# PH415 Assignment 4
## Ising Model Simulation

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## Problem

Write a program for a Monte Carlo (MC) simulation to study the phase transition in 2-dimensional Ising model on a square lattice (128 × 128) with periodic boundary conditions. Set the interaction strength J = 1 and the Boltzmann constant kB = 1. Implement the single spin flip Metropolis algorithm for sampling. The critical temperature of the 2d Ising model is $T_c = 2\ln(1+\sqrt{2}) = 2.269185$.

i Plot Magentisation, m(t) and Energy, E(t) for $t_{max}$ = 50,000 at $T < T_c$, $T = T_c$, $T > T_c$. Print Final lattice configuration for all three temperatures.

ii Varying Temperature for 1.25 to 3.25 in steps of 0.05, Plot average energy per site, average magnetisation, susceptibility and specific heat.

## General Algorithm

- Step 1: Initialize T = 1.25, and generate a lattice of LxL = 128x128 with random 1's and -1's.
- Step 2: Choose a site and find the number of nearest neighbours in opposite spin. Calculate $\Delta E$ and W = $exp(-\Delta E/T)$.
- Step 3: Generate a random number. If r¡W, flip spin. Repeat from Step 2 $L^2$ times.
- Step 4: Increase t by 1. If t¿1000and t%100=0, store E, m, $m^2$ and $E^2$. If t = $t_{max}$, reset t, increase T by 0.05 and repeat from step 2 till T = 3.25.
- Step 5: Take average value of the expression stored for each T and plot.

## Code

```
Tc = 2/(log(1+sqrt(2)));
L = 128;
Temp = 1.25:0.05:3.25;
lat = rand(L,L);
p=0.5;
lat = sign(lat-p);
e = zeros(L,L);
tmax = 50000;
E = zeros(tmax,1);
mag = zeros(tmax,1);
E2avg = zeros(length(Temp),1);
Eavg = zeros(length(Temp),1);
mavg = zeros(length(Temp),1);
m2avg = zeros(length(Temp),1);
sus = zeros(length(Temp),1);
sh = zeros(length(Temp),1);
for k = 1:length(Temp)
    count = 0;
    t = 0;
```

```
    while t < tmax
        for i = 1:L
            for j = 1:L
                e(i,j) = -lat(i,j)*(lat(mod(i-2,L)+1,j)+lat(i,mod(j-2,L)+1)+lat(mod(i,L)+1,j)+lat(i,mod(j,L)+1));
                dE = -2*e(i,j);
                p = exp(-dE/Temp(k));
                r = rand();
                if r <= p
                    lat(i,j) = -lat(i,j);
                end
            end
        end

        mag(t+1) = abs(sum(sum(lat))/(L*L));
        E(t+1) = sum(sum(e))/2;
        if t > 1000 && mod(t,100) == 0
            count = count + 1;
            Eavg(k) = Eavg(k) + E(t+1);
            mavg(k) = mavg(k) + mag(t+1);
            E2avg(k) = E2avg(k) + E(t+1)*E(t+1);
            m2avg(k) = m2avg(k) + mag(t+1)*mag(t+1);
        end
        %disp(t);
        t = t + 1;
    end
    % figure;
    % plot(0:tmax-1,mag);
    % title('Magnetization');
    % xlabel('Time');
    % ylabel('Magnetization');
    % figure;
    % plot(0:tmax-1,E);
    % title('Energy');
    % xlabel('Time');
    % ylabel('Energy');
    % figure;
    % imagesc(lat);
    % title('Lattice');
    disp(Temp(k))
end
Eavg = Eavg/count;
mavg = mavg/count;
m2avg = m2avg/count;
E2avg = E2avg/count;
for i = 1:length(Temp)
    sus(i) = L*L*(m2avg(i) - mavg(i)*mavg(i))/(Temp(i));
    sh(i) = (E2avg(i) - Eavg(i)*Eavg(i))/(Temp(i)*Temp(i));
end

figure;
plot(Temp,mavg);
figure;
plot(Temp,Eavg/(L*L));
figure;
plot(Temp,sus);
figure;
plot(Temp,sh);

writematrix([mavg Eavg sh sus], 'data.csv')
```

