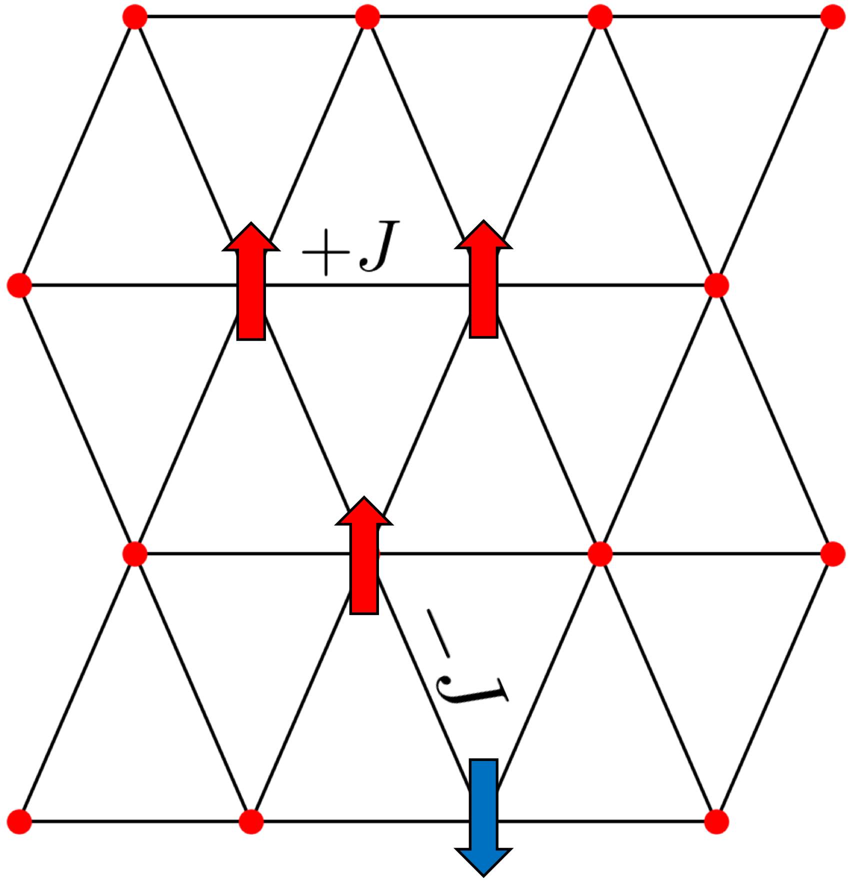
The Anatomy of a Spin:

A Frustrated Ising Model

Benjamin Cohen-Stead

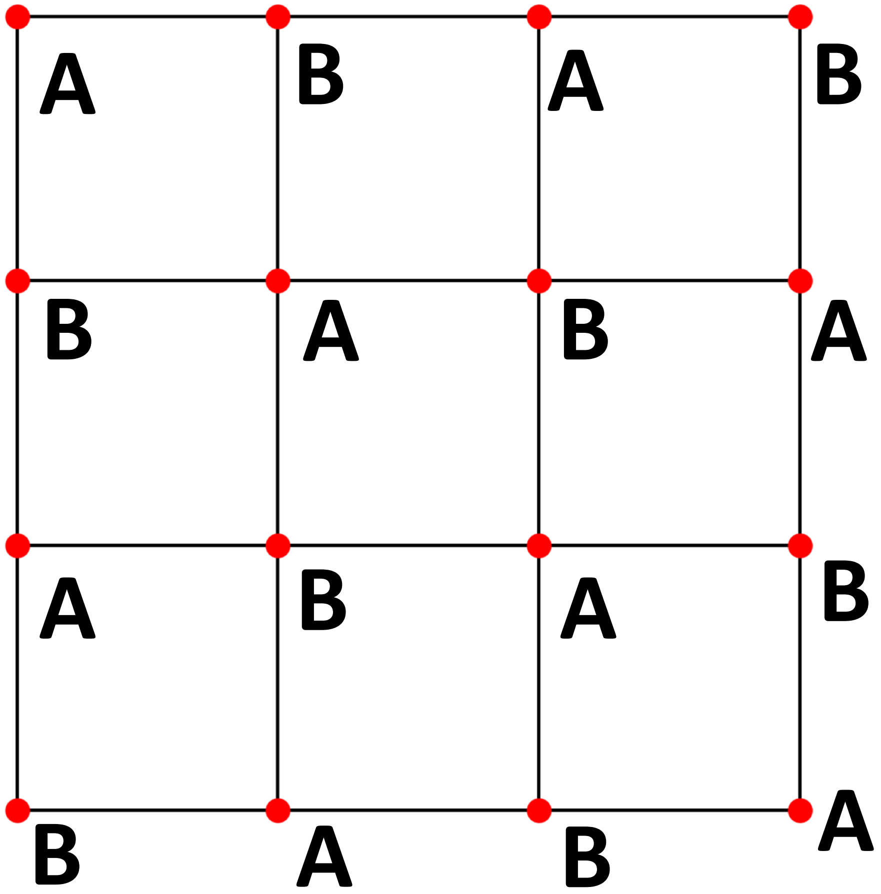
THE SYSTEM: The Triangular Antiferromagnetic Ising Model?

