Module. 3 Assignment: Ising model: corrections from 16^{th} March, 2023. Write your answers and attach the Fig1-Fig9 in one .pdf file.

Implement a Ising model in 3-d, such that you have a L*L*L cubic lattice with periodic boundary conditions. Write the code such that the length of the lattice L is a input parameter of simulation. Moreover, the number of iterations (niter) at a particular temperature T are also input parameters. Thermal energy k_BT is measured in units of J_ising, where J_ising=1.0. N=L*L*L.

Run the simulation for the parameters given below for each question and answer the following questions. (+/-) : signiifies that the value could be either positive or negative depending on the sequence of random numbers generated

Q1. Suppose all the spins in the lattice were pointing in the same direction (i.e. -1) in the initial configuration. L=20. The total magnetic moment (in simulation units) of the entire lattice in this initial configuration will be

Ans:

Q2. Suppose all the spins in the lattice were pointing in the same direction (i.e. +1) in the initial configuration. L=10. The total energy (in simulation units where J_ising=1) of the entire lattice will be

Ans:

Q3. For Parameters k_BT=4.9, L =10, niter =50000. The instantaneous magnetization per spin (value of magnetic moment per spin in a microstate: M) fluctuates around the value:

Ans: value and Fig.1

Q4. Parameters k_BT=3.9, L =10, niter =50000. The instantaneous energy per spin (value of the energy per spin in a microstate: E) fluctuates around the value:

Ans: value and Fig. 2

Q5. Parameters k_BT=4.05, L =10, niter =50000. The instantaneous magnetization M per spin and instantaneous energy E per spin fluctuates around the value:

Ans: Value and Fig. 3.

Q6. Show the fluctuations in the value of M per spin and E per spin at T=3.9 for L = 8, 9, 10 (fig.4)

<u>Questions-1-6 and Figs.1-4 : 3 marks.</u>

Run the simulation for L=7, L=8, L=9 for Temperature (T) range of of k_B T =4.7 to 3.8. Change T in in steps of 0.02. At each value of T, use 10000 MCS for equilibration. After equilibration at each temperature, collect statistical data each MCS for 1 million iterations for thermodynamic averaging.

Calculate specific heat suscptibility (\chi) at each T using fluctuations of the M_L, where M_L is the instantaneous magnetization of ALL (L x L x L) the spins on lattice (and NOT magnetization per spin) corresponding to lattice size L. Also calculate magnetization per spin (M_L/N) at each value of T and plot this versus T for different values of L in **fig 5.**

Similarly calculate heat capacity Cv for N spins using E_L, where E_L is the energy for N spins. Also calculate energy per spin for the system, and plot this quantity for 3 different L **(fig. 6)**

(You can expect L=9 to take around 50 minutes. I just RE-checked that L=9 system takes 1 minutes if I run 20K iterations at each value of T)

Plot chi x versus T for different values of L, **(fig 7)**. Repeat for Cv vs T. **(fig8)** then answer the following questions

Q7. The value of the quantity \chi at the temperature T=4.50000d0 , for the different values of L are approximately : .
Ans:

Q8. The value of Cv at the peak position for L=8 is (approximately):
Ans:

Q9. The value of Cv at the peak position for L=9 is (approximately) : _______

Q10. At temperature 3.8, the value for magnetization per spin for L=7 :

<u>The figures 5-8 and Q7-Q10: 5 marks.</u>

Q11: Binders cumulant plot **(Fig 9)** : <u>1 mark.</u>

Q5. There are multiple energy levels (E_1, E_2,... E_n....) in a system in equilibrium at temperature T. The average number of particles in Energy level E_5 is 100, and the average number of particles in E_10 is 50. The value of energy at level E_10 is greater than that of energy level E_5. The number of particles jumping from E_5 to E_10 is 10 per second. Then the number of particles jumping per second from E_10 to E_5 is: <u>1mark.</u>