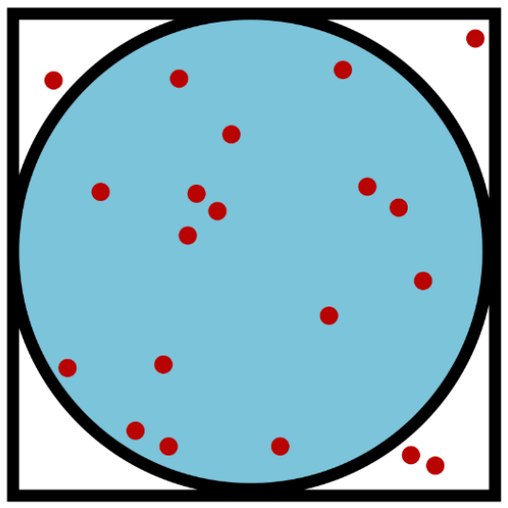
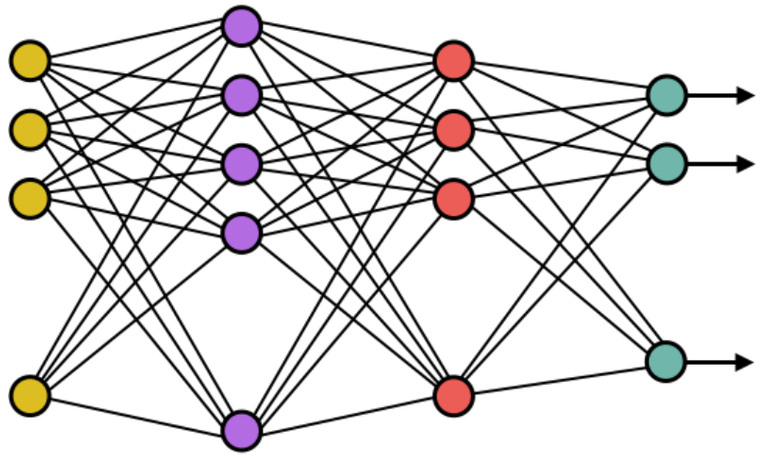
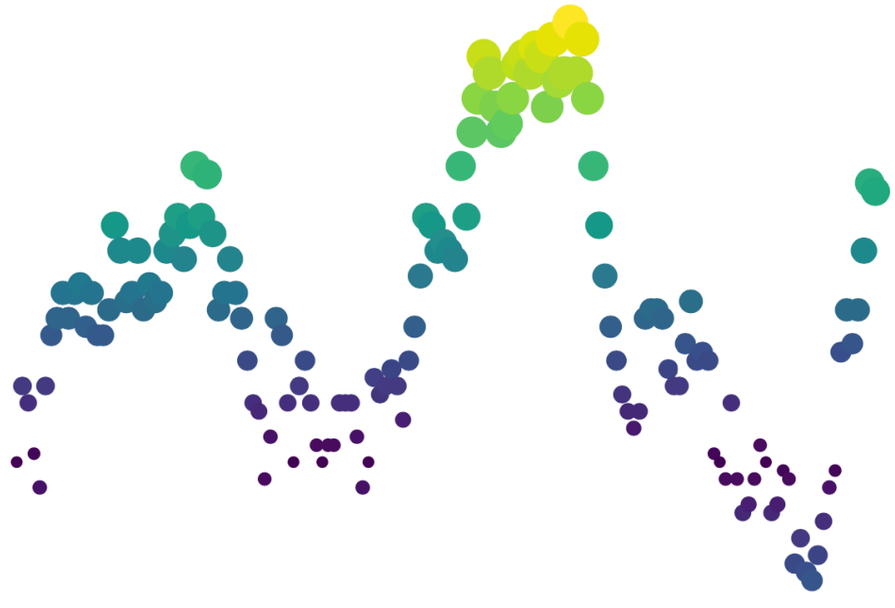
Numerical Methods



