School of Physics & Astronomy

Modelling and Visualisation in Physics

PHYS10035 (SCQF Level 10)

Wednesday 30$^{\text{th}}$ April, 2014 09:30 – 12:30
(May Diet)

Please read full instructions before commencing writing.

Examination Paper Information

Answer all six questions overleaf.
Completed codes should be uploaded via Learn as a single zip file immediately after the examination has finished. Alternatively, 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 the supplied 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 calculators
- School supplied Constant Sheets
- School supplied barcodes

Chairman of Examiners: Prof S Playfer
External Examiner: Prof G Lafferty

A simple model for the normal fluid to superfluid transition in a mixture of He^3 and He^4 can be formulated in terms of a variant of the Ising model. Here, each spin can take on the values 0, for He^3 (which is a normal fluid), or ± 1, for He^4 (which can become superfluid). The Hamiltonian, or energy function, characterising the system can be written down as

$$E = -J \sum_{\langle ij \rangle} S_i S_j$$

where $J > 0$ and S_i is the spin at the i-th lattice point, which as anticipated can take any of the values -1, 0 or 1, while $\langle ij \rangle$ denotes that the sum is performed over spin pairs which are nearest neighbours on the lattice.

According to the Boltzmann distribution, when the system is in thermal equilibrium with a bath at temperature T, the probability of observing a given spin configuration $\mathcal{C}$ is given by

$$P(\mathcal{C}) = \exp\left[-E(\mathcal{C})/(k_B T)\right]$$

where k_B is the Boltzmann constant and $E(\mathcal{C})$ is the energy corresponding to the spin configuration $\mathcal{C}$.

We wish to simulate a mixture of He^3 and He^4 in thermal equilibrium with a bath at temperature T, where the fraction of sites which are He^4 is c (therefore $0 \leq c \leq 1$). In order to do so, you should set up a Monte-Carlo algorithm where you attempt to update the systems as follows. Each time step, (i) either you select a site randomly, and attempt to change the sign of its spin (which will create a new state only when selecting He^4 sites); or (ii) you select a pair of lattice points (for simplicity, avoid the case in which these are nearest neighbours) and attempt to swap their spins. A useful quantity which we sometimes refer to below is the magnetisation, M, which is defined as

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

where N is the total number of spins in the lattice.

1. Explain why the two update moves referred to as (i) and (ii) above allow us to sample the configurations sampled by the system while keeping c constant. **[2]**

2. Write a Java program to sample via Monte Carlo the equilibrium states in this model superfluid mixture on an $L \times L$ two-dimensional square lattice, where you should use periodic boundary conditions, and take $L = 50$ throughout. You can further set $J = k_B = 1$ for all runs. Your program should provide some means to change the value of the temperature T, and of the fraction of He^4 sites, c. It should also display the state of the system in real time as it is running. To initialise the system with the desired fraction c of He^4 sites, you can use the following method: each state is a spin 0, with probability $1 - c$, or a $\pm$ 1 spin, with probability c (in which case it is, for instance, +1 or -1 with equal probability). Although this gives a fraction c of He^4 (± 1 spins) only approximately, it is acceptable to do so in our case. You can then set up the Monte-Carlo algorithm by choosing with equal probability, at each time step, either of the update moves (i) or (ii) detailed above. **[25]**

3. Describe what happens in your system for the following parameter choices: (a) $c = 0.8$, $T = 5$; (b) $c = 0.8$, $T = 1.3$; (c) $c = 0.8$, $T = 0.1$. Within this model, one

can have either a disordered phase (normal fluid), or a magnetised ("superfluid") phase, when the ± 1 spins on average align with each other, so that there is an extensive (proportional to N) magnetisation on average. Furthermore, one can observe either a mixed phase, where spin 0 (He^3) sites and spin ± 1 (He^4) sites are on average uniformly distributed, or a demixed phase, where they segregate. Using this terminology, how would you characterise each of the states in (a), (b), (c) as superfluid/normal fluid and mixed/demixed? **[4]**

4. For a fixed value of $c = 0.8$, use your code to compute the average energy, and the specific heat at constant volume, C_V, defined as

$$C_V = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2},$$

for a range of temperature (e.g. from 0.1 to 3). Plot the specific heat C_V versus temperature, with error bars. Your plot of the specific heat should have two peaks: at what temperatures are they? What do these correspond to? **[8]**

5. Now, for the same value of $c = 0.8$ and the same temperature range as before, compute the magnetic "susceptibility" χ, defined as

$$\chi = \frac{\langle M^2 \rangle - \langle M \rangle^2}{k_B T}.$$

Plot the susceptibility χ versus temperature (you do not need error bars this time). Your plot should now have a single peak. Why do you think this is the case? **[5]**

6. Now set $c = 0.2$. Repeat the calculation of the specific heat, C_V, and plot it versus temperature (you do not need error bars). How many peaks are there now? Why do you think this is the case? Using the results you have found, sketch a possible "phase diagram" in the c-T plane, indicating the regions where you think the phases you have found previously are stable. **[6]**