## Results

### For $T < Tc$

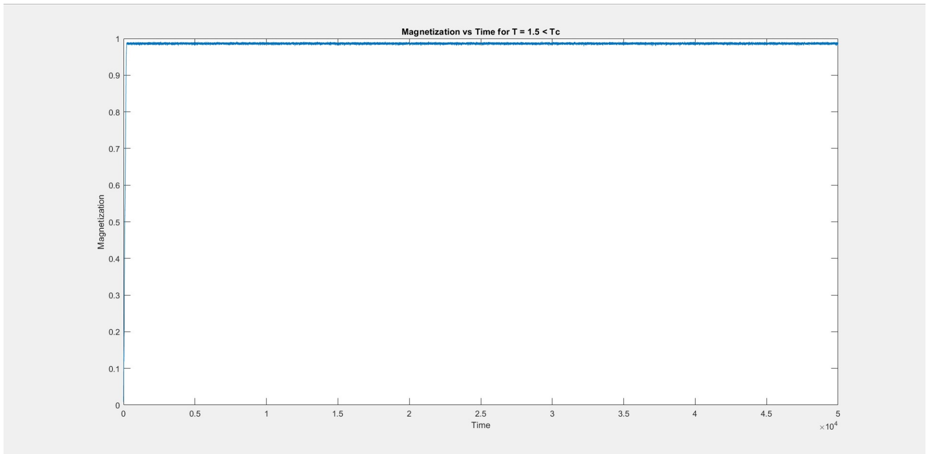


Figure 1: Magnetisation vs Time for an initial Random Configuration for T=1.5

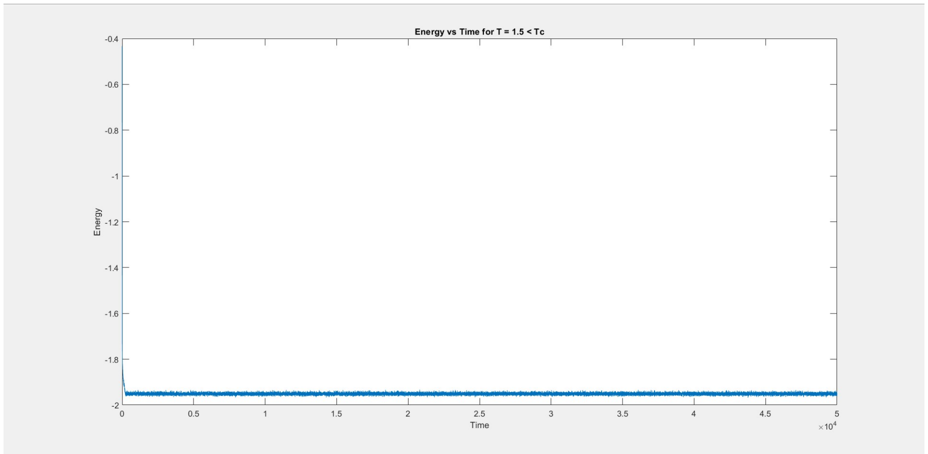


Figure 2: Energy vs Time for an initial Random Configuration for T=1.5

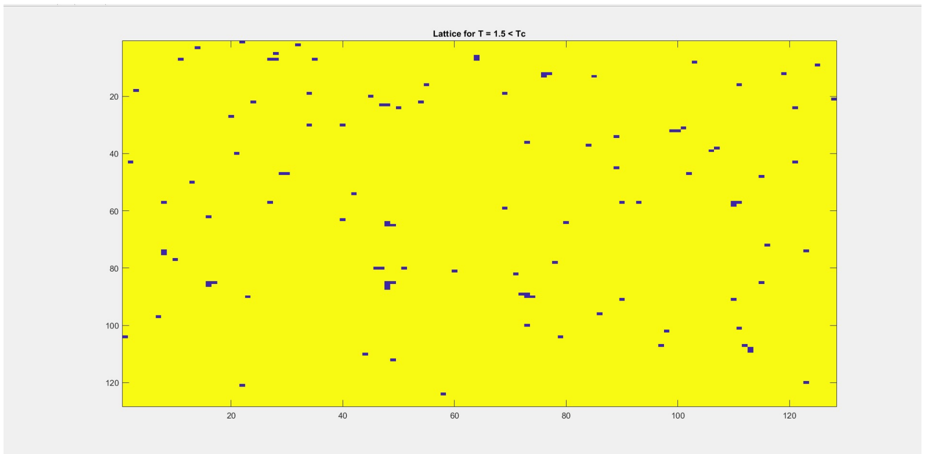


Figure 3: Final Lattice Configuration for T=1.5. Here Blue $\implies$ spin down and yellow $\implies$ spin up.

