

# Experiments

Robin

February 16, 2021

**Motivation:** We wish to study the transport of  $M$  interacting particles within a square lattice of size  $N$ . This can likely be realized by applying a field onto the surface of spin ice in the ground state. In that case, the particles are magnetic monopoles.

$$H(m) = - \sum_{(i,j)} J_{i,j} m_i m_j \quad i, j \in \{1, \dots, N\} \quad m_i \in \{0, 1\} \quad \sum_i m_i = M$$

From now on, let  $J_{i,j} = \begin{cases} J & j \in \text{nbr}(i) \\ 0 & j \notin \text{nbr}(i) \end{cases}$ ,  $\beta = \frac{J}{T}$  and  $|\text{nbr}(i)| = q \forall i$ .

**Mean field theory:** Suppose  $m_i = \langle m_i \rangle + \delta m_i = m + \delta m_i$ , where  $\delta m_i = m_i - m$  is a small fluctuation, then we can simplify the Hamiltonian considerably.

$$\begin{aligned} H(m) &= -J \sum_{(i,j)} m_i m_j \\ &= -J \sum_{(i,j)} (m + \delta m_i)(m + \delta m_j) \\ &\approx -J \sum_{(i,j)} (m^2 + m \delta m_i + m \delta m_j) \\ &= -\frac{J}{2} \sum_{j \in \text{nbr}(i)} \sum_i (m^2 + 2m \delta m_i) \\ &= -\frac{Jq}{2} \sum_i (m^2 + 2m (m_i - m)) \\ &= -\frac{Jq}{2} \left( 2m \sum_i m_i - \sum_i m^2 \right) \\ &= -\frac{Jq}{2} (2Mm - Nm^2) \end{aligned}$$

There is no interaction, which means that the only possible phase is a disordered phase. Similarly, adding a term  $\propto \sum_i m_i$  to the Hamiltonian only changes it

by a constant. Therefore, the Hamiltonian is invariant under application of a constant external field. Note that this analysis is to be taken with a great of salt because in many cases applying an external field will change the number of particles in the lattice.

**For simulation:** Choose an edge  $(i, j)$  randomly. Choose whether to exchange  $m_i$  and  $m_j$  using the Metropolis algorithm. The energy per temperature of an edge of the lattice is given by  $-\frac{E(i,j)}{T} = \beta(m_i m_j + \sum_{i' \neq j} m_i m_{i'} + \sum_{j' \neq i} m_j m_{j'} - m_i m_j)$ .

Let's compute the change in energy when  $m_i$  and  $m_j$  are exchanged:

$$\begin{aligned}
-\frac{\Delta E(i,j)}{T} &= \beta((m_i + \Delta m_i) \left( \sum_{i'} m_{i'} + \Delta m_j \right) + (m_j + \Delta m_j) \left( \sum_{j'} m_{j'} + \Delta m_i \right) \\
&\quad - (m_i + \Delta m_i) (m_j + \Delta m_j) - m_i \sum_{i'} m_{i'} - m_j \sum_{j'} m_{j'} + m_i m_j) \\
&= \beta(\Delta m_i \sum_{i'} m_{i'} + \Delta m_j \sum_{j'} m_{j'} + \Delta m_i \Delta m_j) \\
&= \beta \Delta m_i \left( \sum_{i'} m_{i'} - \sum_{j'} m_{j'} - \Delta m_i \right) \\
&= \beta \Delta m_i \left( \sum_{i'} m_{i'} - m_j - \sum_{j'} m_{j'} + m_i \right) \\
&= \beta(m_j - m_i) \left( \sum_{i' \neq j} m_{i'} - \sum_{j' \neq i} m_{j'} \right)
\end{aligned}$$

