

# DESIGNER SPIN SYSTEMS VIA INVERSE STATISTICAL MECHANICS

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

- 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.

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# APPLICATIONS OF THE INVERSE PROBLEM

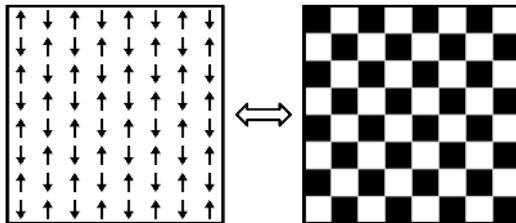
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# APPLICATIONS OF THE INVERSE PROBLEM

- 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, . . .

# A BRIEF OVERVIEW OF THE ISING MODEL

- Used to describe the 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, Segev, Bialek, Nature (2006). Braunstein, Pagnani, Weigt, Zecchina, J. Stat. Mech. (2008). Torquato, Phys. Biol. (2011).*



# 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.

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# THE STANDARD/SIMPLEST ISING SPIN MODEL

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- The standard Ising Hamiltonian takes on the following form:

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

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).

# A GENERALIZED ISING SPIN MODEL

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

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

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

$$\theta_3^2(\lambda) = 1 + 4\lambda + 4\lambda^2 + 4\lambda^4 + 8\lambda^5 + 4\lambda^8 + 4\lambda^9 + 8\lambda^{10} + \dots$$

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*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.*

# A GENERALIZED ISING SPIN MODEL

- It is now convenient to define the  $\mathbf{S}_2$  vector, a quantity closely related to the spin-spin correlation function,  $\langle \sigma_i \sigma_j \rangle$ , with components given by:

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

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- This formalism allows for direct computation of the energy per spin,  $\epsilon$ , via the scalar product of  $\mathbf{S}_2$  with  $\mathbf{J}$ ,

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



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

# SOLVING THE INVERSE SPIN PROBLEM

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

*Rechtsman, Stillinger, Torquato, Phys. Rev. E (2006).*

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Mona Lisa (RGB→GS→B/W)

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

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# SOLVING THE INVERSE SPIN PROBLEM

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

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

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

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

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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.  $\epsilon^{\mathcal{T}} < \epsilon^{C_k} \forall k$ , *if this potential exists.*
- **STEP 2:** SA-MC employs this potential to find a new competitor  $C_{k+1}$  s.t.  $\epsilon^{C_{k+1}} \leq \epsilon^{\mathcal{T}}$ , *if this competitor exists.*
- **STEPS 1 and 2** are then iterated until:
  - For a given  $\{C_k\}$ , LP is unable to generate a potential that favors  $\mathcal{T}$ . **GO TO 1**
  - For a given  $\{J(R)\}$ , SA-MC is unable to locate a competitor that is lower in energy than  $\mathcal{T}$ . **EXIT**

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



# ANALYZING THE SOLUTIONS

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

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- **CLASS II:** Solutions in which a potential was found that generates  $\mathcal{T}$  as a *non-unique* ground state, with degenerate spin configurations having the same  $\mathbf{S}_2$  as  $\mathcal{T}$  ( $\mathbf{S}_2$ -type degeneracies). *Remark:*  $\mathbf{S}_2$ -type degeneracies remain isoenergetic for *any* choice of the spin-spin interaction potential.

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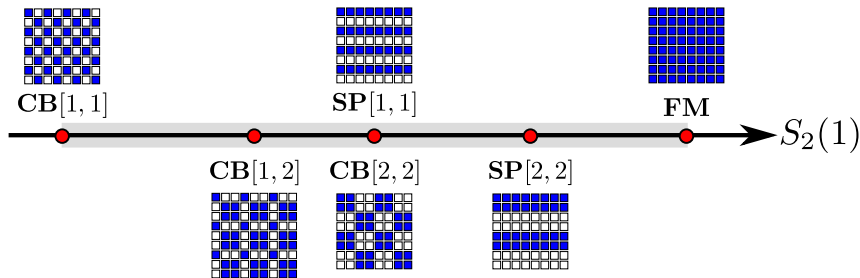
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- **CLASS III:** Solutions that are not contained in either Class I or II as defined above.