Lauren Hayward
PSI Start Online School





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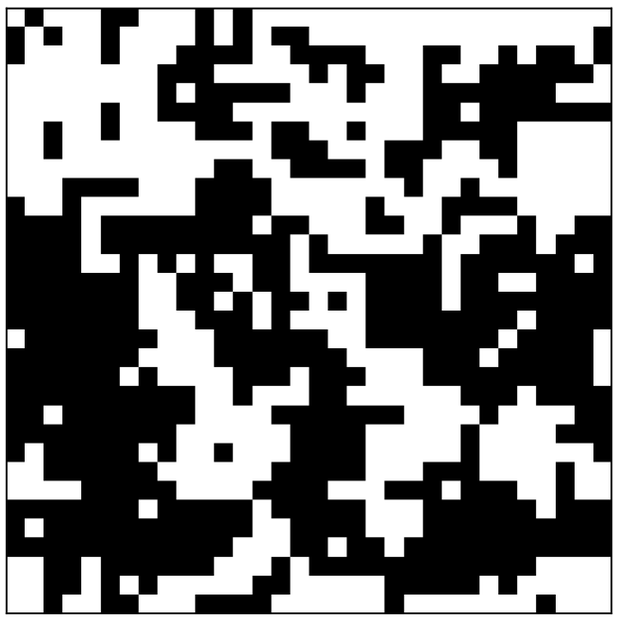
Outline

- Statistical physics and the Ising model

LAST LECTURE

- Monte Carlo methods in statistical physics

TODAY



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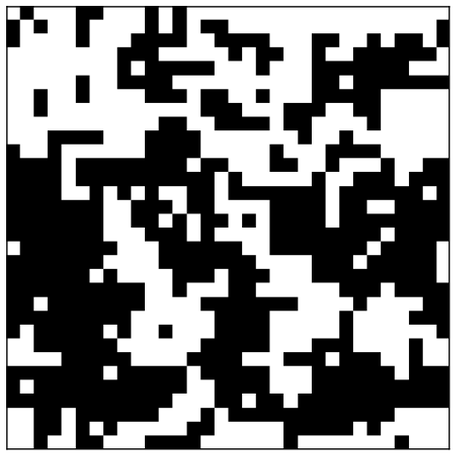
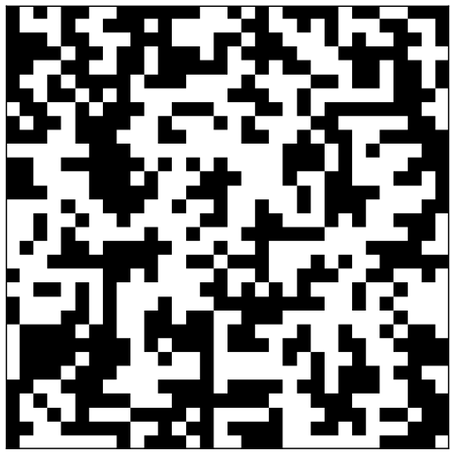
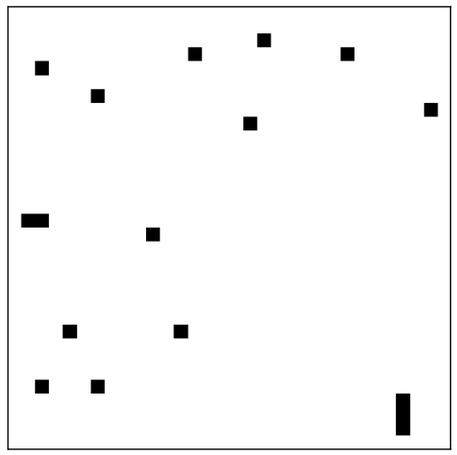
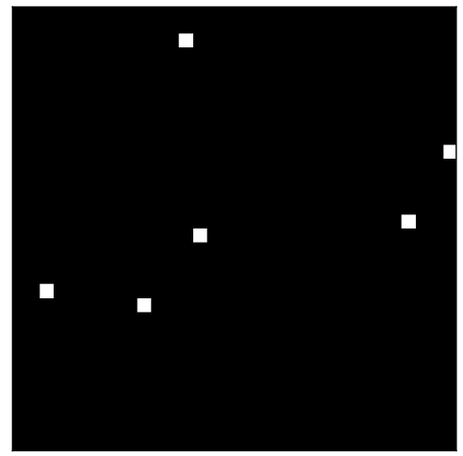
Last lecture: 2D Ising model

$$E = -J \sum_{\langle ij \rangle} s_i \, s_j$$

$s_i =$ **+1** or **-1**

(■ or □)

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Expectation values of observables

In the canonical ensemble, our system is in thermal equilibrium with a heat bath at fixed temperature T.