## For T=Tc

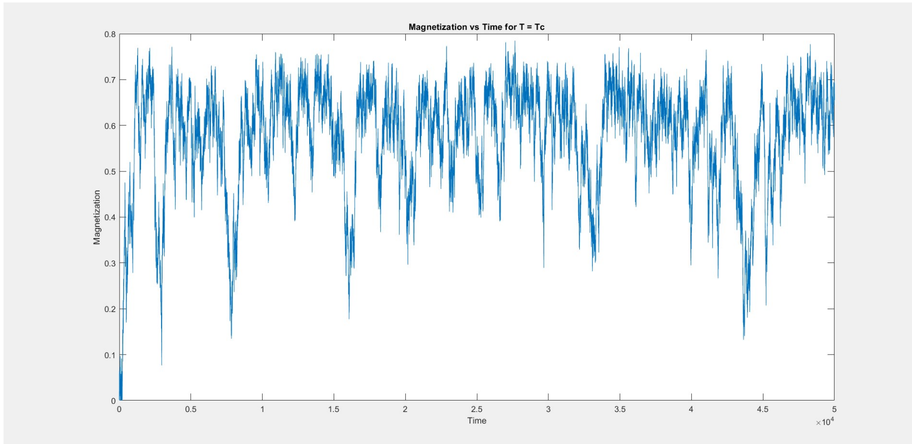


Figure 4: Magnetisation vs Time for an initial Random Configuration for T=Tc

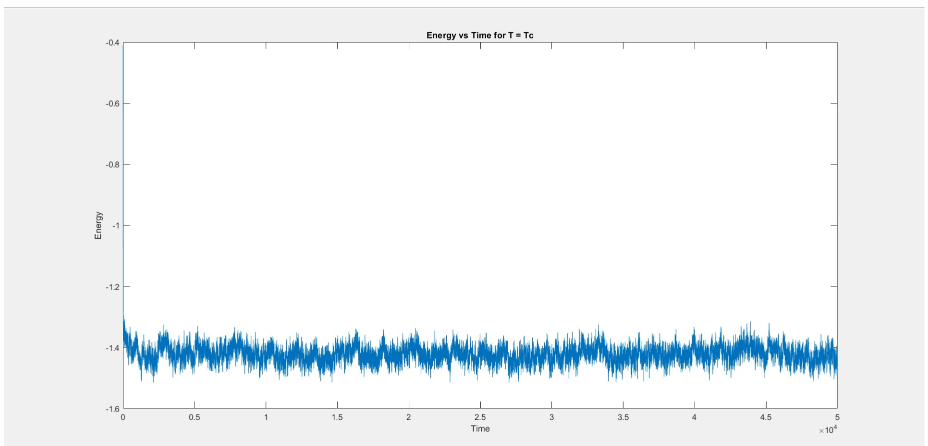


Figure 5: Energy vs Time for an initial Random Configuration for T=Tc

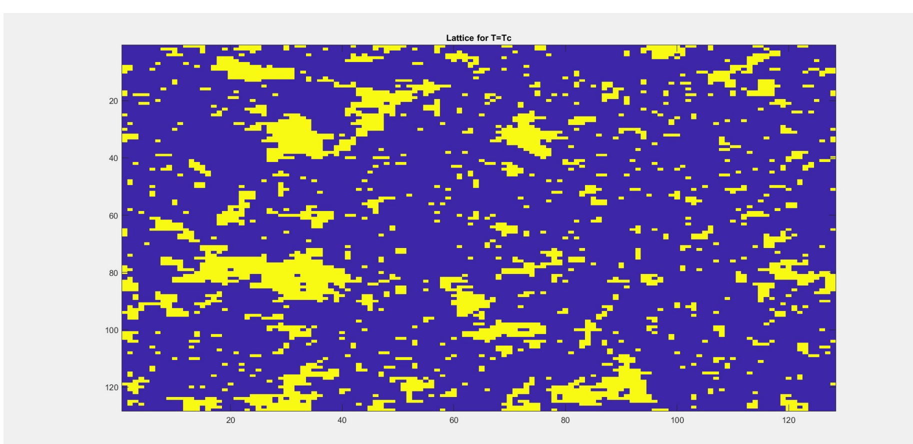


Figure 6: Final Lattice Configuration for T=Tc. Here Blue $\implies$ spin down and yellow $\implies$ spin up.

