Introduction

In this assessment piece, you will be guided through a numerical simulation of ferromagnetic materials using the Ising model, and investigating various thermodynamic properties with your simulation. You will start by simulating a finite line of spins whose spin direction depends only on nearest-neighbour interactions (a 1D Ising model), and eventually will simulate a 2D Ising model with periodic boundary conditions (which, in effect, approximates an 'infinite' 2D lattice of spins). You will then measure some thermodynamic properties of these systems using your simulation. Like all good physicists, we will request that you report any uncertainties or variance in your simulations, as well as to compare your simulated results to expected physical quantities and phenomenon.

The purpose of this assessment is not to get everything perfect, nor is it to simulate absolutely realistic models of atomic spin—that would be too difficult in a third year undergraduate course whose focus isn't just on computational simulations. Instead, it is to introduce you to concepts and approaches in writing and measuring physical simulations. It is also to cement some of the concepts you are studying in PHYS3020 by having you "discover" these properties yourself. Furthermore, it should convince you how powerful simulations are in physics as you will see how even very complicated physical phenomenon can emerge out of simple "rules". Finally, it will also allow you to demonstrate your insight and creativity in ways that other assessment pieces simply couldn't.

We recommend that you perform your simulations in MATLAB, a powerful scientific programming language. Support will be offered in lectures and tutorials to assist you in learning how to use the language, and there is a general MATLAB guide (including some exercises on physics simulations using MATLAB) available on the LearnX platform. You should feel free to use an alternative programming language if you are experienced with one. However, be aware that tutor/staff assistance may be more limited in this case. For all questions, you should provide any code snippets that are relevant inside the body of your answer. You should also upload your entire code as a separate m-file in your submission.

For those of you enrolled in the postgraduate version of the course (PHYS7021), this project is an opportunity to learn graduate attributes including *The ability to work and learn independently and effectively* and *The ability to formulate and investigate problems, create solutions, innovate and improve current practices*. The grade you receive will be based partly on your demonstration of these attributes.

Project structure and grading

Core project: Questions 1 and 2 form the core of the project. The idea is that you'll submit the core project in your first submission, due September 12, 2pm, via a Blackboard submission portal. Each answer should not exceed five pages (so you may use up to 10 pages total, limited to five pages for each question), though you may include an appendix for additional working and code. You will be provided feedback and may, if you wish, resubmit improved answers to be remarked together with your project extension for your second submission. You may submit the entire project instead, but note that Question 3 has a 10 page limit (not 5).

Open-ended extension: Question 3 extends the core of the project to more open-ended simulations. This question should be submitted with the second submission, due October 17, 2pm, via a Blackboard submission portal. Your answer to Question 3 should not exceed ten pages, though you may include an appendix for additional working and code.

Grading and Style: The report is marked out of a total of 100%, with Questions 1 and 2 graded holistically out of 70%, and Question 3 graded out of 30%. Importantly, note that the core project marks are not evenly split; the idea is that you will attempt to write a good report first and foremost, rather than merely answering the questions asked. As such, keep in mind that the format of the submission should be a report-style, similar to a lab report. If it helps, you can think of your simulation as the experiment—though of course, you should provide code snippets, where relevant, to aid in completing the tasks required of you.

As always, please try and keep your work readable, relevant and concise. This is a good habit to get into as future physicists. It also makes the marking easier and quicker for the tutors! And, where relevant, don't forget to include data analysis (error bars, discussion of sources of error, error propagation and estimation, linking simulation results to, or explaining discrepancies from, theory, etc.).

Background Physics

Ferromagnets and the Ising Model

A simple model of a paramagnet is a substance consisting of magnetic dipoles, whose spin may align in one of two directions (we will call these spin-up or spin-down). For these substances, there is no inherent preference for dipoles to align parallel or anti-parallel to their neighbours unless an external magnetic field is applied.

However, not all substances are like paramagnets since, In the real world, dipoles are influenced by their neighbours' spin direction. Without considering the complicated physical reasons for it, let's just introduce into our model an energy contribution to the system's Hamiltonian depending on the relative alignment of neighbouring dipoles.

When these energy contributions cause neighbouring dipoles to align parallel to each other, we call the substance *ferromagnetic* (the most famous example being iron, Fe). When they cause them to align antiparallel, we call the substance *antiferromagnetic* (for example, nickel oxide (NiO)). By merely adding some neighbouring interactions, we will see that—under certain conditions—a net, long-range magnetisation can emerge within our lattice.

Of course, iron is not ordinarily a permanent magnet because a lump of iron consists of millions of domains (microscopic regions containing billions of dipoles). The net spins of each domain align in different directions from one another, and hence the entire material has no net magnetisation. However, we can make a lump of iron a permanent magnet by heating it in an external magnetic field, then cooling it back down to room temperature. This 'permanent' magnet, of course, is not truly permanent, since heating our lump of iron above a certain temperature (called the Curie temperature, which is 1043 K for iron) will cause it to become a paramagnet.