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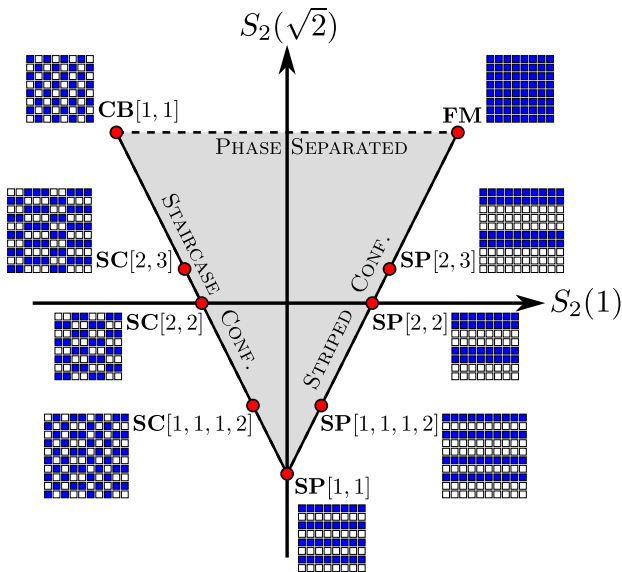
# MAPPING SPIN CONFIGURATIONAL SPACE ONTO $S_2$

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



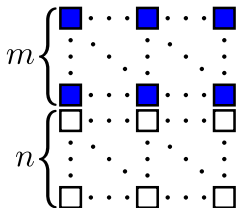
- Nearest-neighbor  $S_2$  values for select spin configurations.
- The gray shading represents the **entire spectrum** of possible spin configurations discretized on a periodic square lattice.

# MAPPING SPIN CONFIGURATIONAL SPACE ONTO $S_2$



# TARGET STRUCTURES: STRIPED PHASES

Graphical depiction of the  $\mathbf{SP}[m, n]$  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.

# THE $\text{SP}[N,N]$ SPIN CONFIGURATIONS

- Systematic study of  $n = 1, 2, \dots, 10$  revealed that all  $\text{SP}[n, n]$  spin configurations are *unique* ground states (Class I).

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

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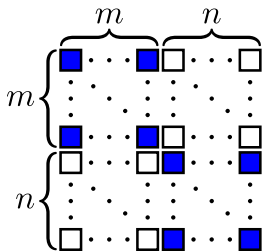
- Systematic study of  $n = 1, 2, \dots, 10$  revealed that all **SP** $[n, n]$  spin configurations are *unique* ground states (Class I).
- These finite-range potentials (of length  $n$ ) are discrete by construction and have compact support.
- Alternative to the infinite-range interactions known to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

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



# TARGET STRUCTURES: BLOCK CHECKERBOARDS

Graphical depiction of the  $\mathbf{CB}[m, n]$  block checkerboard spin configuration



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

# THE $\mathbf{CB}[N,N]$ SPIN CONFIGURATIONS

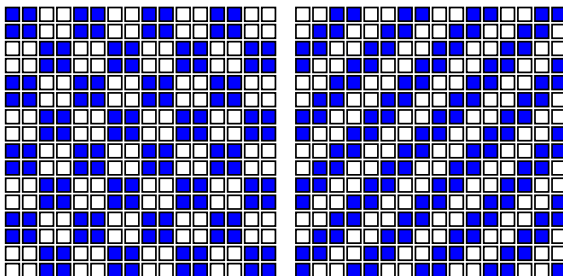
- With the exception of  $\mathbf{CB}[1, 1]$ , a systematic study of  $n = 2, 3, \dots, 10$  revealed that all  $\mathbf{CB}[n, n]$  spin configurations are *degenerate* ground states (Class II).

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- Like the  $\mathbf{SP}[n,n]$  cases, the *shortest* radial interaction potentials are of length  $n$ .
- As Class II solutions, the  $\mathbf{CB}[n, n]$  spin configurations have a finite set of  $S_2$ -degeneracies.

