Computational Physics

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Ex.10 : Monte Carlo for the 2D Ising model on a square lattice.

We will consider the Ising model for a 2D square lattice of $N = L \times L$ sites. Each spin s_i may point up ($s_i = 1$) or down ($s_i = -1$). The energy is given by the sum over nearest neighbour interactions (indicated by the symbol $\Sigma_{<ij>}$)

$$E = -J\Sigma_{<ij>} s_i s_j \tag{1}$$

where J is the coupling constant which we take $J = 1$. The total magnetization is simply $M = \Sigma_i s_i$. It is convenient to define a magnetization per spin $m = M/N$ and an energy per spin $\epsilon = E/N$.

At low temperatures and zero applied magnetic field, the ground state magnetization per spin is $m = 1$ (or equivalently $m = -1$) since all spins are aligned. The ground state energy per spin is $\epsilon = -2J$ (because each spin has four neighbours but interactions should not be counted twice). At high temperatures, both the average energy and magnetization tend to zero. The critical temperature from the phase transition from the ordered low temperature phase to the disordered high temperature phase is $T_c = 2,269J$.

Study of behaviour of magnetization by use of Metropolis algorithm

The basic program to run a Monte Carlo simulation with the Metropolis algorithm for a 20×20 lattice of spins in contact with a heath bath at constant temperature (canonical ensemble) is given in the program *mc.f* (written in fortran 77). You need also to copy the file *mc.inc* which is needed by *mc.f*. Besides, a second program *mcini.f* can be used to generate an initial configuration of assigned magnetization. These programs have been written for didactical purposes by Dr. M. P. Allen, University of Bristol. They are easy to read and well documented and you will appreciate the implementation of the algorithm. Notice that periodic boundary conditions are used. A sweep (or a MC step) consists of N attempts to flip a spin chosen at random. The averages are done on all the moves. I suggest to start by using the program as it is and change it afterwards if you wish.

1) Read the program and try to understand how it works. Give particular attention to the implementation of the Metropolis algorithm and to the evaluation of averages. Check that also if a spin flip is not accepted, the configuration is added to the number of configuration on which averages are performed.
2) Compile the programs with f77. Generate with *mcini.f* an initial configuration with average magnetization $m = 0$. Run *mc.f* for $T = 2.0$ (below T_c). Change the program to write the quantities which appear on the screen into files to plot them afterwards. In doing this try not to change drastically the lay-out of the program. Keep the lines of comment in the output, with a # in front to use gnuplot.

3) Study the behaviour of magnetization as function of MC steps for $T = 1.$ and $T = 3.5$ starting in each case both with initial magnetization $m = 1$ and $m = 0$, using the same initial seed and same number of steps. A reasonable run could be of a total of 5000 MC steps for each temperature divided in *nblock* blocks of *nstep* MC steps. Estimate of the errors are done as described for random walks.

   In this way, one gets a feeling of the relaxation time needed to reach the equilibrium value of the magnetization at each temperature, depending on the initial conditions.

4) Make a plot of the magnetization as a function of temperature from $T = 1.$ to $T = 3.5$. In doing this one should, in principle, discard all MC steps before equilibration before starting to compute the average value of the magnetization.

Domain formation, Kawasaki dynamics with constant magnetization

When considering single spin flips, as done in the previous point, the magnetization is not conserved and one can study the relaxation of the system. It is interesting to consider another approach which conserves the magnetization, the so-called Kawasaki dynamics. Instead of attempting single spin flips, a move consists in exchanging the spin of two neighboring sites with opposite spins. Our aim is to show that if we start with a configuration with zero magnetization (typical of high temperature) and the temperature is lowered well below T_c domain formation (clustering of up and down spins) occurs in the system.