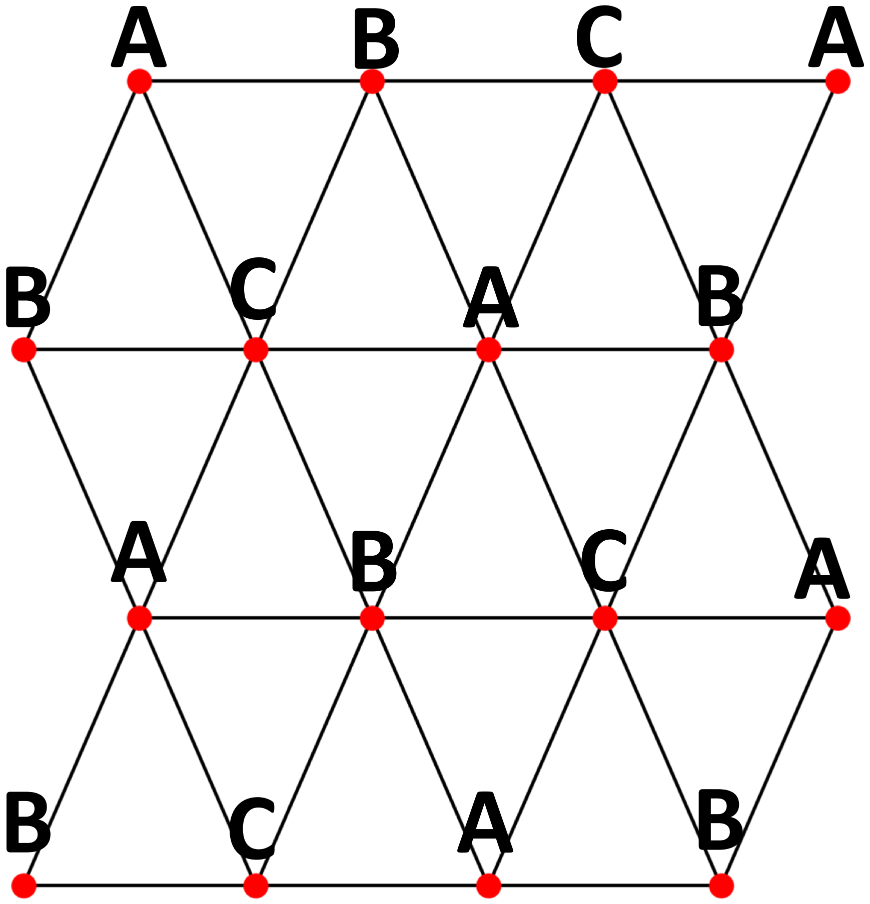
$$H = J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \text{ where } J > 0 \text{ and } \sigma_i = \pm 1$$



THE SYSTEM: The Triangular Antiferromagnetic Ising Model?

