HomeWork 4 : Ising Spins

Most of this homework has to be done on a computer, with the language of your choice. Present your results with graphs, plots, and data.

We consider $i = 1 \dots N$ spins taking values $S_i = \pm 1$, on a two-dimensional grid of size $L \times L$, with $N = L^2$. We shall use periodic boundary conditions. The Hamiltonian reads

$$\mathcal{H} = -\sum_{\langle i,j \rangle} S_i S_j \tag{1}$$

where $\langle i, j \rangle$ denote the complete set of links i, j on the two-dimensional grid. We work here with the convention that $k_b = J = 1$, so that $\beta = 1/T$.

1 The Metropolis rule

1. Implement the *classical* metropolis sampling strategy, where one choose one spin at random, propose a flip and accept it with a probability such it that satisfies the detailed balanced property with the Metropolis rule. We shall define the time t as moving from t to $t + 1/N$ every time we attempt to move a single spin.
   From Onsager, we now that there is a phase transition at $T_c = \frac{2}{\ln(1+\sqrt{2})} \approx 2.26918$. How does the system looks like after few steps at large $T > T_c$? And at small $T < T_c$?
2. Start with a perfectly ordered configuration, with a system size not too small ($L > 20$ at least). Plot how the energy and the magnetization evolve in time for different value of the temperature $T > T_c$. Do you notice anything special around T_c ?
3. Start with a random configuration. Plot how the energy and the magnetization evolve in time for different value of the temperature $T < T_c$. Look at how the configurations of spins evolve : do you always reach a perfect configuration at $T = 0$?

2 The Wolff algorithm

1. We shall now implement the Wolff strategy, which we recall here (notations are from https ://arxiv.org/pdf/cond-mat/0311623.pdf)

Algorithm 1 Wolff Cluster

$i \leftarrow random(N)$
$\mathcal{C} \leftarrow \{i\}$
$\mathcal{F}_{\text{old}} \leftarrow \{i\}$
while $\mathcal{F}_{\text{old}} \neq \{\}$
    $\mathcal{F}_{\text{new}} \leftarrow \{\}$
    for $\forall i \in \mathcal{F}_{\text{old}}$ do
        $\forall j$ neighbor of i with $S_i = S_j$, and j not in $\mathcal{C}$ do
            with probability p : add j to $\mathcal{F}_{\text{new}}$ and to $\mathcal{C}$.
    $\mathcal{F}_{\text{old}} \leftarrow \mathcal{F}_{\text{new}}$
for $\forall i \in \mathcal{C}$ do $S_i = -S_i$
$t \leftarrow t + \text{size}(\mathcal{C})/N$

2. Compare the performance with metropolis by repeating Q1.2 and Q1.3. Compare the time needed to reach equilibrium in both methods.

3 Finite Size Scaling

For the last problem, we need to generate some good estimates of the average magnetization and of the energy, for many different sizes.

1. The first thing you will have to do is run the Wolff algorithm a long time, at different temperatures (above and below T_c) and sizes L, to get some estimate of

$$
\begin{aligned}
m_{\text{abs}} &= \mathbb{E}[|\sum S_i/N|] && (2)\\
m_2(L,T) &= \mathbb{E}[(\sum S_i/N)^2] && (3)\\
m_4(L,T) &= \mathbb{E}[(\sum S_i/N)^4] && (4)\\
e(L,T) &= \mathbb{E}[(\mathcal{H}(\{S\})] && (5)\\
g_{\text{Binder}}(L,T) &= \frac{m_4(L,T)}{3m_2(L,T)^2} && (6)
\end{aligned}
$$

   You can do this by running your algorithm long enough such that these quantity do not evolve in time and then performing averages with many configuration (let us not worry too much about the error bar in this homework)

2. Compare the value of the magnetization (absolute) and energy with respect to the exact Onsager solution at $N \to \infty$ [1]

3. Try to do a finite size scaling plot for the magnetization and the binder cummulant with the following scaling assumptions :

$$
\begin{aligned}
m_{\text{abs}}(L,T) &= L^{-\frac{\beta}{\nu}} g_1(|T-T_c|L^{\frac{1}{\nu}}) && (7)\\
g_{\text{Binder}}(L,T) &= g_2(|T-T_c|L^{\frac{1}{\nu}}) && (8)
\end{aligned}
$$

   Find the best value of T_c, ν and β by tryong to manually experimenting with different values (the goal is to observe a nice Data collapse on a single curve), and compare with the exact results from the Onsager solution.

1. you can find them here, with the exact value of the critical exponents : `http://www.nyu.edu/classes/tuckerman/stat.mech/lectures/lecture_26/node2.html`.