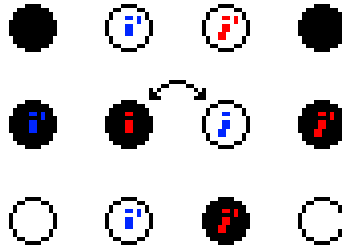
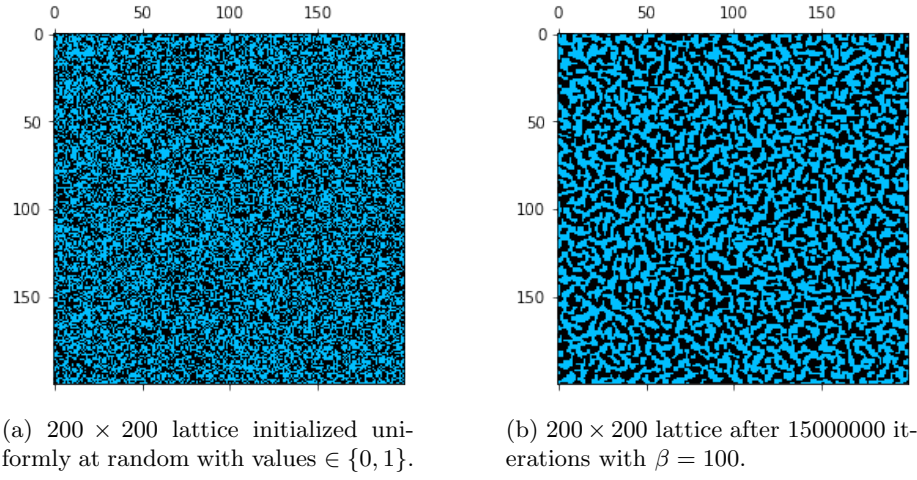


Figure 2: Sketch of the interaction between  $i$ ,  $j$  and neighbouring sites.  $i$  interacts with the blue sites, and  $j$  with the red ones.

**For exact solution:** Work out the 1D problem.

$$\begin{aligned}
 H(m) &= -J \sum_i m_i m_{i+1} \quad \text{if } m \text{ is a cycle, } J \neq 0 \text{ iff } j = i + 1 \\
 &= -J \sum_i k_i \quad \text{where } k_i = 1 \text{ if } m_i = m_{i+1} = 1, k_i = 0 \text{ otherwise}
 \end{aligned}$$

This system has  $\binom{N}{M}$  allowed configurations. To compute the partition function we must first find the degeneracy of all values of  $K = \sum_i k_i$ . This is equivalent to computing the number  $c(K, M, N)$  of induced subgraphs with  $M$  vertices and  $K$  edges in a cycle of length  $N$ .

Let's conceptualize a cycle of length  $N - 1$  as an open string of length  $N$  with periodic boundary conditions. We'll start with an empty string and calculate the number of ways to put  $M$  particles and  $K$  interacting pairs in it. Now let's take a vertex at one end of the string. We can either fill in with a particle or leave it empty. This observation gives us a simple way to divide the length  $N$  problem into two smaller problems. One of them is the calculation of the number of ways to put  $M - 1$  particles and  $K$  interacting pairs in a length  $N$  string with both ends filled. The other one is the calculation of the number of ways to put  $M$  particles and  $K$  interacting pairs in a length  $N$  string with one end filled and the other end empty. Repeating the process, we find that  $c(K, M, N) = f(K, M - 1, N - 1) + \sum_{O=1}^{N-2} g(K, M - 1, O)$ , where  $f(K, M, N)$  and  $g(K, M, N)$  are the calculations on smaller strings we mentioned. Similarly to how we decomposed  $c(K, M, N)$  in a combination of  $f(K, M, N)$  and  $g(K, M, N)$ ,  $f(K, M, N)$  and  $g(K, M, N)$  can be shown to obey the following recurrences:

$$\begin{aligned}
f(K, M, N) &= f(K - 1, M - 1, N - 1) + g(K, M, N - 1) \\
g(K, M, N) &= f(K, M - 1, N - 1) + g(K, M, N - 1) \\
\Rightarrow f(M, N, K) - g(M, N, K) &= f(M - 1, N - 1, K - 1) - f(M - 1, N - 1, K) \\
&\Rightarrow g(M, N - 1, K) = f(M, N - 1, K) - f(M - 1, N - 2, K - 1) \\
&\quad + f(M - 1, N - 2, K) \\
&\Rightarrow f(M, N, K) = f(M - 1, N - 1, K - 1) + f(M, N - 1, K) \\
&\quad + f(M - 1, N - 2, K) - f(M - 1, N - 2, K - 1)
\end{aligned}$$