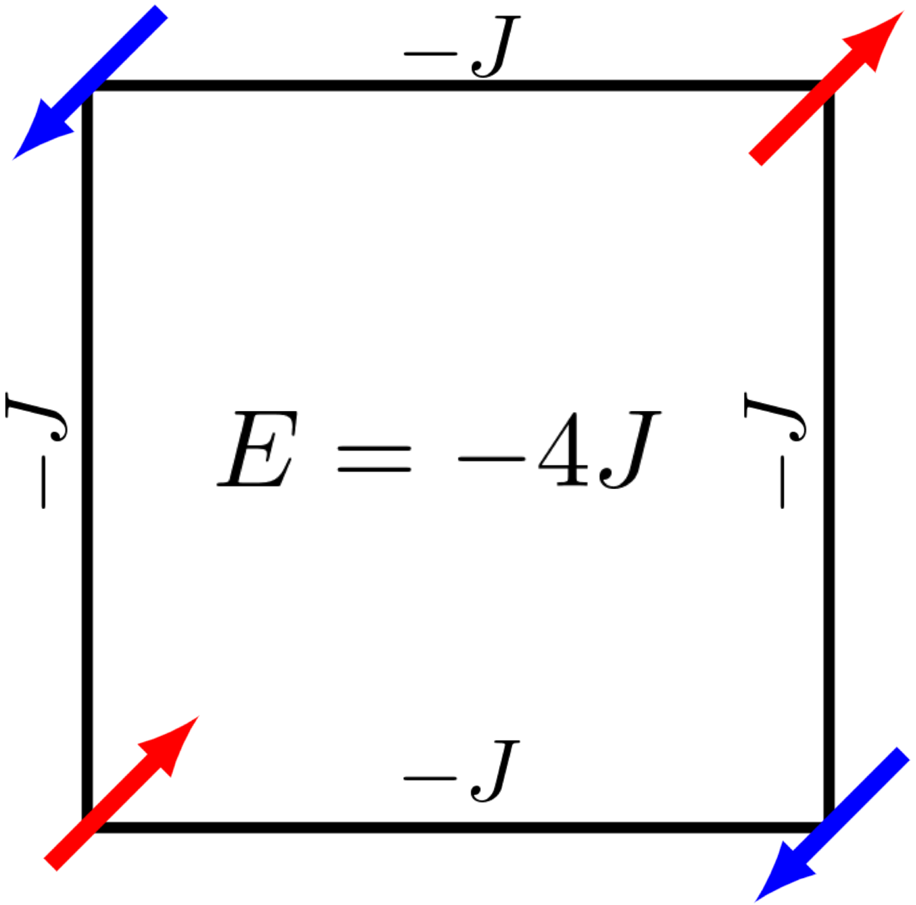
$$H = J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \text{ where } J > 0 \text{ and } \sigma_i = \pm 1$$

