School of Physics & Astronomy

Modelling and Visualisation in Physics

PHYS10035 (SCQF Level 10)

Friday 29th April, 2016 09:30 – 12:30
(May Diet)

Please read full instructions before commencing writing.

Examination Paper Information

Answer all questions overleaf.
Completed codes should be uploaded via Learn as a single zip file immediately after the examination has finished. If technical problems arise with the submission process, you can email the zip file to dmarendu@ph.ed.ac.uk.
Figures should also be submitted electronically, they should also be described in the script book.
You may use any resources available on the internet at the beginning of the examination, or present in your CPlab home directory but you may not communicate with any other person electronically or otherwise.

Special Instructions

- Only authorised Electronic Calculators may be used during this examination.
- A sheet of physical constants is supplied for use in this examination.
- Attach supplied anonymous bar codes to *each* script book.

Special Items

- School supplied Constant Sheets
- School supplied barcodes

Chairman of Examiners: Prof S Playfer
External Examiner: Prof S Clark

A simple model for an antiferromagnet under an external magnetic field can be formulated in terms of the Ising model, as follows. The Hamiltonian, or energy function, characterising the system can be written down as

$$E(\{S_i\}) = -J \sum_{\langle ij \rangle} S_i S_j - h \sum_i S_i$$

where $J < 0$ is the coupling between neighbouring spins (notice this is the *opposite* sign for J with respect to the standard Ising model!) and $h \geq 0$ is the magnetic field, while S_i is the spin at the i-th lattice point, which can take either the values -1, or 1. Finally, $\langle ij \rangle$ denotes that the sum is performed over spin pairs which are nearest neighbours on the lattice.

We want to simulate the physics of the antiferromagnet in a field, in two dimensions. In order to do so, you should set up a Monte-Carlo algorithm where you attempt to update the systems by selecting a site randomly at each time step, and by attempting to change the sign of its spin (i.e., flip its spin) – the move is then accepted or rejected according to the Metropolis test.

Two useful quantities which we refer to below are the "magnetisation", M, and the "staggered magnetisation", M_s. These are defined as follows:

$$M = \sum_{i=1}^{N} S_i,$$

and

$$M_s = \sum_{i=1}^{N} \mathrm{sgn(i)S_i},$$

where N is the total number of spins in the square lattice, and sgn(i), the sign of the $i-$th lattice point is defined as

$$\mathrm{sng(i)} = (-1)^{\mathrm{row(i)+col(i)}},$$

where row(i) and col(i) are the number of the row and column on the lattice which identify the point i (e.g., in a square lattice with L rows and columns, so that $N = L^2$, row(i) and col(i) run from 1 to L).

a. Describe what states you expect for: (i) J large and negative, $h = 0$; (ii) $J = -1$, and h large and positive. What would you expect the values of M and M_s should be in the cases (i) and (ii)? Here and in what follows you can set $k_B = T = 1$, where k_B is the Boltzmann constant, and T is the temperature. **[5]**

b. Write a Java program to sample via Monte Carlo the equilibrium states in this model antiferromagnet on an $L \times L$ two-dimensional square lattice, with periodic boundary conditions. You should take $L = 50$ throughout; you can further set $J = -1$ for all runs. [Recall also $k_B = T = 1$ from part (a).] Your program should provide some means to change the value of the magnetic field h; it should also display the state of the system in real time as it is running. To initialise the system you can start with a random state with equal probability of having a spin equal to -1 or +1 at all lattice points. You can then set up the Monte-Carlo algorithm by attempting to flip a spin at each time step. **[25]**

c. Use your code to compute the following quantities: (i) the average and the variance of the magnetisation, (ii) the average and the variance of the staggered magnetisation, (iii) the average of the energy of the system (you will not need the variance of the energy). Recall that the variance of a quantity, say A, is given by

$$\mathrm{Var}(A) = \langle A^2 \rangle - \langle A \rangle^2,$$

where $\langle \cdot \rangle$ denotes averaging (here, over configurations of the system). You should plot the quantities (i), (ii) and (iii) as a function of h, for the fixed values of J and T specified previously; your plot should cover the range between $h = 0$ and $h = 10$ (e.g., with uniformly separated points, where h is changed by 0.5 between two different points). Your plot for the variances of the magnetisation and staggered magnetisation should each display a peak – you should say what these correspond to. **[10]**

d. Modify your code so that the external field can depend both on position and time. If we identify with x and y the positions along the horizontal and vertical directions in the lattice (i.e., x and y are equal to the previously defined $\mathrm{row}(i)$ and $\mathrm{col}(i)$ functions respectively, and they vary between 1 and L), and we denote by n the current time, measured in units of Monte-Carlo sweeps (recall that a sweep is equal to $N = L^2$ attempted flips), we are interested in the following functional form for the external field,

$$h(x, y, n) = h_0 \cos(2\pi x/P) \cos(2\pi y/P) \sin(2\pi n/\tau)$$

where P is the spatial period, and τ is the time period.

Fix $P = 25$, $\tau = 10000$, and $h_0 = 10$. Run your code with this parameter set and describe the spin patterns that you observe as a function of time. What is the typical pattern at the times when $\sin(2\pi n/\tau)$ factor is approximately equal to: (i) -1, (ii) 0, and (iii) 1? You can either sketch these on your exam script book, or save suitable data files or snapshots on the computer. **[5]**

e. Run your code for the same parameter values, and write in a file the value of the maximal field strength over space at a give time, $h_0 \sin(2\pi n/\tau)$, and that of the instantaneous staggered magnetisation, as a function of time. You should plot the staggered magnetisation as a function of time, and of field, for two values of the spatial period: $P = 25$ and $P = 10$. What happens as you decrease the spatial period? **[5]**