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FYS4150
Project 4 - deadline November 15

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Introduction

Method

To be able to start programming, one first needs to find the expressions for the partition function Z with its corresponding energy values E, the mean magnetic moment M, the specific heat C_V and the susceptibility X as functions of the temperature T. All of this using the periodic boundary condition. The partition function Z is giving by:

$$Z = \sum_{i=1}^{M} e^{-\beta * E_i}$$

where β is the inverse temperature given by $\beta = \frac{1}{kT}$ where k is the Boltzmann constant and T is the temperature, so every expression containing β is dependent on the temperature T. E_i is the energy for different spin settings given by:

$$E = -J \sum_{<kl>}^{N} s_k s_l$$

where J is the coupling constant and N is the total number of spins. s_k and s_l are the spins of two neighbouring objects in a lattice. Since we are working 2x2 lattice, the total number of combinations are given by $2^4 = 16$, considering we are working with the Ising model where the spins can only be -1 or 1.
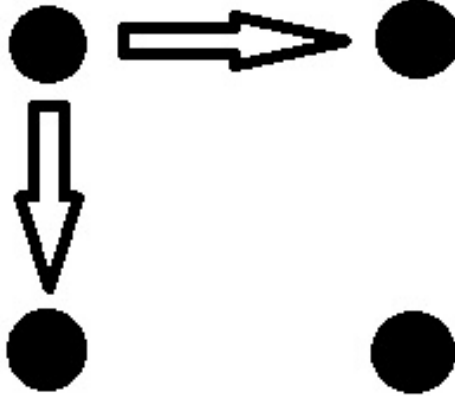

Figure 1: A two by two lattice and how they interact using the Ising model

From figure 1 we see how the Ising model works on a 2x2 lattice and from this the energy is calculated. One can observe that energy is non-zero on lattices where all the objects have the same spin $(-8J)$ and where the two diagonals have opposite spin from each other $(8J)$. All other settings have zero energy. Knowing the energy values we can calculate the mean energy $< E >$ with our specific partition function:

$$<E> = \frac{1}{Z} \sum_{i=1}^{M} E_i e^{-\beta E_i}$$

$$= \frac{1}{2e^{-8} + 2e^8 + 12} \sum_{1}^{16} E_i e^{-\beta E_i}$$

$$= \frac{16e^{-8} - 16e^8}{2e^{-8} + 2e^8 + 12} = -7.983928$$

Now we can simply put the same energy values into our partition function:

$$Z = e^{-\beta*-8J} + e^{-\beta*-8J} + e^{-\beta*8J} + e^{-\beta*8J} + 12 * e^0$$

$$Z = 2e^{-8J\beta} + 2e^{8J\beta} + 12$$

The magnetization is given by:

$$M = \sum_{j=1}^{N} s_j$$

Unlike in the energy case, the magnetization does not depend the lattice having the same spin or that the diagonals have opposite spin. The only case where the magnetization is zero in a 2x2 lattice is when half of the objects in the lattice opposite spins. Therefore we get the magnetization values:

$$M_i = [4 + 2 + 2 + 2 + 2 + 0 + 0 + 0 + 0 + 0 + 0 + -2 + -2 + -2 + -2 + -4]$$

To calculate the mean magnetic moment or mean magnetization we use the equation below with our calculated magnetic moment and energy values:

$$|M| = \frac{1}{Z} \sum_{i}^{M} M_i e^{-\beta E_i}$$

$$= \frac{1}{2e^{-8} + 2e^8 + 12} \sum_{1}^{16} M_i e^{-\beta E_i}$$

$$= \frac{8e^8 + 16}{2e^{-8} + 2e^8 + 12} = 3.994643$$

To calculate the the specific heat, one only needs to know the total number of spins of the lattice. In the 2x2 lattice case the total number of spins is 4, and remember also that $\beta J = 1$ and $k = 1$. The specific heat is then:

$$C_V = \frac{1}{kT^2}(<E^2> - <E>^2)$$

4

$$= \frac{1}{kT^2}(\frac{128e^{-8} - 128e^8}{2e^{-8} + 2e^8 + 12} - (\frac{16e^{-8} - 16e^8}{2e^{-8} + 2e^8 + 12})^2)$$

$$= 0.128329$$

The term $< E^2 > - < E >^2$ is also called the variance of the energy and is precisely calculated just as shown above. The same variance calculation can be applied to calculating the susceptibility, but the energy terms have to be substituted for mean magnetization. Let's calculate the variance separate from the desired equation this time:

$$\sigma_M^2 = < M^2 > - < M >^2 = \frac{1}{Z} \sum_{i=1}^{M} M_i^2 e^{-\beta E_i} - (\frac{1}{Z} \sum_{i=1}^{M} M_i e^{-\beta E_i})^2$$

$$= \frac{32}{2e^{-8} + 2e^8 + 12}(e^{-8} + 1) - (\frac{8e^8 + 16}{2e^{-8} + 2e^8 + 12})^2 = 0.010853$$

Remember that the $\beta = 1$ in the 2x2 lattice case, so the susceptibility would be the same as the variance in that case. We would usually have to calculate the susceptibility with the following equation:

$$X = \frac{1}{k_b T}(< M^2 > - < M >^2) = \frac{1}{k_b T}\sigma_M^2 = 0.010853$$

Results

From the general equations in the method, the following analytical and numerical values were found:

$$Analytical, Numerical$$

$$< E >= -7.983928, < E >= -7.984$$

$$< M >= 3.994643, < M >= 3.99599$$

$$C_V = 0.128329,$$

$$X = 0.010853, X = 0.0133519$$

To get good results for mean energy and mean magnetic moment took very few Monte Carlo, or MC, cycles, only about 100 000. Then the values would be off only by a factor of about 10^{-3}. The susceptibility and the specific heat took many more MC cycles and correct results started showing around 10^8 for susceptibility and XXX for specific heat.