We'll use the method of characteristic functions to find  $f$  and  $g$ . Let  $F(x, y, z) = \sum_{K, M, N} f(K, M, N) x^K y^M z^N$ ,  $G(x, y, z) = \sum_{K, M, N} g(K, M, N) x^K y^M z^N$  and  $f(1, 0, 0) = g(0, 0, 0) = 1$ ,  $f(K, M, 0) = g(K, M, 0) = 0$  for all other  $K, M$ . We need to calculate  $F(x, y, z)$  on subsets with one or two arguments equal to 0 before we're able to fully calculate  $F(x, y, z)$  and  $f(K, M, N)$ . Directly from initial conditions, we get  $g(0, 0, N) = f(0, 0, N) = 1$  and  $f(K, 0, N) =$

$$g(K, 0, N) = \begin{cases} 1 & K = 0 \\ 0 & K \neq 0 \end{cases} \text{ when } N \neq 0. \text{ This result allows us to calculate}$$

$F(x, 0, z)$  and  $G(x, 0, z)$ .

$$\begin{aligned}
F(x, 0, z) &= \sum_{K, N} f(K, 0, N) x^K z^N \\
&= x + \sum_{N \neq 0} z^N \\
&= x + \frac{z}{1-z} \\
G(x, 0, z) &= \sum_{K, N} g(K, 0, N) x^K z^N \\
&= 1 + \frac{z}{1-z}
\end{aligned}$$

Calculating  $F(0, y, z)$  and  $G(0, y, z)$  is a bit more complicated.

$$\begin{aligned}
f(0, M, N) &= g(0, M, N-1) \\
g(0, M, N) &= f(0, M-1, N-1) + g(0, M, N-1)
\end{aligned}$$

$$\begin{aligned}
\sum_{M, N} f(0, M, N+1) y^M z^N &= \sum_{M, N} g(0, M, N) y^M z^N \\
\frac{1}{z} \left( \sum_{M, N} f(0, M, N) y^M z^N - \sum_M f(0, M, 0) y^M \right) &= \sum_{M, N} g(0, M, N) y^M z^N \\
\frac{1}{z} \sum_{M, N} f(0, M, N) y^M z^N &= \sum_{M, N} g(0, M, N) y^M z^N \\
F(0, y, z) &= zG(0, y, z) \\
\sum_{M, N} g(0, M+1, N+1) y^M z^N &= \sum_{M, N} f(0, M, N) y^M z^N + \sum_{M, N} g(0, M+1, N) y^M z^N \\
\frac{1}{yz} \left( \sum_{M, N} g(0, M, N) y^M z^N - \frac{1}{1-z} \right) &= \sum_{M, N} f(0, M, N) y^M z^N + \frac{1}{y} \left( \sum_{M, N} g(0, M, N) y^M z^N - \frac{1}{1-z} \right) \\
G(0, y, z) - \frac{1}{1-z} &= yzF(0, y, z) + zG(0, y, z) - \frac{z}{1-z}
\end{aligned}$$

$$\begin{aligned}
G(0, y, z) &= yz^2G(0, y, z) + zG(0, y, z) + 1 \\
G(0, y, z) &= \frac{1}{1-z-yz^2} \\
F(0, y, z) &= \frac{z}{1-z-yz^2}
\end{aligned}$$

$$\begin{aligned}
G(0, y, z) &= \sum_{n=0}^{\infty} (z + yz^2)^n \\
&= \sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k} z^{n-k} y^k z^{2k} \\
&= \sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k} y^k z^{n+k} \\
&= \sum_{M, N} g(0, M, N) y^M z^N \text{ where } g(0, M, N) = \begin{cases} \binom{N-M}{M} & M \in \{0, N/2\} \\ 0 & M \notin \{0, N/2\} \end{cases}
\end{aligned}$$

$$F(0, y, z) = \sum_{M, N} g(0, M, N) y^M z^N \text{ where } g(0, M, N) = \begin{cases} \binom{N-M-1}{M} & M \in \{0, N/2-1\} \\ 0 & M \notin \{0, N/2-1\} \end{cases}$$

