Question 3 (Unit 10IM) – 90 marks

This question relates to ***Simulations of the Ising model (Unit 10IM)****.*

Many parts of this question require you to modify existing Python code, from the computer session, or write your own code. You should ensure that any modifications or additions are appropriately commented. You should also annotate any graphs that you create, ensuring that the axes and all plots of your graph are labelled appropriately.

Note that in parts (b), (c), (d) and (e) of this question, you are required to use units where both the exchange constant J and Boltzmann constant k_B are equal to 1.

(a) Consider a two-state system that can be in *state 1* with energy 0, or in *state 2* with energy ε. Assume that the system is in thermodynamic equilibrium according to Boltzmann's distribution.

(i) Calculate the mean energy $\langle E \rangle$. [*3*]

(ii) Calculate the mean-square energy $\langle E^2 \rangle$. [*3*]

(iii) Take the number of atoms to be $N = 1$ and show that the specific heat capacity can be written as

$$c = \frac{1}{k_B T^2} \frac{\varepsilon^2 e^{-\varepsilon/(k_B T)}}{\left(1 + e^{-\varepsilon/(k_B T)}\right)^2}.$$

[*4*]

(b) The task for this part is to implement and run a simulation of the 2D ferromagnetic Ising model using the Metropolis–Hastings algorithm. To do this you should appropriately modify the code supplied in Computer session 10IM.1.

Consider a 2D ferromagnetic Ising model on a square lattice, with periodic boundary conditions and no external field, using units in which $J = 1$ and $k_B = 1$.

(i) Create a single graph displaying four plots of the magnetisation per spin, m, as a function of the temperature in the range $T = 0.2$ to $T = 4.0$, for lattices of size $N = L \times L$ with $L = 30, 40, 50, 60$.
(*Hint*: for every temperature, you are advised to allow the system to relax for a minimum of 500 sweeps before 'taking measurements'.) [*12*]

(ii) On the same graph as part (i), additionally plot the mathematically exact magnetisation per spin, m, which, for this system, in the limit of an infinite number of spins, is given by

$$m(T) = \begin{cases} \left(1 - \sinh(2J/(k_B T))^{-4}\right)^{1/8} & T \leq T_c, \\ 0 & T > T_c, \end{cases}$$

where

$$T_c = \frac{2J}{k_B \ln(1 + \sqrt{2})} \simeq 2.26918.$$

Note that Python may give a warning when calculating the exact magnetisation, but this can be ignored. [*5*]

(iii) Briefly comment on the comparison between the simulation results in part (i) and the exact values in part (ii). [*3*]

Parts (c) and (d):

In parts (c) and (d) we consider the effect of an external magnetic field, with component B, applied to the ferromagnetic Ising model, using units in which $J = 1$ and $k_B = 1$. The Hamiltonian is

$$E(\mathbf{s}, J, B) = -J \sum_{\langle i,j \rangle} s_i s_j - B \sum_i s_i.$$

In part (c) we consider the effect of an external field on the **1D model**, and in part (d) we consider the effect on the **2D model**.

Note that for all the Monte Carlo simulations in parts (c) and (d) it is sufficient to allow the system to relax for 500 sweeps before 'taking any measurements'.

(c) **Ising model in 1D:** Consider a 1D Ising model, with periodic boundary conditions in the presence of an external magnetic field B.

(i) In Subsection 5.3 of Unit 10IM we derived a simple expression, equation (25), for the change in energy when a single spin is flipped, for the case when $B = 0$. Show that for the 1D model in the presence of an external magnetic field B, the change in energy when the spin s_k is flipped is given by

$$E_b - E_a = 2s_k \left(J \sum_{i\,\text{n.n.of}\,k} s_i \; + \; B \right),$$

where the sum is over the nearest neighbour spins of s_k. [5]

(ii)
- For $B = 0.1$, create a single graph displaying four plots of the magnetisation per spin, m, versus temperature in the range $T = 0.2$ to $T = 4.0$, for lattices of size $N = 8, 16, 32, 64$. [7]
- For $B = 0.5$, create a second graph of four plots using the same parameters as above. [3]
- On each of the plots in the two graphs above, additionally plot the mathematically exact magnetisation per spin, m, which, for this system, in the limit of an infinite number of spins, is given by

$$m(T, B) = \frac{\sinh(\beta B)}{\sqrt{\cosh^2(\beta B) - 2e^{-2\beta J}\sinh(2\beta J)}}, \qquad \beta = \frac{1}{k_B T}.$$ [3]

(d) **Ising model in 2D:** Consider a 2D ferromagnetic Ising model on a square lattice, with periodic boundary conditions in the presence of an external field B.

(i) Show that for the 2D model in the presence of an external magnetic field B, the change in energy when the spin s_k is flipped is given by

$$E_b - E_a = 2s_k \left(J \sum_{i\,\text{n.n.of}\,k} s_i \; + \; B \right),$$

where the sum is over the nearest neighbour spins of s_k. [4]

(ii) For a lattice of size $N = 32 \times 32$:

- Create a single graph displaying four plots of the mean total energy versus temperature in the range $T = 0.1$ to $T = 10$, with $B = 0.0, 0.2, 0.4, 0.6$. [9]

- Comment on whether the external non-zero field lowers or raises the energy in comparison to the $B = 0$ case. Suggest an explanation for the observed effect based on the action of the external field on the individual spins. [*3*]

(iii) For a lattice of size $N = 64 \times 64$:

- Create a single graph displaying three plots of the specific heat capacity versus temperature in the range $T = 0.5$ to $T = 4$, with $B = 0.0, 0.2, 0.4$.
  (*Hint*: For every temperature, calculate average values over no fewer than 2000 sweeps.) [*4*]
- Comment briefly on the effect of the external field on the specific heat capacity. [*2*]

(e) This part is less prescriptive than other parts of this TMA question and it requires you to use your judgement and initiative to explore the 3D Ising model. For all the simulations you are advised to allow the system to relax for at least 400 sweeps before 'taking measurements', and you should also use at least 2000 sweeps to estimate average values. Try to ensure that the execution time for each of your codes does not exceed about 2 minutes (for a typical computer).

Consider a 3D ferromagnetic Ising model on a cubic lattice, $\mathcal{L} = \{l\mathbf{i} + m\mathbf{j} + n\mathbf{k}\}$ with $l, m, n = 1, 2, \ldots, L$. Assume periodic boundary conditions and the presence of an external field B, using units in which $J = 1$ and $k_B = 1$.

(i) For $B = 0$, use Monte Carlo simulations to estimate the value of the critical temperature T_c in the infinite system. [*12*]

(ii) By considering values of B in the range $B = 0.005$ to $B = 0.5$, describe the effect of a non-zero magnetic field on the magnetisation of the system. [*8*]