Assignment 3.

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Due Oct 24

1. (a) We can define a reference temperature as

$$\epsilon = k_B T_r$$

Dividing the current temperature by the reference gets you the dimensionless temperature.

$$T^* = \frac{T}{\frac{\epsilon}{k_B}}$$

(b)

$$\beta = \frac{1}{k_B T}$$

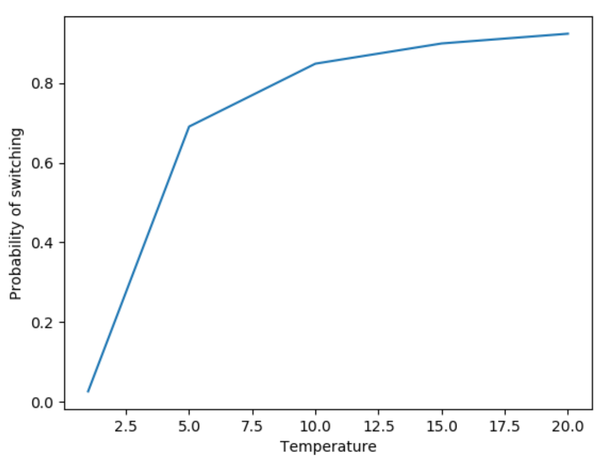
Now, $k_B T_r$ is a constant. So, we define

$$\beta^* = \epsilon\beta = k_B T_r \beta = \frac{1}{T^*}$$

(c)

$$\Delta E^* = \frac{\Delta E}{\epsilon}$$

2. (a) For the 5 temperatures (1,5,10,15,20), the ratio is plotted below.

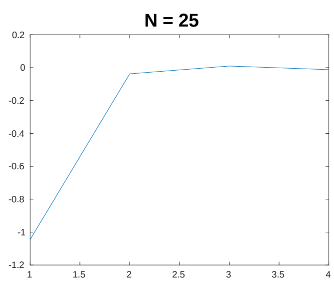


(b) As the temperature increases, the probability of switching goes to 1. This is because the energy $\beta\epsilon$ goes to zero with increasing temperature. Thus, the random variable in the Metropolis algorithm will always be less than e^0 and switching would happen nearly always.

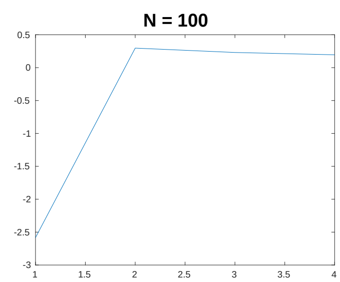
3. (a) i. magnetization measures the number of positive spins minus the number of negative spins.

   ii. Average magnetization measures the average magnetization over nsteps.

   (b) The average magnetization as a function of temperature for a 1-D lattice. It seems arbitary for smaller lattice size but it does get clear when the size of the lattice gets bigger.



(a) 25



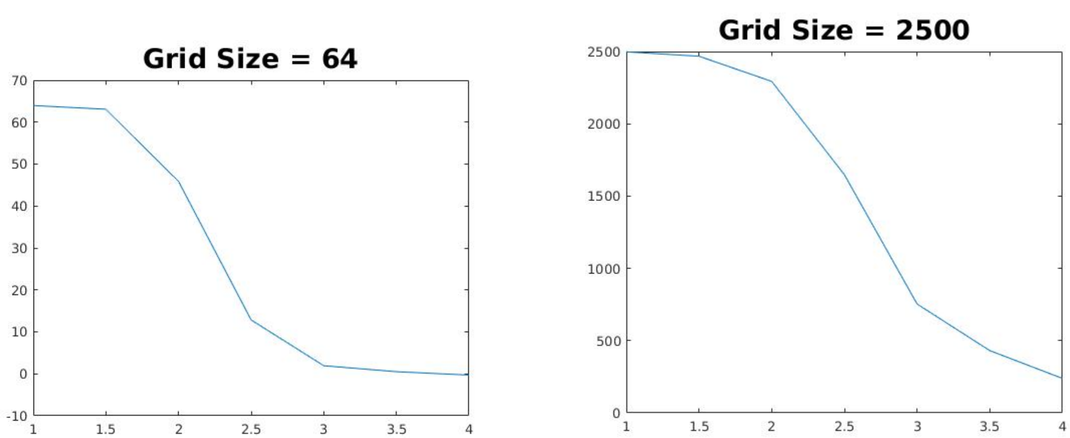
(b) 100

Figure 1: 1-d lattice

(a) 500 (b) 1000

Figure 2: 1-d lattice with very large lattice sizes

The average magnetization as a function of temperature for a 2-D lattice.



(a) 8x8 (b) 50x50

Figure 3: 2-d lattice

(c) i. It looks like in the 2-d lattices, at lower temperature, the spins are all in the same direction. I think this is because the increased number of neighbours in 2-d makes the synchronized same spin state more desirable. The 1-d lattices don't seem to show that behaviour for smaller lattice size and it is only seen consistently for large lattice sizes.

ii. As the size of the lattice increases, the jump becomes more and more abrupt. The critical temperature is about $T^* = 2.5$ for a 2-d lattice and $T^* = 3$ for a 1-d lattice.

iii. As the size of the lattice increases, the same spin state gets more desirable. This can be seen especially in the 1-d lattice where the number of states with same spin increase with the lattice

4. Magnetization is lost on increasing temperature. Iron is magnetic at room temperature. So,

$$\frac{\epsilon}{k_B T_r} >> 0$$

So, we would expect

$$\frac{\epsilon}{k_B T_r} > 1$$

$$\alpha k_B T_r > k_B T_r$$

So,

$$\alpha > 1$$

Let's see if it's true. Iron loses magnetization at 1024 K. So,

$$\frac{4\epsilon}{k_B 1024} \approx 0$$

$$\frac{4\epsilon}{k_B 1024} < 1$$

$$\epsilon < 3.5 * 10^{-21} J$$

We would guess ϵ around $1.4 * 10^{-20}$ which is still bigger than $k_B T_r$

So, α should be greater than 1.