It takes a bit more work to calculate  $G(x, y, z)$ .

$$\begin{aligned}
\sum_{K, M, N} f(K+1, M+1, N+1) x^K y^M z^N &= \sum_{K, M, N} f(K, M, N) x^K y^M z^N + \sum_{K, M, N} g(K+1, M+1, N) x^K y^M z^N \\
\frac{1}{xyz} \left( F(x, y, z) - \frac{z}{1-z-yz^2} - x \right) &= F(x, y, z) + \frac{1}{xy} \left( G(x, y, z) - \frac{1}{1-z-yz^2} \right) \\
F(x, y, z) - x &= xyzF(x, y, z) + zG(x, y, z)
\end{aligned}$$

$$\begin{aligned}
\sum_{K, M, N} g(K, M+1, N+1) x^K y^M z^N &= \sum_{K, M, N} f(K, M, N) x^K y^M z^N + \sum_{K, M, N} g(K, M+1, N) x^K y^M z^N \\
\frac{1}{yz} \left( G(x, y, z) - 1 - \frac{z}{1-z} \right) &= F(x, y, z) + \frac{1}{y} \left( G(x, y, z) - 1 - \frac{z}{1-z} \right) \\
G(x, y, z) - 1 - \frac{z}{1-z} &= yzF(x, y, z) + zG(x, y, z) - z - \frac{z^2}{1-z} \\
G(x, y, z) &= yzF(x, y, z) + zG(x, y, z) + 1
\end{aligned}$$

$$\begin{aligned}
F(x, y, z) &= \frac{z}{1 - xyz} G(x, y, z) + \frac{x}{1 - xyz} \\
G(x, y, z) &= \frac{yz^2}{1 - xyz} G(x, y, z) + \frac{xyz}{1 - xyz} + zG(x, y, z) + 1 \\
\frac{1 - xyz - yz^2 - z + xyz^2}{1 - xyz} G(x, y, z) &= \frac{1}{1 - xyz} \\
G(x, y, z) &= \frac{1}{1 - xyz - yz^2 - z + xyz^2} \\
&= \sum_{n=0}^{\infty} (z + yz^2 + xyz - xyz^2)^n
\end{aligned}$$

$$\begin{aligned}
G(x, y, z) &= \sum_{n=0}^{\infty} (z + yz^2 + xyz - xyz^2)^n \\
&= \sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k} (z + yz^2)^k (xyz - xyz^2)^{n-k} \\
&= \sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k} \sum_{l=0}^k \binom{k}{l} z^{k-l} y^l z^{2l} \\
&\quad \sum_{m=0}^{n-k} \binom{n-k}{m} (-1)^m x^{n-k-m} y^{n-k-m} z^{n-k-m} x^m y^m z^{2m} \\
&= \sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k} \sum_{l=0}^k \binom{k}{l} y^l z^{k+l} \sum_{m=0}^{n-k} \binom{n-k}{m} (-1)^m x^{n-k} y^{n-k} z^{n-k+m} \\
&= \sum_{n=0}^{\infty} \sum_{k=0}^n \sum_{l=0}^k \sum_{m=0}^{n-k} \binom{n}{k} \binom{k}{l} \binom{n-k}{m} (-1)^m x^{n-k} y^{n-k+l} z^{n+m+l}
\end{aligned}$$

$$K = n - k$$

$$M = n - k + l$$

$$N = n + m + l$$

$$\begin{aligned}
&= \sum_{K,M,N} \sum_{m=0}^K \binom{N-m-M+K}{N-m-M} \binom{N-m-M}{M-K} \binom{K}{m} (-1)^m x^K y^M z^N \\
&= \sum_{K,M,N} \sum_{m=0}^K \frac{(N-m-M+K)!}{(N-m-2M+K)!} \binom{K}{m} (-1)^m \frac{1}{K!} \frac{1}{(M-K)!} x^K y^M z^N \\
&= \sum_{K,M,N} \sum_{m=0}^K (-1)^m \binom{K}{m} \binom{N-m-M+K}{N-m-2M+K} \frac{M!}{K!(M-K)!} x^K y^M z^N \\
&= \sum_{K,M,N} \sum_{m=0}^K (-1)^m \binom{K}{m} \binom{N-m-M+K}{M} \binom{M}{K} x^K y^M z^N \\
&= \sum_{K,M,N} \binom{N-M}{M-K} \binom{M}{K} x^K y^M z^N \text{ by Wolfram}
\end{aligned}$$

$$g(K, M, N) = \begin{cases} \binom{N-M}{M-K} \binom{M}{K} & M \in \{0, N\} \\ 0 & M \notin \{0, N\} \end{cases}$$