We will model the behaviour of a ferromagnetic domain using a very simple model: the Ising model. We account only for the neighbouring interactions between dipoles, but ignore any long-range magnetic interactions between them. We will also assume a preferred axis of magnetisation, and that dipoles can only align parallel or antiparallel to this axis.

Next, we introduce some notation: let N be the total number of dipoles, and s_i be the spin of the ith dipole, where $s_i = 1$ signifies spin-up, and $s_i = -1$ signifies spin-down. The energy contribution when neighbouring dipoles are aligned parallel will be $+\epsilon$, and when aligned antiparallel will be $-\epsilon$. Hence, regardless of spin direction, the energy contribution can be written as $-\epsilon s_i s_j$, where j is the spin of the jth dipole (assumed to be a neighbouring dipole). The total energy of the system due to all nearest-neighbour interactions is thus:

$$U = -\epsilon \sum_{\substack{\text{neighbouring} \\ \text{pairs } i,j}} s_i s_j. \tag{1}$$

Now, to predict the thermal behaviour of the system, we should compute the partition function (in accordance with canonical formalism):

$$Z = \sum_{\{s_i\}} e^{-\beta U}, \tag{2}$$

where $\beta = 1/kT$, with $k = 1.38\times10^{-23}$ J/K is Boltzmann's constant, and T is the temperature of the system. Note that this sum is over all possible sets of dipole alignments. For N dipoles, each with two possible alignments, the number of terms in the sum is 2^N. For even relatively small values of N, adding up all the terms by brute force is not practical.

Monte Carlo Simulations

Consider an Ising model with about 100 dipoles. Even the fastest computer in the world couldn't compute the probabilities of all possible states (at least, not within our lifetimes), but then maybe it isn't necessary to consider *all* states. Perhaps a random sampling of about a million states is sufficient to compute the values we need. This is the idea behind Monte Carlo methods (named after the Casino de Monte-Carlo in Monaco): by repeated random sampling of possible states from deterministic systems, we can build up a sufficiently large sample to compute the values we are interested in.

This procedure (called the *naive* Monte Carlo method) does not work for the Ising model, however. Recall that the fundamental assumption of statistical mechanics is that, given enough time, an isolated system in a given macrostate has an equal likelihood of being in any of the microstates that produce that macrostate. However, the naive Monte Carlo method implicitly assumes that every possible microstate (drawn from every possible macrostate of our system) is equally probable (despite the fact that the macrostates themselves are not equally probable, and hence nor are the microstates, since this is a canonical ensemble and not a microcanonical one). Hence, even if we compute a billion states, this only represents a tiny fraction of the states for an Ising model with $N = 100$ (wherein there are about 10^{21} such states). Even worse, at low temperatures where we are interested in the important (and most probable) states which are strongly magnetised, we are likely to miss such states entirely (since, even though these states are the most probable, a billion states is simply too small a sample to ensure it is representative of the actual distribution of possible states).

A better idea is to use the Boltzmann factors themselves to weight our random distribution. For the Ising model, this can be achieved as follows: first, start with any state you like. Secondly, choose a dipole at random (using a uniform random distribution). Thirdly, compute the energy difference resulting from the flip: if $\Delta U \leq 0$, go ahead and flip it (thus generating the next system state); otherwise, if $\Delta U > 0$, decide at random whether to flip the dipole, where the probability of a flip is $e^{-\beta\Delta U}$. If the dipole isn't flipped, then the next state is the same as the last one. Otherwise, the next state has that dipole flipped. In either case, we then choose another dipole at random (using a uniform random distribution) and repeat the process until every dipole has had many chances to be flipped. This method is called either the Metropolis algorithm, or Monte Carlo summation with importance sampling.

The Metropolis algorithm generates a subset of states where low-energy states are more common than high-energy ones. Indeed, it can be shown that the probability of a transition to a new state using this algorithm is identical to the probability of a transition according to the Boltzmann probabilities for that system (in other words, it avoids "clumping" of highly improbable states by "weighting" the states with more probable energy values in our random distribution). Thus, our subset of states better represents the distribution of possible macrostates for our system than with the naive Monte Carlo method.

There is one caveat: this method will only generate states with the precisely correct Boltzmann probabilities once the algorithm has been running long enough for every state to have been generated multiple times. We want to run it for a much shorter time than this (such that almost all states are never generated at all). Under such circumstances, there is no guarantee that the subset of states actually generated accurately represents all possible system states. But then again, this is analogous to what happens in the real world where a large system never has time to explore all its possible microstates. So—provided we give every dipole many chances to flip (say, between 10^3 and 10^5 such chances for each dipole)—we can be relatively sure our simulation will represent the expected thermodynamics of a real-world system.

To mitigate any edge effects of our system (since the edges have fewer neighbouring dipoles), it is a good idea to include periodic boundaries on our lattice. In the 1D case, this involves setting, e.g., the right neighbour of the last dipole as being the first dipole (such that the lattice effectively 'wraps around' on itself, like a closed loop). This approximates an infinite lattice, with the approximation improving as the number of dipoles increases.