The expectation value of a quantity Q is:

$$\langle Q \rangle = \sum_{\mu} Q_\mu p_\mu$$

where:

- μ represents a microstate of the system
- $p_\mu = \frac{1}{Z} e^{-\beta E_\mu}$
- E_μ is the energy of state μ
- $Z = \sum_{\mu} e^{-\beta E_\mu}$
- $\beta = \frac{1}{k_B T}$

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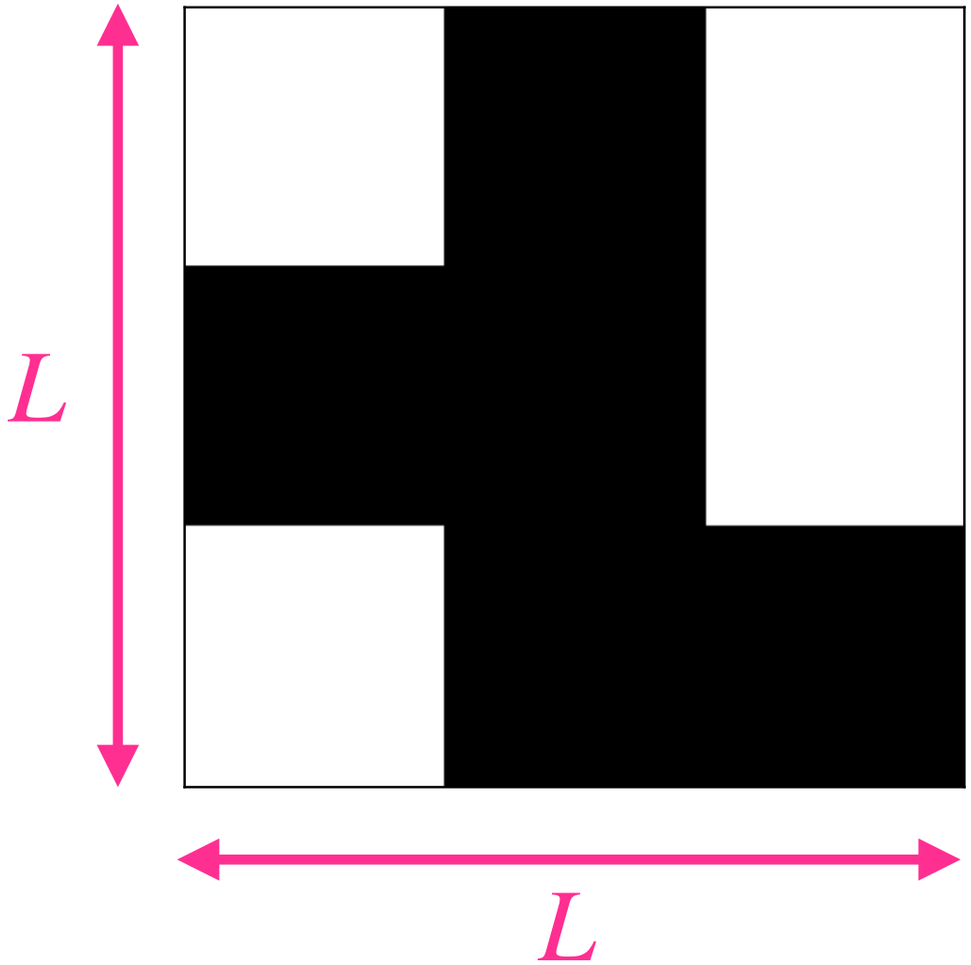
Statistical physics

We would like to study the behaviour of expectation values in the limit where the number of particles N is large.

Consider the Ising model on a square lattice:



$$N = L^2$$

The total number of accessible microstates is:

$$2^N = 2^{(L^2)}$$

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2D Ising model

For *N*=25, the fastest algorithms for computing the sums $\sum_{\mu}$ over all microstates require around a minute. The time to compute this sum directly scales as $2^N = 2^{(L^d)}$

N	time
25	~1 minute
30	~ 30 minutes
35	~ 20 hours
40	~20 days
50	~60 years
80	~ 7×10^{10} years

longer than the age of the universe!