We can easily calculate  $f(K, M, N)$  with the help of the recurrence relations we wrote down at the beginning.

$$\begin{aligned}
f(K, M, N) &= g(K, M+1, N+1) - g(K, M+1, N) \\
&= \binom{N-M}{M-K+1} \binom{M+1}{K} - \binom{N-M-1}{M-K+1} \binom{M+1}{K} \\
&= \binom{N-M-1}{M-K} \binom{M+1}{K} \text{ by Pascal's identity}
\end{aligned}$$

$$\begin{aligned}
c(K, M, N) &= f(K, M-1, N-1) + \sum_{O=1}^{N-2} g(K, M-1, O) \\
&= \binom{N-M-1}{M-K-1} \binom{M}{K} + \sum_{O=M-1}^{N-2} \binom{O-M+1}{M-K-1} \binom{M-1}{K}
\end{aligned}$$



$$\begin{aligned}
\sum_{O=M-1}^{N-1} \binom{O-M+1}{M-K-1} &= \sum_{O=M-1}^{N-2} \binom{O-M+2}{M-K} - \sum_{O=M-1}^{N-2} \binom{O-M+1}{M-K} \\
&= \sum_{O=M}^{N-1} \binom{O-M+1}{M-K} - \sum_{O=M-1}^{N-2} \binom{O-M+1}{M-K} \\
&= \binom{N-M}{M-K} \\
c(K, M, N) &= \binom{N-M-1}{M-K-1} \binom{M}{K} + \binom{N-M}{M-K} \binom{M-1}{K}
\end{aligned}$$

We take the thermodynamics limit  $M \rightarrow \infty$ ,  $N \rightarrow \infty$ ,  $\frac{M}{N} = \rho$ . We'll assume the maximum of  $c(K, M, N)$  along  $K$  is attained when  $K \propto M$  and find the constant of proportionality  $\eta$ .  $\eta$  can be thought of as the number of links per particle.

$$\begin{aligned}
c(K, M, N) &\approx \sqrt{\frac{N-M-1}{2\pi(M-K-1)(N-2M+K)}} \\
&\quad \frac{(N-M-1)^{N-M-1}}{(M-K-1)^{M-K-1}(N-2M+K)^{N-2M+K}} \\
&\quad \sqrt{\frac{M}{2\pi K(M-K)}} \frac{M^M}{K^K(M-K)^{M-K}} \\
&\quad + \sqrt{\frac{N-M}{2\pi(M-K)(N-2M+K)}} \\
&\quad \frac{(N-M)^{N-M}}{(M-K)^{M-K}(N-2M+K)^{N-2M+K}} \\
&\quad \sqrt{\frac{M-1}{2\pi K(M-K-1)}} \frac{(M-1)^{M-1}}{K^K(M-K-1)^{M-K-1}}
\end{aligned}$$

$$\begin{aligned}
Z &= \sum_K c(K, M, N) e^{\beta K} \\
&\approx \sum_K \sqrt{\frac{N-M-1}{2\pi(M-K-1)(N-2M+K)}} \\
&\quad \frac{(N-M-1)^{N-M-1}}{(M-K-1)^{M-K-1}(N-2M+K)^{N-2M+K}} \\
&\quad \sqrt{\frac{M}{2\pi K(M-K)}} \frac{M^M}{K^K(M-K)^{M-K}} e^{\beta K} \\
&\quad + \sum_K \sqrt{\frac{N-M}{2\pi(M-K)(N-2M+K)}} \\
&\quad \frac{(N-M)^{N-M}}{(M-K)^{M-K}(N-2M+K)^{N-2M+K}} \\
&\quad \sqrt{\frac{M-1}{2\pi K(M-K-1)}} \frac{(M-1)^{M-1}}{K^K(M-K-1)^{M-K-1}} e^{\beta K}
\end{aligned}$$