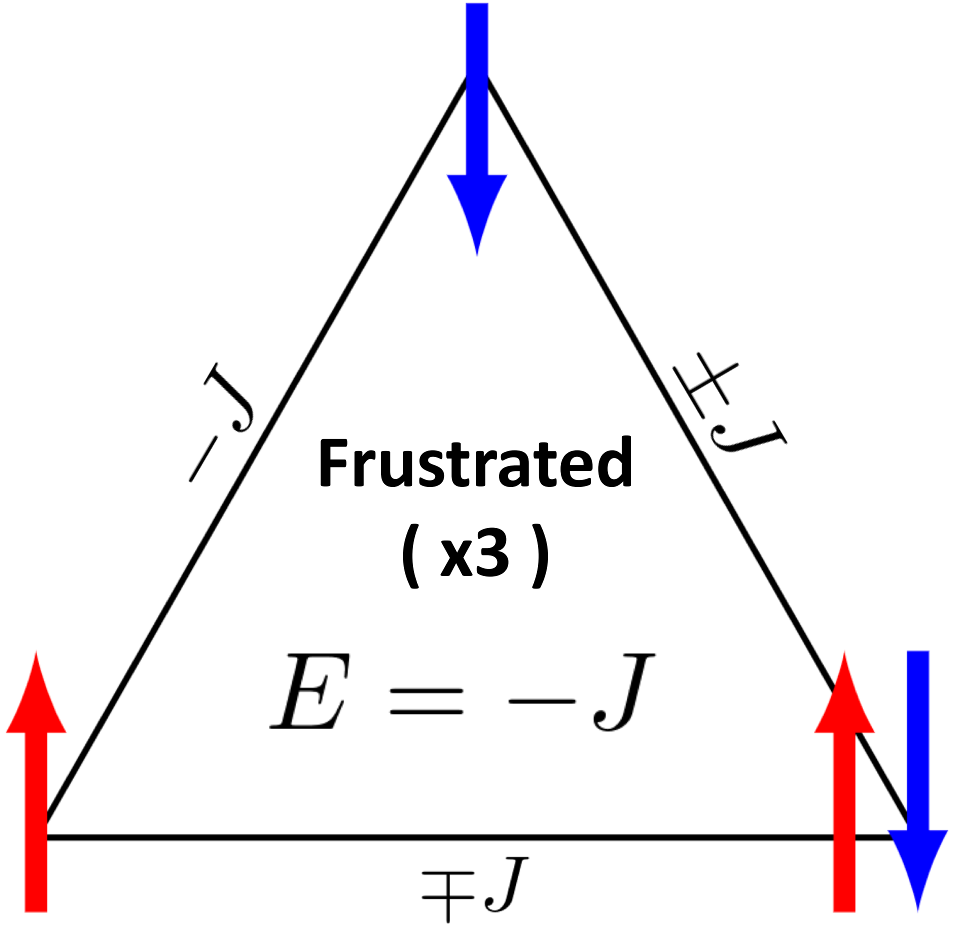




What is Frustration?

$$H = J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \text{ where } J > 0 \text{ and } \sigma_i = \pm 1$$