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Monte Carlo methods in statistical physics

If we try to evaluate the sums $\sum_\mu$ directly, we are limited to $N=50$ to 60, which corresponds to $L=7$ or 8 for the 2D Ising model. We need other methods to study bigger systems!

Monte Carlo methods address this exponential complexity by considering only M microstates $\mu_1, \mu_2, \ldots, \mu_M$ selected at random.

Reference:

Newman & Barkema, "Monte Carlo methods in Statistical Physics"

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Calculating the expectation value $\langle Q \rangle = \sum_{\mu} Q_\mu p_\mu$ using Monte Carlo sampling:

In particular, if each state μ_i $(1 \leq i \leq M)$ is selected from the set of all states according to the desired prob. dist. p_{μ_i}, then:

$$\langle Q \rangle \simeq Q_M = \frac{1}{M} \sum_{i=1}^{M} Q_{\mu_i}$$

This estimate makes use of "importance sampling" (the more probable states are more likely to be selected.)

To implement this sampling, we can use Markov chain Monte Carlo (MCMC).

↳ use the current state μ to propose a move to a new related state ν, and then decide whether to accept or reject the move

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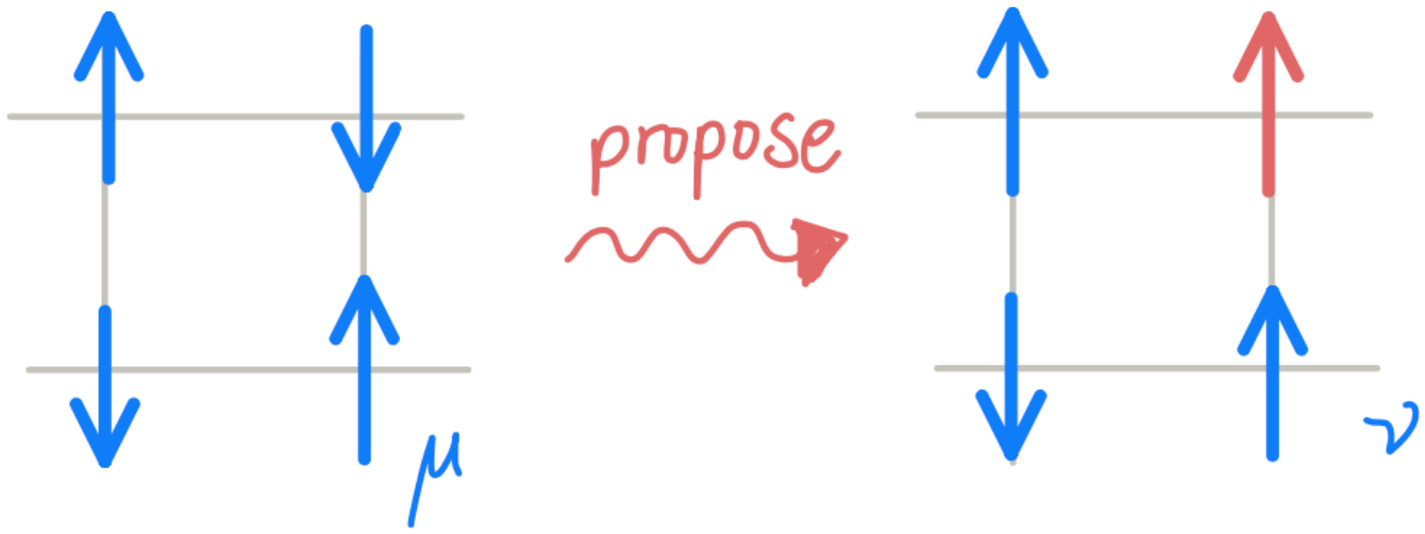
eg) single spin flip moves:

Ising model



Given μ, propose ν where:

- In principle, any proposal is allowed
  - ↳ single-spin flip
  - ↳ non-local "cluster" spin flips
  - ⋮
- Once a proposal is generated, we choose to accept or reject it

The probability of moving from μ to ν is the "transition prob." $T(\mu \to \nu)$, where $\sum_{\nu} T(\mu \to \nu) = 1$

We can choose any set of transition probs. $\{T(\mu \to \nu)\}$ as long as we satisfy two conditions:

1. **Ergodicity:** there is a non-zero probability of transitioning (eventually) from μ to and ν

$$\mu \to \ldots \to \nu$$

2. **Detailed balance (DB)**

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2 Detailed balance (DB):

The rate of transition into and out of any state μ must be equal

$$\underbrace{\sum_{\nu} p_\nu T(\nu \to \mu)}_{\text{rate of transition into } \mu} = \underbrace{\sum_{\nu} p_\mu T(\mu \to \nu)}_{\text{rate of transition out of } \mu}$$

One way to satisfy this condition is:

$$\boxed{p_\nu T(\nu \to \mu) = p_\mu T(\mu \to \nu)} \quad \text{DB}$$

$$p_\nu \, T(\nu \to \mu) = p_\mu \, T(\mu \to \nu)$$

DB

When $p_\mu = \frac{1}{Z} e^{-\beta E_\mu}$, we have:

$$\frac{T(\mu \to \nu)}{T(\nu \to \mu)} = e^{-\beta(E_\nu - E_\mu)}$$

Recall that in MCMC, transitioning from μ to ν involves first proposing and then accepting the move. Let us introduce the notation:

$$T(\mu \to \nu) \equiv \underbrace{g(\mu \to \nu)}_{\text{selection prob.}} \underbrace{A(\mu \to \nu)}_{\text{acceptance prob.}}$$

For a given set of selection probabilities, we would like to make the acceptance probabilities $A(\mu \to \nu)$ as close to 1 as possible so that we are more likely to sample different states.

From DB:

$$\frac{A(\mu \to \nu)}{A(\nu \to \mu)} = \frac{g(\nu \to \mu)}{g(\mu \to \nu)} e^{-\beta(E_\nu - E_\mu)}$$

Metropolis algorithm: $A(\mu \to \nu) = \min\left(1, \frac{g(\nu \to \mu)}{g(\mu \to \nu)} e^{-\beta(E_\nu - E_\mu)}\right)$

↳ ensures that $A(\mu \to \nu)$ or $A(\nu \to \mu)$ is equal to 1.

Pseudocode for Monte Carlo sampling with single-spin-flip Metropolis moves:

(generates *M* samples $\mu_1, \mu_2, \ldots, \mu_M$ from the distribution $p_\mu = \frac{1}{Z} e^{-\beta E_\mu}$)

Choose sample μ_1 at random

for step = 2, ... , M:

  choose a lattice site i at random

  define state ν to be the same as $\mu_{\text{step}-1}$ but with the spin at site i flipped

  calculate ΔE for the proposed move $\mu_{\text{step-1}} \to \nu$

  generate r from a uniform random distribution U[0,1)

  if r < $e^{-\beta \Delta E}$:

    $\mu_{\text{step}} = \nu$ (accept the move)

  else:

    $\mu_{\text{step}} = \mu_{\text{step-1}}$ (reject the move)

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Notes:

- In practice, we ignore the first several samples since they are not truly sampled from p_M.
- When calculating Q_M, we should use states μ_i that are statistically independent. The Markov time required to get indep. samples depends on both the algorithm and the temperature.

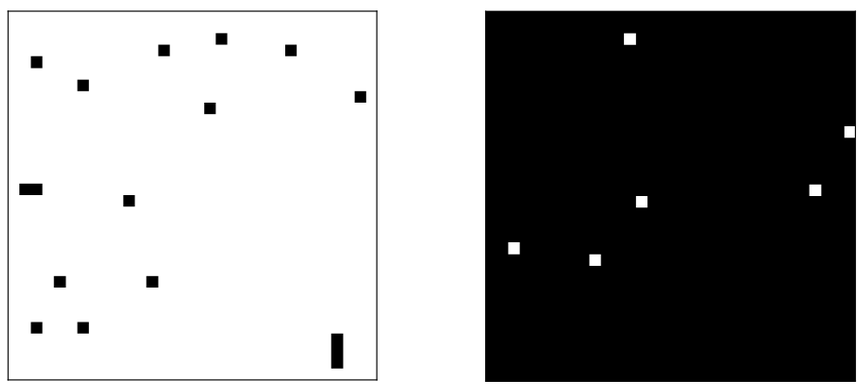
Monte Carlo for the 2D Ising model

$$E = -J \sum_{\langle ij \rangle} s_i \, s_j$$

At high temperatures:

Paramagnetic phase

At low temperatures:



Ferromagnetic phase

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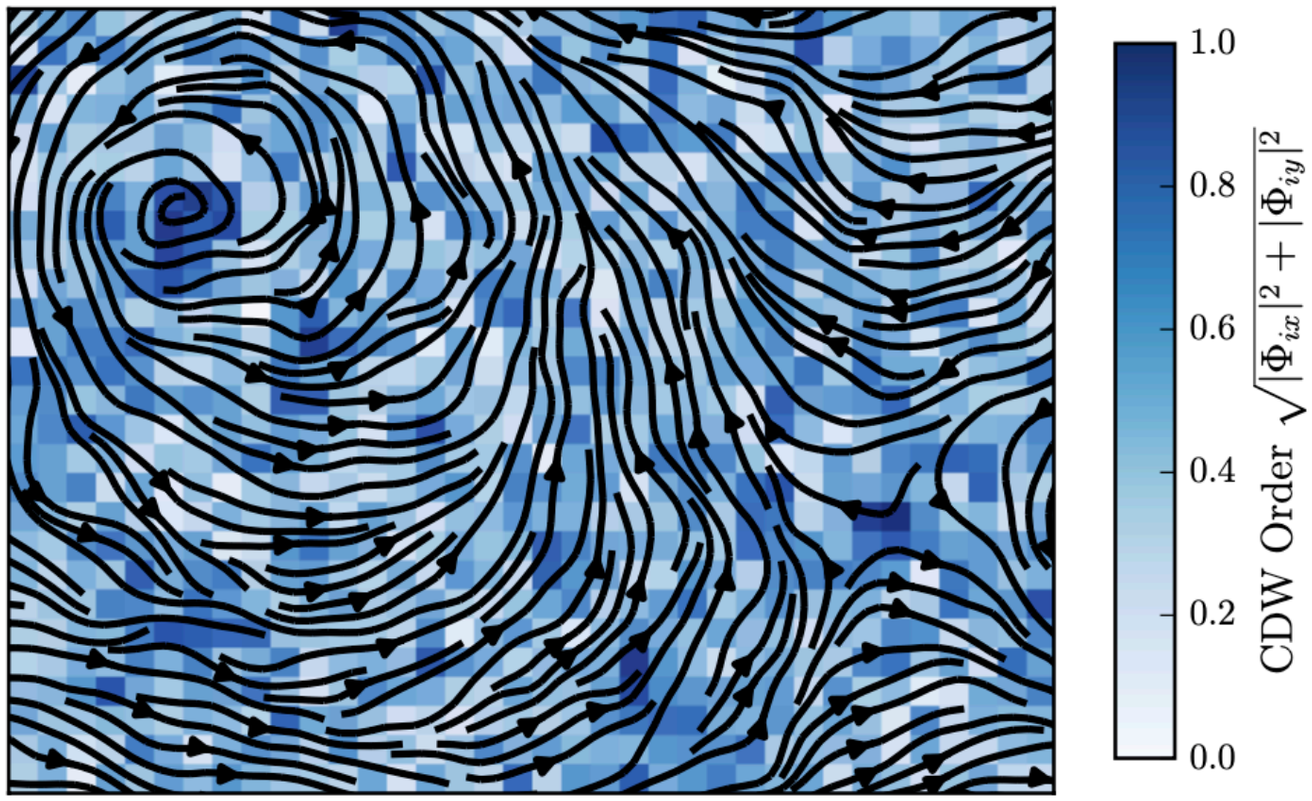
Monte Carlo to study high-temperature superconductivity

$$H = \frac{\rho_s}{2} \sum_{\langle ij \rangle} \left[\sum_{\alpha=1}^{2} (n_{i\alpha} - n_{j\alpha})^2 + \lambda \sum_{\alpha=3}^{6} (n_{i\alpha} - n_{j\alpha})^2 \right]$$

$$+ \frac{\rho_s a^2}{2} \sum_{i} \left[g \sum_{\alpha=3}^{6} n_\alpha^2 + g' \left(\sum_{\alpha=3}^{6} n_\alpha^2 \right)^2 + w \left[\left(n_{i3}^2 + n_{i4}^2 \right)^2 + \left(n_{i5}^2 + n_{i6}^2 \right)^2 \right] \right]$$



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