$$\begin{aligned}
\log(c(K, M, N) e^{\beta K}) &\sim (N-M) \log(N-M) - (M-K) \log(M-K) \\
&\quad - (N-2M+K) \log(N-2M+K) + M \log(M) \\
&\quad - K \log(K) - (M-K) \log(M-K) + \beta K \\
\frac{\partial}{\partial K} \log(c(K, M, N) e^{\beta K}) &= 2 \log(M-K) + 2 - \log(N-2M+K) \\
&\quad - 1 - \log(K) - 1 + \beta \\
&= 2 \log(M-K) - \log(N-2M+K) - \log(K) + \beta \\
0 &= 2 \log(M-K) - \log(N-2M+K) - \log(K) + \beta \\
e^{-\beta} &= \frac{(M-K)^2}{(N-2M+K)K} \\
e^{-\beta} &= \frac{(1-\eta)^2}{(1/\rho - 2 + \eta)\eta}
\end{aligned}$$

$$\begin{aligned}
K &= \frac{\sqrt{(e^{-\beta}-1)M^2 + (e^{-\beta}M - \frac{1}{2}e^{-\beta}N - M)^2 + (e^{-\beta}M - \frac{1}{2}e^{-\beta}N - M)}}{e^{-\beta}-1} \\
\eta &= \frac{\sqrt{(e^{-\beta}-1) + (e^{-\beta} - \frac{1}{2\rho}e^{-\beta} - 1)^2 + (e^{-\beta} - \frac{1}{2\rho}e^{-\beta} - 1)}}{e^{-\beta}-1}
\end{aligned}$$

$$\eta = \sqrt{\frac{1}{|e^{-\beta} - 1|} + \left(1 - \frac{1}{2\rho|e^{\beta} - 1|}\right)^2} + 1 - \frac{1}{2\rho|e^{\beta} - 1|}$$

$$C = -\frac{\partial\eta}{\partial\beta} = \frac{\left(2(\rho - 1)\rho(e^{\beta} - 1) + \sqrt{1 - 4(\rho - 1)\rho(e^{\beta} - 1)} - 1\right)e^{\beta}}{2\sqrt{1 - 4(\rho - 1)\rho(e^{\beta} - 1)}(e^{\beta} - 1)^2}$$

Some interesting limits include  $\beta \rightarrow \infty$ ,  $\beta \rightarrow 0$  and  $\beta \rightarrow -\infty$ .

$$\beta \rightarrow \infty \Rightarrow \eta \rightarrow \sqrt{-1 + 1} + 1$$

= 1 particles are clustering

$$\beta \rightarrow 0 \Rightarrow \eta = \frac{|e^{-\beta} - \frac{1}{2\rho}e^{-\beta} - 1|\sqrt{1 + \frac{e^{-\beta} - 1}{(e^{-\beta} - \frac{1}{2\rho}e^{-\beta} - 1)^2}} + (e^{-\beta} - \frac{1}{2\rho}e^{-\beta} - 1)}{e^{-\beta} - 1}$$

$$\rightarrow \frac{\frac{1}{2\rho}\sqrt{1 + 4(e^{-\beta} - 1)\rho^2} - \frac{1}{2\rho}}{e^{-\beta} - 1}$$

$$\rightarrow \frac{\frac{1}{2\rho} + (e^{-\beta} - 1)\rho - \frac{1}{2\rho}}{e^{-\beta} - 1}$$

$\rightarrow \rho$  particles are distributed randomly

$$\beta \Rightarrow -\infty \Rightarrow \eta \rightarrow \left|1 - \frac{1}{2\rho}\right| + 1 - \frac{1}{2\rho}$$

$$= \begin{cases} 2 - \frac{1}{\rho} & \rho \geq \frac{1}{2} \\ 0 & \rho < \frac{1}{2} \end{cases} \text{ particles avoid contact}$$

The discontinuity indicates a phase transition when  $\beta \rightarrow -\infty$  and  $\rho \rightarrow \frac{1}{2}$ .