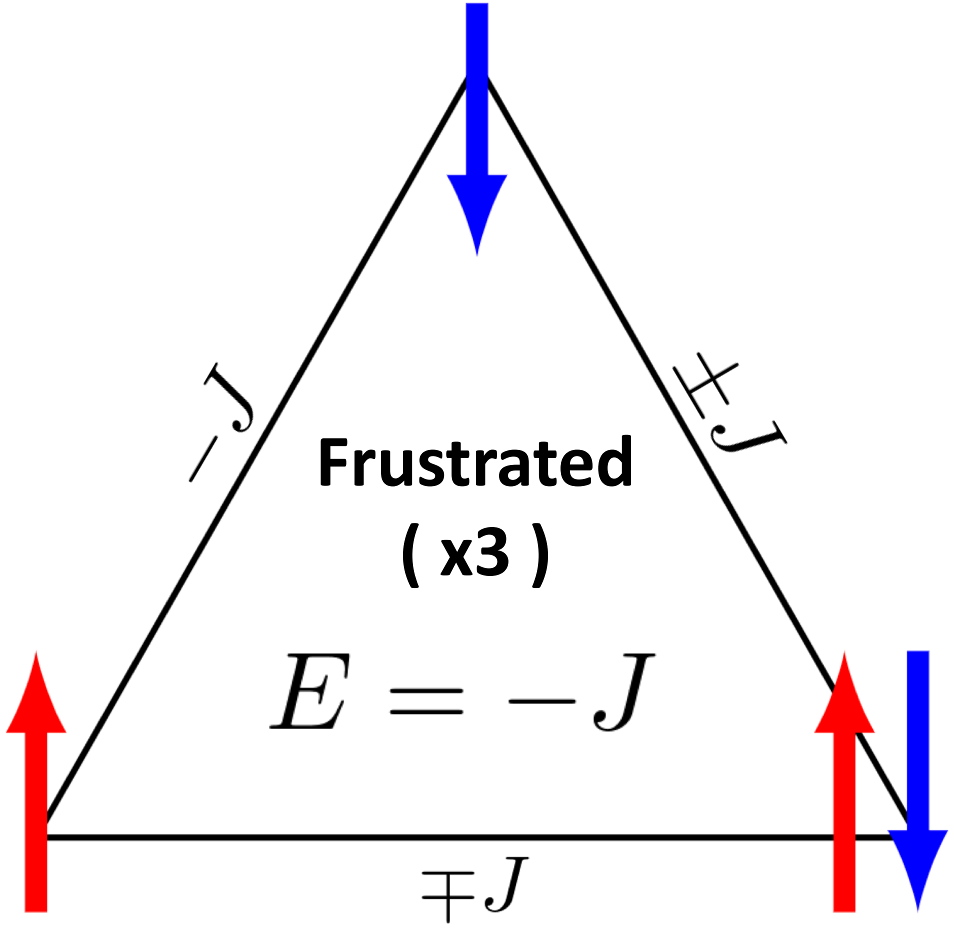


What is Frustration?

$$H = J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \text{ where } J > 0 \text{ and } \sigma_i = \pm 1$$

Why Is Frustration Interesting?

- At T=0 the ground state (lowest energy state) is highly degenerate $\Longrightarrow$ The entropy $H[\boldsymbol{\sigma}] \neq 0$ at $T = 0$
- No finite temperature phase transition.



What Types of Entropies Are There to Look At?

- **Thermodynamic Entropy Density**: $h = \frac{H[\boldsymbol{\sigma}]}{N} = \frac{-1}{N} \sum_{\sigma \in \boldsymbol{\sigma}} p(\sigma) \log_2 p(\sigma)$

- **Isolated Spin Entropy**: $H[\boldsymbol{\sigma}_0] = -p(\uparrow) \log_2 p(\uparrow) - p(\downarrow) \log_2 p(\downarrow)$

- **Total Correlation Density**: Measures how constrained the spin distribution is $\Longrightarrow$ maximized when spins are strongly correlated. $\rho = H[\boldsymbol{\sigma}_0] - h$

What Types of Entropies Are There to Look At?

- **Localized Entropy Density**: The residual entropy per spin; the amount of entropy associated with a given spin that is not shared with its neighbors.

$$r = \frac{1}{N} R[\boldsymbol{\sigma}] = \frac{1}{N} \sum_{i=1}^{N} H[\sigma_i | \sigma_{\setminus i}]$$

- **Bound Entropy Density**: The portion of the thermodynamic entropy density (*h*) that is shared between a spin and the rest of the lattice. $b = r - h$

- **Enigmatic Entropy Density**: $q = \rho - b$

What Types of Entropies Are There to Look At?

