Monte Carlo simulations 2006. Exercise 7

To be handed in Mon Apr 24, solutions given Thu Apr 27 10:15.

1. (30 p or 20 p) Write a program which simulates the 2D square Ising model with the Metropolis Monte Carlo method. Consider an extension of the basic Ising model, which considers both the 4 nearest neighbours (nn) at $(i \pm 1, j)$ and $(i, j \pm 1)$ and the 4 second-nearest neighbours ($2nn$) at $(i \pm 1, j \pm 1)$. The nearest neighbour interaction energy is J_{nn} and the second-nearest neighbour interaction is J_{2nn}. Use periodic boundary conditions in both x and y.

The code should calculate the average magnetization per spin M as a function of temperature T in the absence of an external magnetic field H. Use the normalized units $J_{nn} = 1$ and $k = 1$. Use the code to determine $M(T)$ and from this data a rough estimate of the critical temperature T_c to an accuracy in T of ~ 0.2.

Treat the following 4 cases:

a) $J_{nn} = 1.0$, $J_{2nn} = 0.0$ (the basic 2D Ising model)

b) $J_{nn} = 1.0$, $J_{2nn} = 0.5$

c) $J_{nn} = 1.0$, $J_{2nn} = -0.5$ (a simple model of ferrimagnetism)

d) $J_{nn} = 1.0$, $J_{2nn} = -1.0$ (a simple model of antiferromagnetism)

Report T_c for all cases. Return the code.

You are allowed to do the exercise taking an existing Ising model simulator from anywhere, then modify it to suit this problem. In this case you should clearly state it, give credit to the authors of the original code and indicate which parts you have modified. In this way you can get at most 20 p for the exercise..

Hint. Note that in the absence of an external field, the Ising model can at low temperatures be either all magnetized up or down with equal probability. You need to account for this somehow to get meaningful averages of the magnetization.

2. (10 p) Use your understanding of physics to explain qualitatively why the critical temperature changes as it does in parts b), c) and d) compared to the value in part a).

Even if you can not solve exercise 1, you can solve exercise 2 if you are able to predict the right behaviour.