**For $T > Tc$**

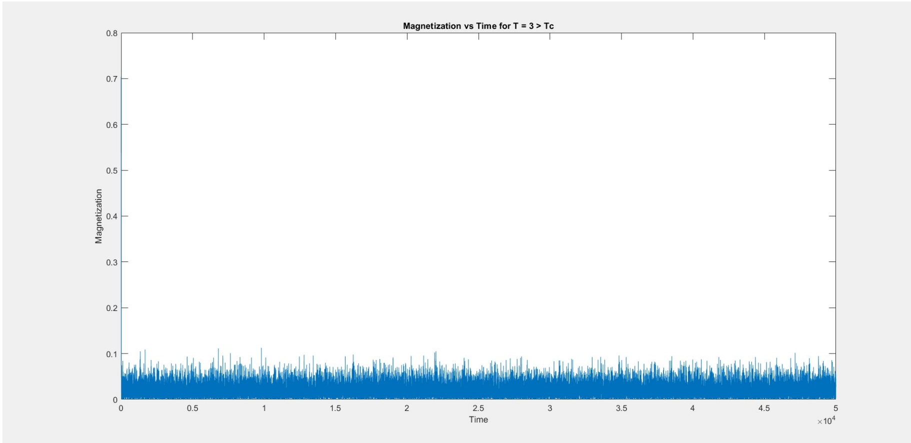


Figure 7: Magnetisation vs Time for initial configuration of all up for T=3

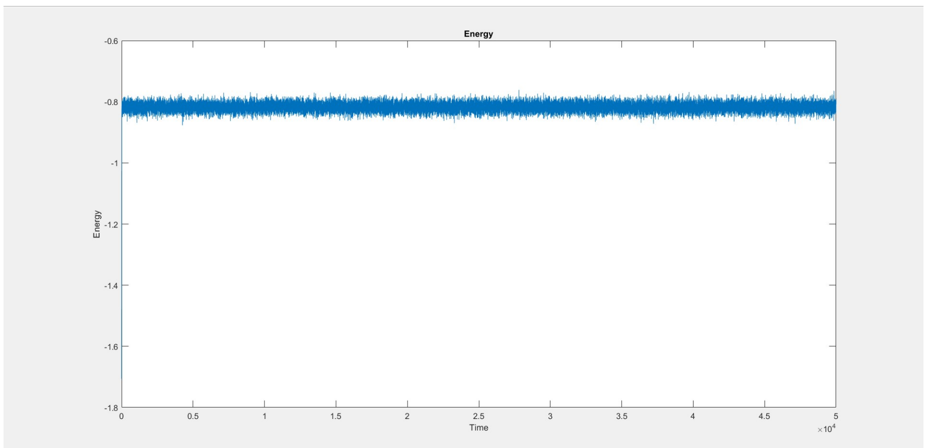


Figure 8: Energy vs Time for initial configuration of all up for T=3

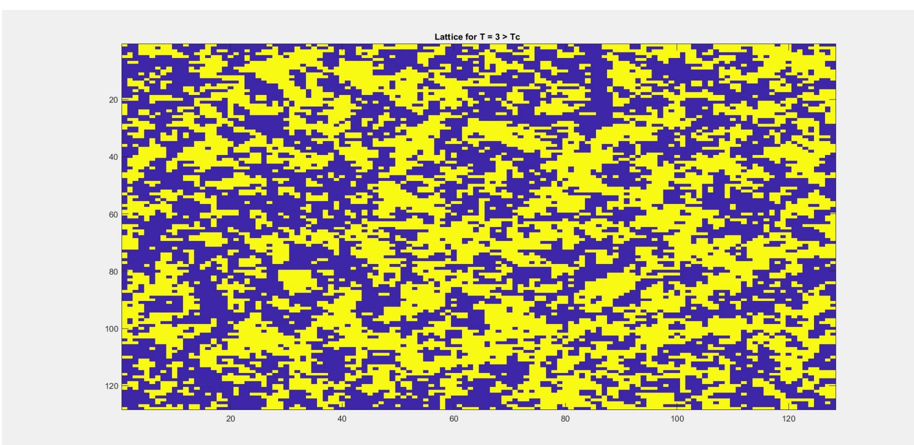


Figure 9: Final Lattice Configuration for T=3.Here Blue $\implies$ spin down and yellow $\implies$ spin up.

