Project 6

Ising model

Consider a 2D square lattice of $N \times N$ atoms. They have a spin $\sigma = \pm 1$, either pointing up or down. The lattice sites can be labelled with some index. Take $N = 50$. The energy of this system is defined as

$$E = -J \sum_{i,j} \sigma_i \sigma_j \tag{1}$$

Here σ_i, σ_j are the spins at nearest neighbor lattice sites i and j. Take $J = 1$. Each neighboring pair is counted only once, each site has four nearest neighbors. Take periodic boundary conditions for the grid.

Start with a random initialization of the spins on the lattice. The probability of finding a particular configuration of spins, denoted by s, depends on it's energy E_s by the Boltzmann relation

$$P(s) \propto \exp\left[-\frac{E_s}{k_B T} \right] \tag{2}$$

Randomly flip spins according to this probability and generate a bunch of configurations that follow this probability distribution using the Metropolis algorithm. Continue this till you have sampled a broad range of the energy distribution and the magnetization becomes steady. The magnetization is defined as

$$M = (\sum_i \sigma_i)/(N^2) \tag{3}$$

Perform this simulation for different values of $k_B T$ ranging from 0.1 to 10. Calculate the magnetization in the equilibriated state. Analyze how the magnetization varies with $k_B T$ and see if there is a phase transition with temperature.