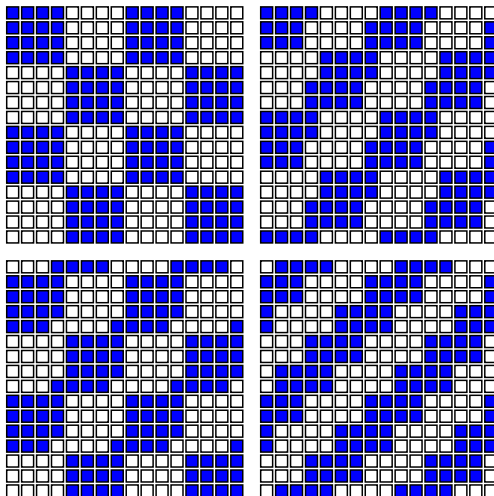
# THE $CB[N,N]$ SPIN CONFIGURATIONS

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



# THE $\text{CB}[N,N]$ SPIN CONFIGURATIONS

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

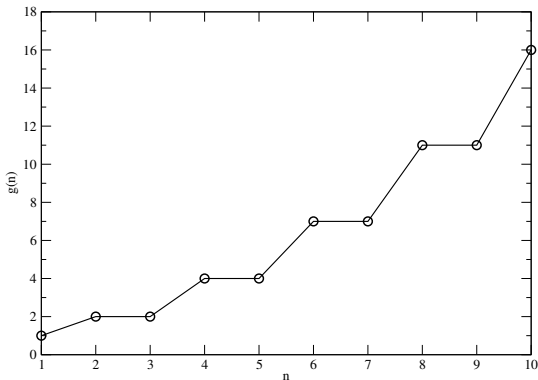


# THE $\mathbf{CB}[N,N]$ SPIN CONFIGURATIONS

The number of  $S_2$ -type degeneracies for the  $\mathbf{CB}[n, n]$  spin configurations  $g(n)$  was found as:

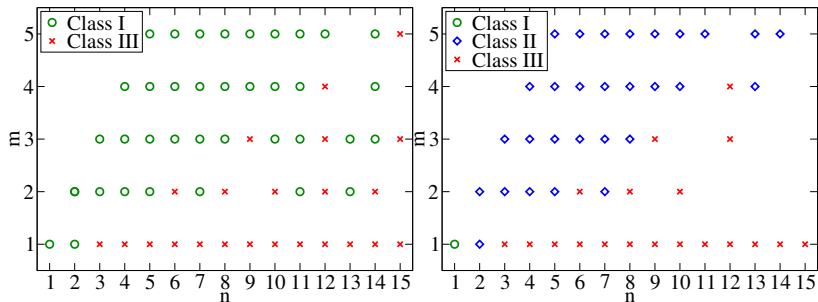
$$g(n) = 1 + \frac{\lfloor \frac{n}{2} \rfloor (\lfloor \frac{n}{2} \rfloor + 1)}{2}$$

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



# THE $\text{SP}[M,N]$ AND $\text{CB}[M,N]$ SPIN CONFIGURATIONS

Solution classes for the  $\text{SP}[m, n]$  and  $\text{CB}[m, n]$  spin configurations.



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

# SOME OPEN QUESTIONS...

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



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- 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.

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- 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?

# GROUND STATE ENUMERATION & CLASSIFICATION

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	$N_I$	$N_{II}$	$N_{III}$	$N_{\text{conf}}$
$1 \times 1$	1	0	0	2
$2 \times 2$	3	0	1	16
$3 \times 3$	3	2	6	512
$4 \times 4$	5	1	266	65,536
$5 \times 5$	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.

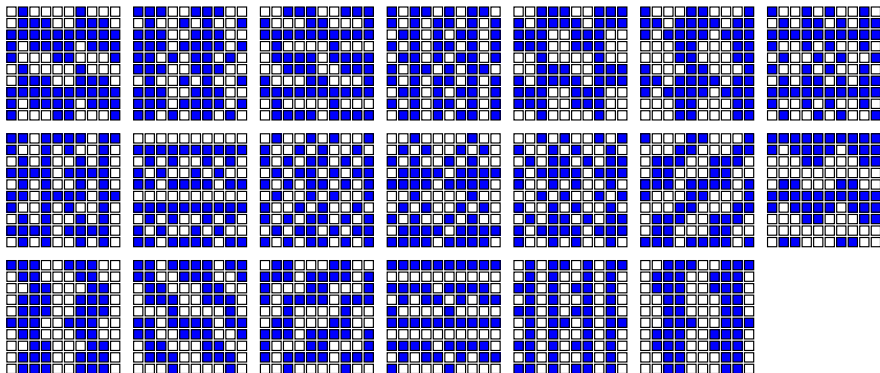
# GROUND STATE ENUMERATION & CLASSIFICATION