## Part B

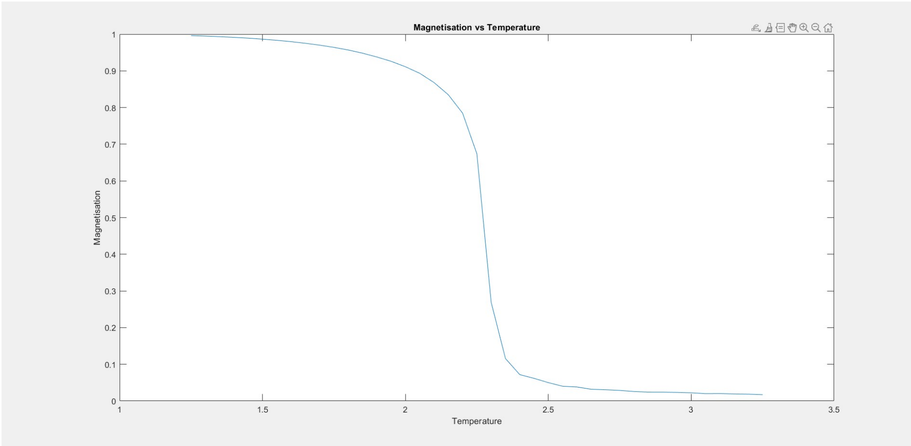


Figure 10: Magnetisation per lattice vs Temperature

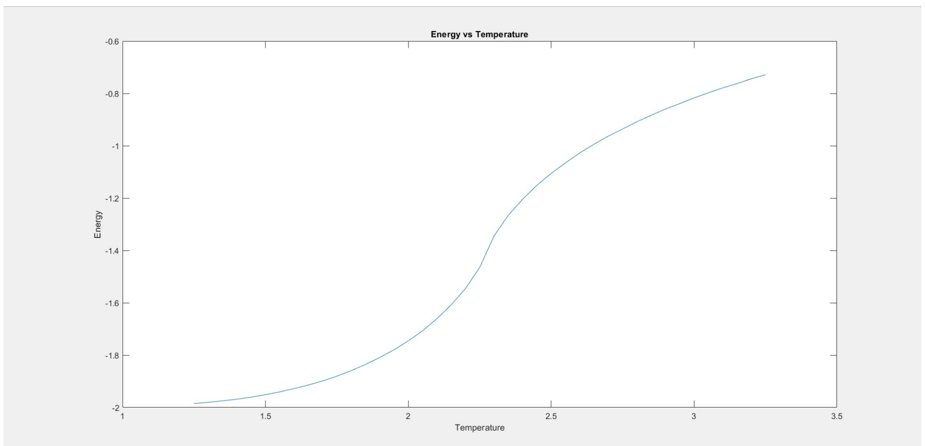


Figure 11: Energy per lattice vs Temperature

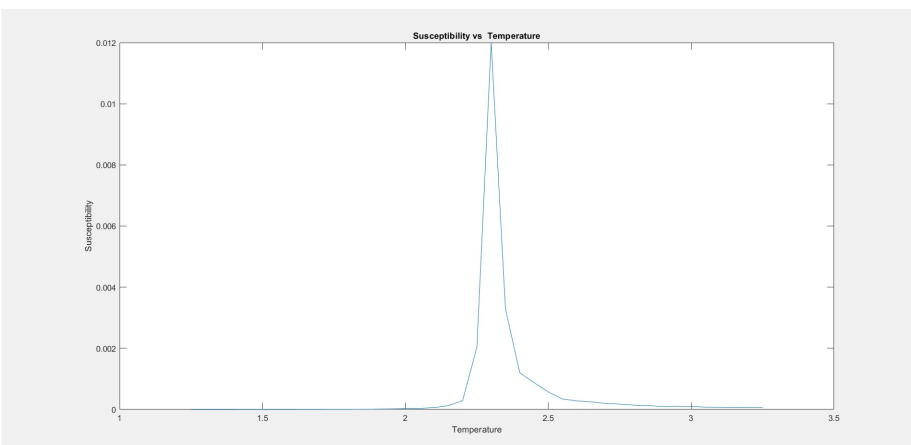


Figure 12: Susceptibility per lattice vs Temperature

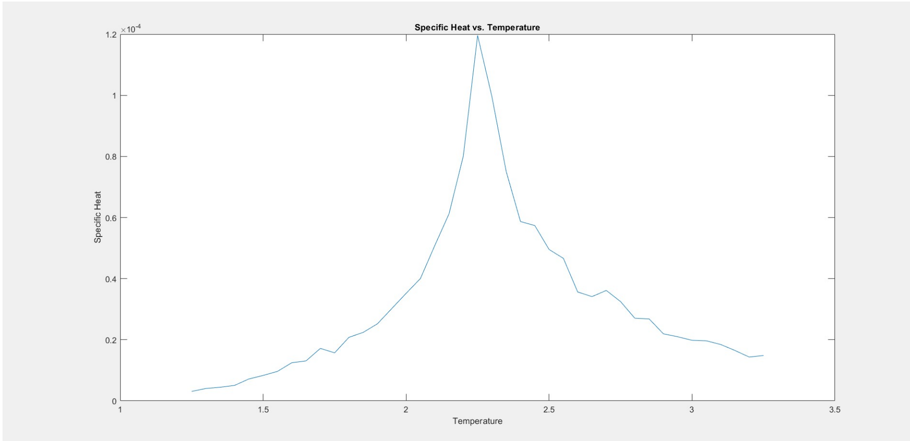


Figure 13: Specific Heat per lattice vs Temperature

# Discussion

- From the plots for $T < Tc$, we can see that the magnetisation of a lattice site of random spins converges to a $m \approx 1$. This implies that all the spins are aligned in the same direction. Similarly, the energy plot takes the minimum value of -2. The final lattice configuration shows that almost all spins are aligned upwards.
- From the plots for $T = Tc$, we can see that the magnetisation of a lattice site of random spins does not converge, and keeps oscillating around an average value of 0.5. This suggests that most spins are in a single direction with some smaller clusters of opposite spins. As such, the energy per lattice also decreases. The final lattice configuration shows these small clusters as expected.
- From the plot for $T > Tc$, we can see that the magnetisation of a lattice site of up spins converges to a $m \approx 0$. This implies that all the spins are aligned randomly. Hence, the energy per lattice also decreases to a value of -0.8. The final lattice configuration also shows that the sites randomly oriented in spin up or spin down.
- The average Magnetisation/Energy vs Temperature plots are plotted by taking average of the expressions after every 100 cycles to avoid correlation. The first 1000 cycles are also skipped to allow the spin simulation to reach equilibrium.
- The magnetisation vs Temperature plot shows that for $T < Tc$, the average magnetisation is close to 1, where for $T > Tc$, the magnetisation is close to 0.
- As the Temperature increases, the average energy per lattice site increases from a minimum of -2. This trend is expected as energy generally increases with Temperature.
- The susceptibility and specific heat show sharp peeks at T=Tc. This is characteristic of a Second order transition.