Experiments

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Motivation: We wish to study the transport of M interacting particles within a square lattice of size N.

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

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

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.

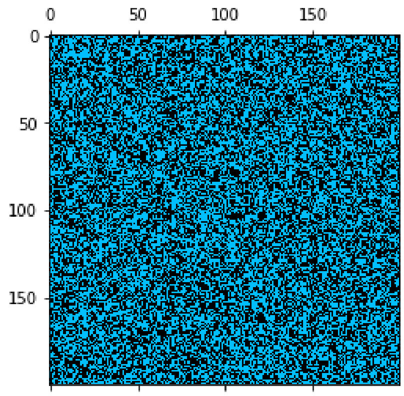
$$\begin{aligned} H(m) &= -J \sum_{(i,j)} m_i\ m_j \\ &= -J \sum_{(i,j)} (m + \delta m_i)(m + \delta m_j) \\ &\approx -J \sum_{(i,j)} (m^2 + m\ \delta m_i + m\ \delta m_j) \\ &= -\frac{J}{2} \sum_{j \in \mathrm{nbd}(i)} \sum_i (m^2 + 2m\ \delta m_i) \\ &= -\frac{Jq}{2} \sum_i (m^2 + 2m\ (m_i - m)) \\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

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.

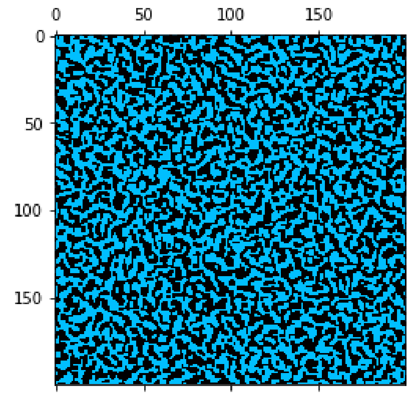
For simulation: Choose an edge (i, j) randomly. Choose whether to exchange m_i and m_j using the Metropolis algorithm. The energy per temperature of an edge of the lattice is given by $-\frac{E_{(i,j)}}{T} = \beta(m_i\ m_j + \sum_{i' \neq j} m_i\ m_{i'} + \sum_{j' \neq i} m_j\ m_{j'} = m_i \sum_{i'}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

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

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



(a) 200×200 lattice initialized uniformly at random with values $\in \{0, 1\}$.



(b) 200×200 lattice after 15000000 iterations with $\beta = 100$.

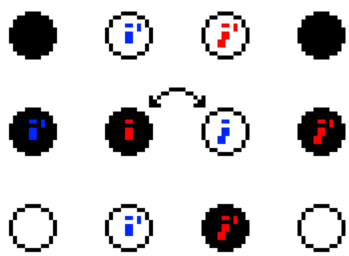


Figure 2: Sketch of the interaction between i, j and neighbouring sites. i interacts with the blue sites, and j with the red ones.

For exact solution: Work out the 1D problem.

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

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 one 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 $f(K, 0, N) = g(K, 0, N) = \begin{cases} 1 & K = 0 \\ 0 & K \neq 0 \end{cases}$ when $N \neq 0$. 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.

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

$$\begin{aligned}
\sum_{M,N} f(0,M,N+1)y^M z^N &= \sum_{M,N} g(0,M,N)y^M z^N \\
\frac{1}{z}\Big(\sum_{M,N} f(0,M,N)y^M z^N - \sum_{M} f(0,M,0)y^M\Big) &= \sum_{M,N} g(0,M,N)y^M z^N \\
\frac{1}{z}\sum_{M,N} f(0,M,N)y^M z^N &= \sum_{M,N} g(0,M,N)y^M z^N \\
F(0,y,z) &= zG(0,y,z)
\end{aligned}$$

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

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

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

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

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

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

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

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

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

$$
\begin{aligned}
K &= n-k \\
M &= n-k+l \\
N &= n+m+l
\end{aligned}
$$

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

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

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

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

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

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

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

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

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

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

$$\begin{aligned}
\beta \to \infty \Rightarrow \eta &\to \sqrt{-1+1}+1 \\
&= 1 \text{ particles are clustering} \\
\beta \to 0 \Rightarrow \eta &= \frac{|e^{-\beta} - \frac{1}{2\rho}e^{-\beta} - 1|\sqrt{1 + \frac{e^{-\beta}-1}{(e^{-\beta}-\frac{1}{2\rho}e^{-\beta}-1)^2}} + (e^{-\beta} - \frac{1}{2\rho}e^{-\beta} - 1)}{e^{-\beta}-1} \\
&\to \frac{\frac{1}{2\rho}\sqrt{1+4(e^{-\beta}-1)\rho^2} - \frac{1}{2\rho}}{e^{-\beta}-1} \\
&\to \frac{\frac{1}{2\rho} + (e^{-\beta}-1)\rho - \frac{1}{2\rho}}{e^{-\beta}-1} \\
&\to \rho \text{ particles are distributed randomly} \\
\beta \Rightarrow -\infty \Rightarrow \eta &\to \left|1 - \frac{1}{2\rho}\right| + 1 - \frac{1}{2\rho} \\
&= \begin{cases} 2 - \frac{1}{\rho} & \rho \geq \frac{1}{2} \\ 0 & \rho < \frac{1}{2} \end{cases} \text{ particles avoid contact}
\end{aligned}$$

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