$ \langle \sigma \rangle $	$N_I$	$N_{II}$	$N_{III}$
0.04	28	25	1737
0.12	16	4	1690
0.20	17	0	1415
0.28	4	0	1226
0.36	4	0	903
0.44	4	0	623
0.52	0	0	357
0.60	0	0	169
0.68	0	0	64
0.76	0	0	19
0.84	0	0	5
0.92	0	0	1
1.00	1	0	0

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

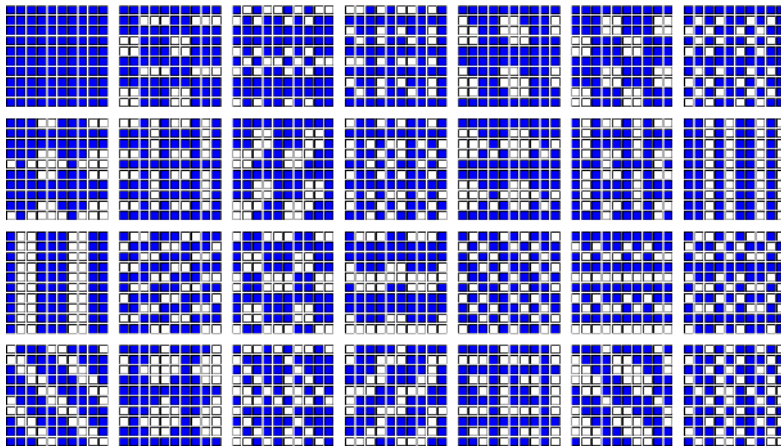
# GROUND STATE ENUMERATION & CLASSIFICATION

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



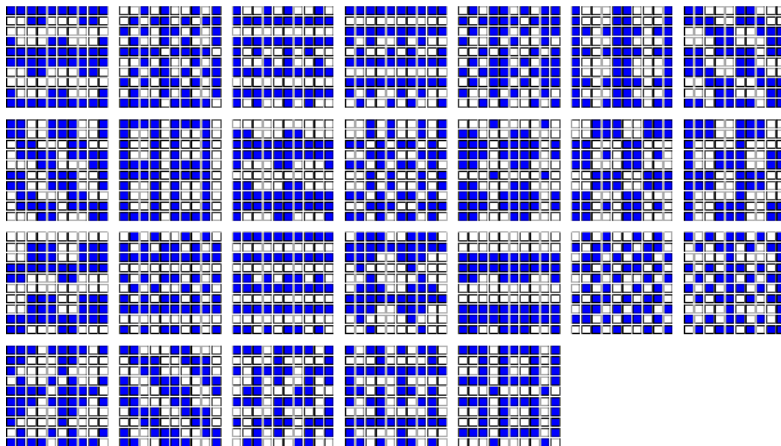
All  $5 \times 5$  Class I spin configurations ( $N = 20$ ) that are **not** left invariant under any combination of symmetry operations, displayed left-to-right, top-to-bottom, in order of decreasing absolute magnetization  $|\langle \sigma \rangle|$ .

# GROUND STATE ENUMERATION & CLASSIFICATION



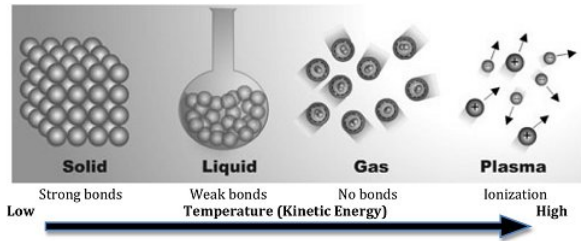
All  $5 \times 5$  Class I spin configurations ( $N = 54$ ) that are left invariant under some combination of symmetry operations, displayed left-to-right, top-to-bottom, in order of decreasing absolute magnetization  $|\langle \sigma \rangle|$ .