$\mathrm{H}\left[\boldsymbol{\sigma}_0\right]$ Isolated Spin Entropy

h Entropy Density

ρ Total Correlation Density

r Localized Density

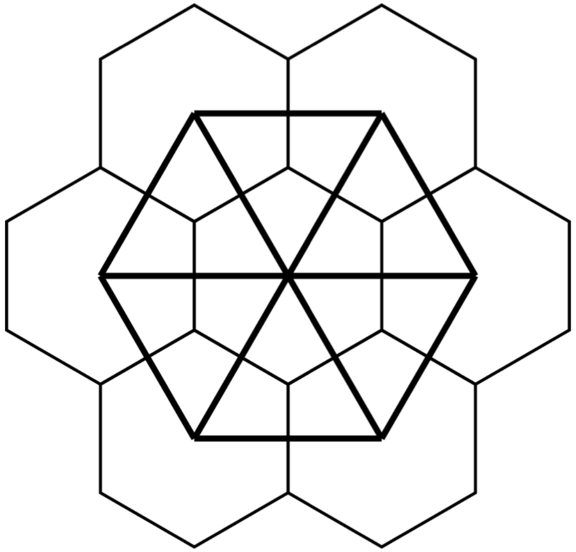
b Bound Density

b Bound Density

q Enigmatic Density

V. S. Vijayaraghavan, R. G. James, and J. P. Crutchfield, Entropy 19, 114 (2017).

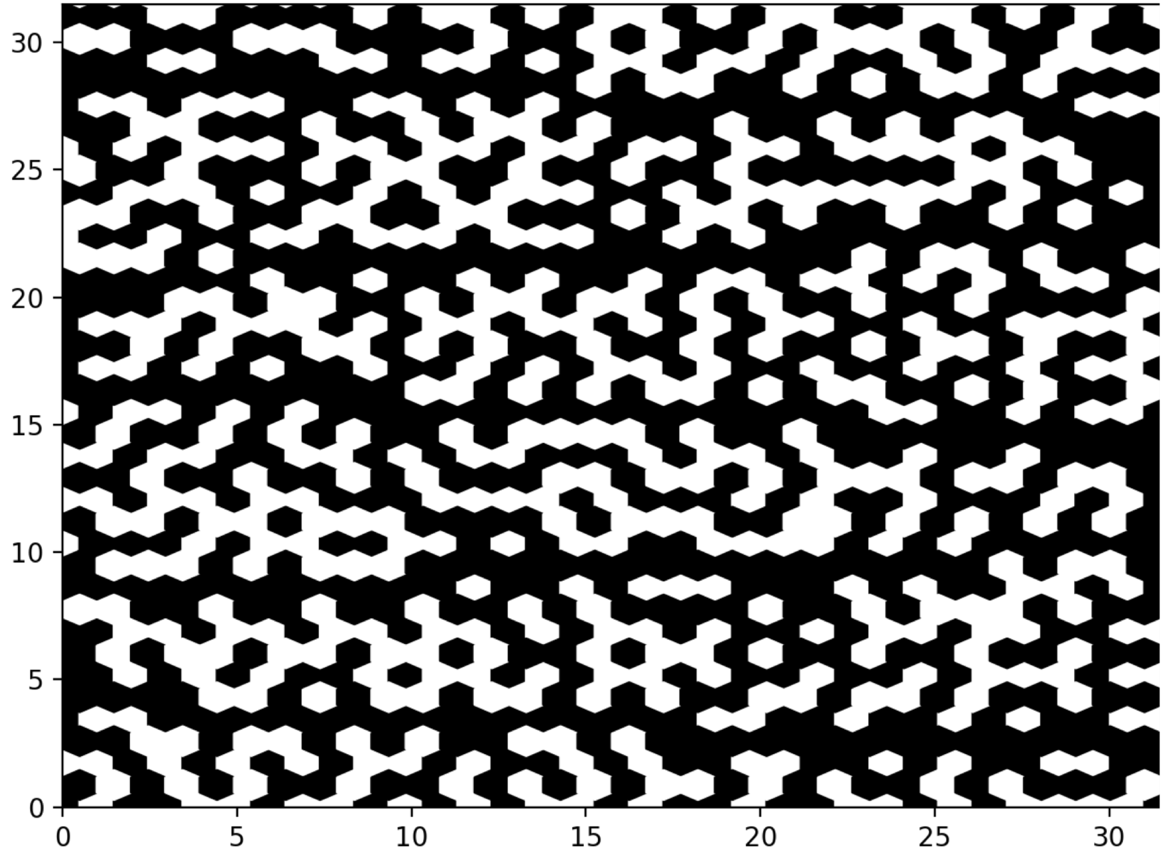
Method: How Do I Actually Measure These Quantities?



1. Monte Carlo Simulations used to generate a representative sample of Lattice Configurations.

- Lattice Size: 30x30
- Temperature Range: 0.40, 0.45, 0.50, … , 2.00
- Duration: 10,000 + 100,000 Monte Carlo Sweeps.
- Sample Size: 10,000 saved configurations.
- Metropolis-Hastings used for spin-flip decision.

