

Week 5: Assignment Ising-2. Comp-Physics (lec of 13-19Sept, 2021).

Implement a Ising model in **3-d**, such that you have a $L \times L \times L$ 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 $k_B T$ is measured in units of J_{ising} , where $J_{\text{ising}}=1.0$. $N=L \times L \times L$. Thermal energy $k_B T$ is measured in units of J_{ising} , where $k_B=1$.

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 10^6 iterations for thermodynamic averaging. Calculate specific heat susceptibility (χ) at each T using fluctuations of the energy M_L , where M_L is the instantaneous magnetization of ALL 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 . Similar calculate heat capacity C_v for N spins using E_L , where E_L is the energy for N spins. Also calculate energy per spin for the system.

(You can expect the runs to take around 15 to 45 minutes depending on the value of L . All numbers are specified in simulation units)

Plot $\chi \times T$ versus T for different values of L , and then answer the following questions

Q1. The value of the quantity χ at the temperature $T=4.50000d0$, for the different values of L are approximately : .

Ans:

Q2. The value of C_v at the peak position for $L=8$ is (approximately):

Ans:

Q3. The value of C_v at the peak position for $L=9$ is (approximately) : _____

Q4. At temperature 3.8, the value for magnetization per spin for $L=7$: _____

Q5. There are multiple energy levels ($E_1, E_2, \dots, E_n, \dots$) 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:

Q6. Calculate and plot Binder cumulant for different lattice sizes, thereby find the actual transition temperature.