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All  $5 \times 5$  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  $|\langle \sigma \rangle|$ .

# PHASES (STATES) OF MATTER

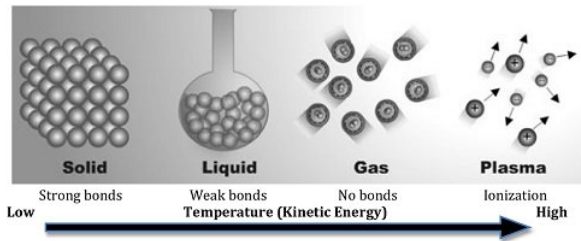


## Traditional Criteria

- 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



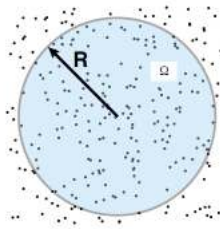
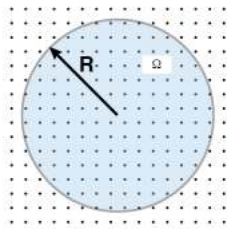
# PHASES (STATES) OF MATTER



## Non-Traditional/Broader Criteria

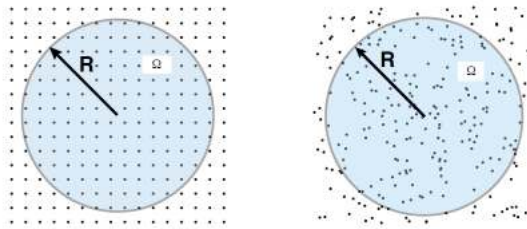
- Reproducible long-lived metastable or non-equilibrium phases, *e.g.*, spin and structural glasses
- Interacting entities need not be microscopic, can include larger building blocks, *e.g.*, colloids and metamaterials
- Endowed with unique properties

# NEW PHASES (STATES) OF MATTER



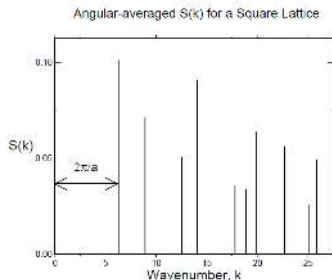
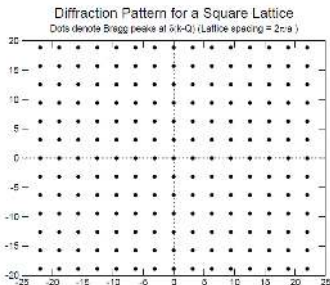
- Let  $\Omega$  be a spherical window of radius  $R$  in  $\mathbb{R}^d$  and  $\sigma^2 \equiv \langle N^2(R) \rangle - \langle N(R) \rangle^2$  be the **number variance**.
- For Poisson and many disordered point patterns:  $\sigma^2 \sim R^d$ .

# NEW PHASES (STATES) OF MATTER



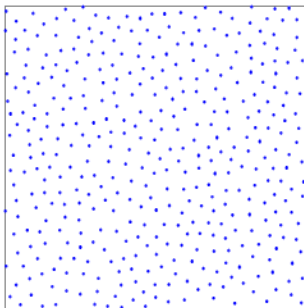
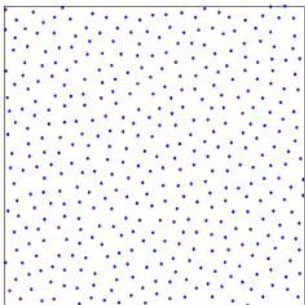
- Let  $\Omega$  be a spherical window of radius  $R$  in  $\mathbb{R}^d$  and  $\sigma^2 \equiv \langle N^2(R) \rangle - \langle N(R) \rangle^2$  be the **number variance**.
- For Poisson and many disordered point patterns:  $\sigma^2 \sim R^d$ .
- **Hyperuniform** point patterns:  $\sigma^2$  grows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

# ALL CRYSTALS ARE TRIVIALY HYPERUNIFORM

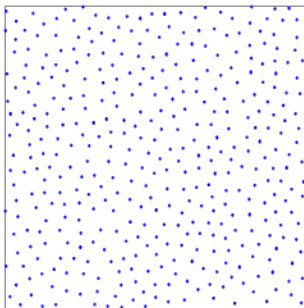
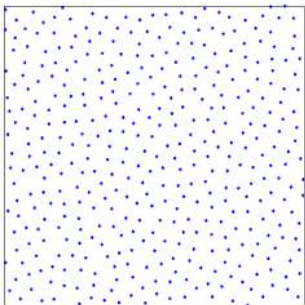


- All perfect crystals are hyperuniform in that  $\sigma^2 \sim R^{d-1}$ .
- The degree to which they suppress large-scale density fluctuations varies.