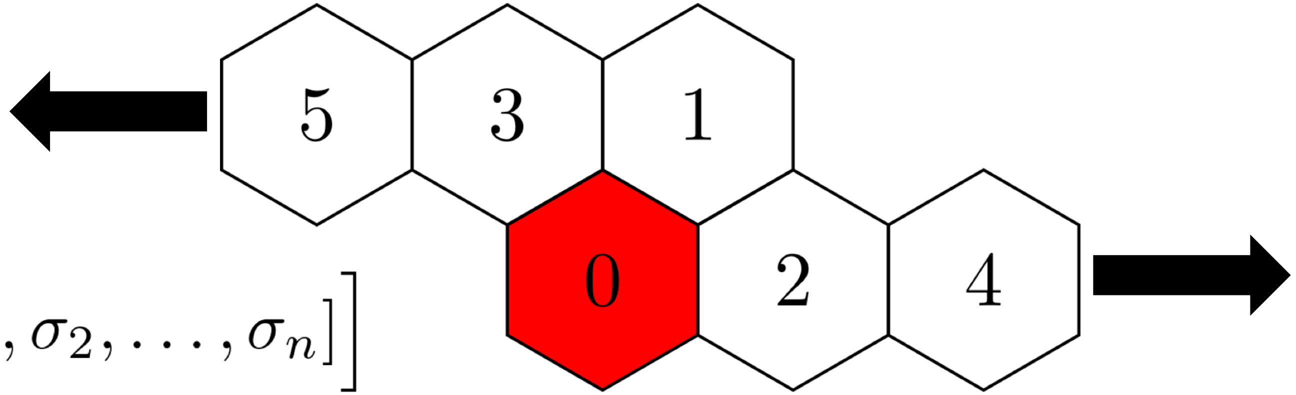
$$P_{flip} = \min\left(1, e^{-\Delta E_{flip}/T}\right)$$



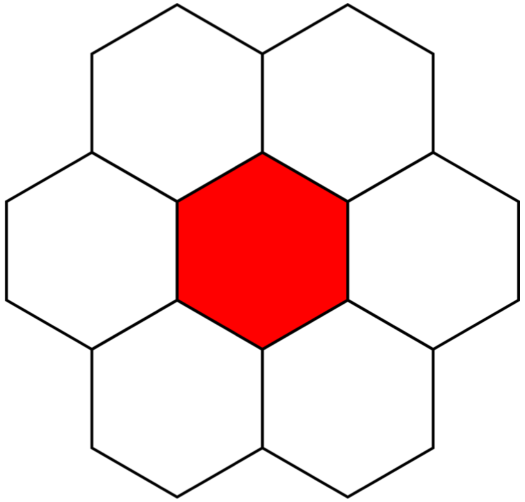
Method: How Do I Actually Measure These Quantities?

2. Using sampled configurations, calculate estimates for the different entropic quantities.

$$
\begin{aligned}
h &= \lim_{n\to\infty} H[\sigma_0|\sigma_1,\sigma_2,\ldots,\sigma_n] \\
&= \lim_{n\to\infty} \Big[H[\sigma_0,\sigma_1,\sigma_2,\ldots,\sigma_n] - H[\sigma_1,\sigma_2,\ldots,\sigma_n]\Big]
\end{aligned}
$$



$$
r = \frac{1}{N}R[\boldsymbol{\sigma}] = \frac{1}{N}\sum_{i=1}^{N} H[\sigma_i|\sigma_{\backslash i}] = \frac{1}{N}\sum_{i=1}^{N} H[\sigma_i|\sigma_{nn}]
$$



Method: How Do I Actually Measure These Quantities?