# WHICH POINT PATTERN IS HYPERUNIFORM?

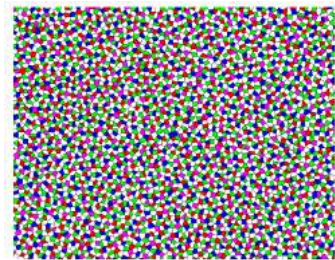


# WHICH POINT PATTERN IS HYPERUNIFORM?



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

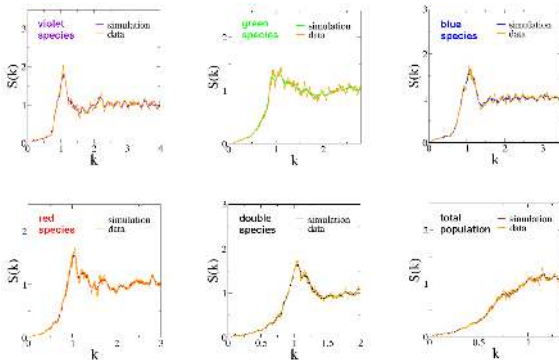
# HYPERUNIFORM AVIAN CONE RECEPTORS



- 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).*

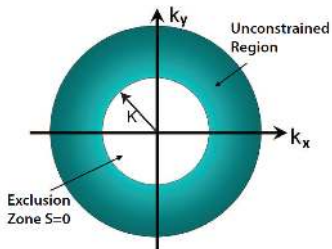
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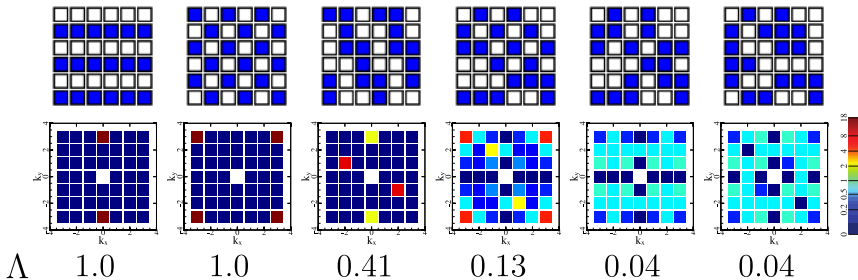
# ALL STEALTHY PATTERNS ARE HYPERUNIFORM



- “Stealthy” point patterns take hyperuniformity one step further and are characterized by  $S(k) = 0$  for  $0 < k \leq K$ .
- 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  $K_1 < k \leq K_2$  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...

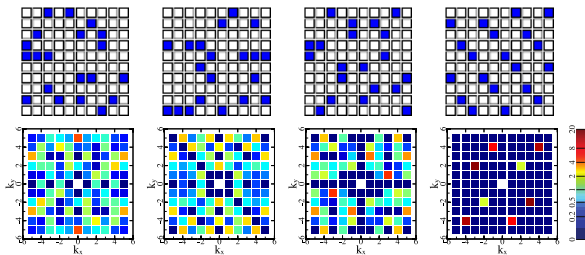


$$\Lambda = \sum_{\mathbf{k}} [S(\mathbf{k}) - 1]^2$$

- 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?



$K$	1	$\sqrt{2}$	2	$\sqrt{5}$
$\Lambda$	75.5	81.0	137.5	1039

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

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

- 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.

# ACKNOWLEDGMENTS



Frank Stillinger



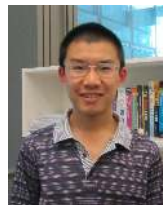
Salvatore Torquato



Roberto Car



Étienne Marcotte



Ge Zhang

# 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](mailto:distasio@cornell.edu) for more details.