2. Using sampled configurations, calculate estimates for the different entropic quantities.

Isolated Spin Entropy $\mathrm{H}\left[\boldsymbol{\sigma}_0\right] = -p(\uparrow)\log_2 p(\uparrow) - p(\downarrow)\log_2 p(\downarrow)$

h **Entropy Density**

Total Correlation Density ρ

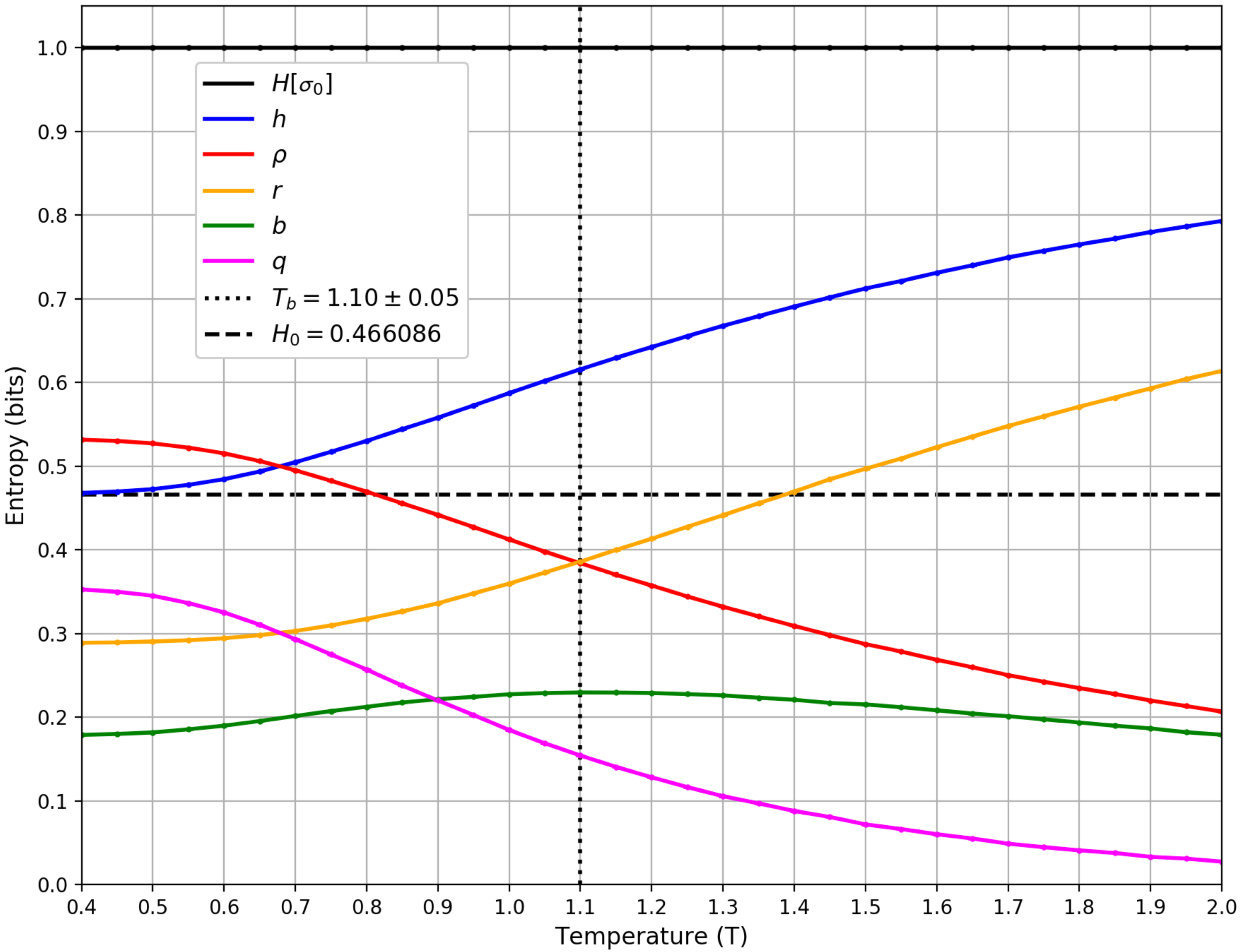
Localized Density r

Bound Density b

b

q **Enigmatic Density**

Results



$H[\sigma_0]$
h
ρ
r
b
q
$T_b = 1.10 \pm 0.05$
$H_0 = 0.466086$
Entropy (bits)
Temperature (T)
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0