Relevant Equations and the Effect of Dimensionality

Although this model seems rather simple, attempting to solve it exactly can prove tedious and difficult. Hence, we present the exact results without their derivations (although these can be easily found online and in textbooks).

In one dimension, our spins are organised in a line, and each dipole only has 2 neighbours (its left and right neighbour, respectively). The average energy of the system from nearest-neighbour interactions is:

$$\langle U \rangle = -N\epsilon \tanh \beta\epsilon, \tag{3}$$

which goes to $-N\epsilon$ as $T \to 0$ and goes to 0 as $T \to \infty$. Thus, the dipoles are all parallel at $T = 0$, and are all randomly aligned at high temperatures. The transition to alignment is gradual and continuous, however, and so it does not exhibit the spontaneous alignment we expect of true ferromagnetic systems.

Let's turn to two dimensions now. Here, we will note that there are four neighbours—one above, one below, one to the left and one to the right (we assume diagonal neighbours don't interact). Unfortunately, though an exact solution for the energy exists in two dimensions, there are no closed-form representations of it. Something that does emerge is the spontaneous alignment of the dipoles at a non-zero *critical* temperature, given by:

$$T_c = \frac{2\epsilon}{k \ln(1+\sqrt{2})} \approx 2.27\epsilon/k. \tag{4}$$

This temperature is the temperature at which a *phase transition* occurs for our 2D Ising model, and is analogous to the Curie temperature for ferromagnetic materials.

Let us now consider the number of neighbours as a function of dimensionality. Note that in 3 dimensions, there are 3 different simple lattice structures we could adopt. The number of

nearest neighbours (represented by n) is then:

$$n = \begin{cases} 2 & \text{in one dimension;} \\ 4 & \text{in two dimensions (square lattice);} \\ 6 & \text{in three dimensions (simple cubic lattice);} \\ 8 & \text{in three dimensions (body-centred cubic lattice);} \\ 12 & \text{in three dimensions (face-centred cubic lattice).} \end{cases} \tag{5}$$

In general, our Hamiltonian for the energy is then given by:

$$H = -\epsilon \sum_{\langle i,j \rangle} s_i s_j - \mu_B B \sum_i s_i, \tag{6}$$

where $\langle i, j \rangle$ refers to a sum over all neighbouring pairs, μ is the magnetic moment of each dipole, and B is the strength of the external magnetic field. Note that this is the same as Equation 1, with an added term for the energy from an external magnetic field (and it reduces to the same thing when either B or μ_B equals 0). Note also that $\langle U \rangle$ is given by the time average value of H.

Further, we define the net magnetisation as:

$$M = \mu_B N \overline{s}, \tag{7}$$

where $\overline{s} = \frac{1}{N} \sum_i s_i$ is the average spin of our lattice. We also note that the heat capacity for our system is:[1]

$$C = \left(\frac{\partial U}{\partial T} \right)_{N,V,B} = \frac{\langle U^2 \rangle - \langle U \rangle^2}{kT^2}. \tag{8}$$

Our entropy can be computed using the definition:

$$S = k \ln \Omega, \tag{9}$$

where Ω is the multiplicity for our system (the number of microstates corresponding to a particular macrostate). With $\langle U \rangle$, T and S, we can then compute the Helmholtz free energy F from the definition:

$$F = U - TS. \tag{10}$$

This is all the information you need to get started on the core project. As such, you don't *need* to look up external literature to help you (though of course you are more than welcome to). For the open-ended extension, however, we recommend you do some external reading.

[1] This equality holds since we assume that our system is in equilibrium with a reservoir at temperature T; for more information, see Schroeder, *An Introduction to Thermal Physics* (3rd ed.), Problem 6.18

Question 1

(Core project. Five pages maximum. Questions 1 & 2 graded together out of 70%.)

In this question, you will simulate a 1D Ising model, and compare your results to exact solutions that you will derive from Z. You will also discuss the behaviours of finite and infinite 1D Ising models based on your simulations. There are five parts in this question.

(a) Code up a one-dimensional Ising model with periodic boundaries using the Metropolis algorithm for $N = 100$; for the time being, ignore any effects from an external magnetic field. Provide the initial and final outputs from the simulation for at least three different temperatures (we recommend $T = 2.0$, $T = 1.0$ and $T = 0.5\ \epsilon/k$). We recommend storing your spin values in a ***row*** vector labelled `s`, where spin-up is 1 and spin-down is -1, and using the `image` command in MATLAB as follows:

```
image('CData',s*256)
colormap('gray')
xlim([1 length(s)]
set(gcf,'position',[200 200 600 200])
```

If you see a blank plot, remember that `s` has to be a row vector. Your output, provided your simulation is working, should look like a barcode at sufficiently high temperatures. Make sure you give every dipole many chances to flip to ensure the system has reached approximate thermodynamic equilibrium (we recommend at least 1,000 chances for every dipole to flip). What do you notice about the size of the 'chunks' of colour at low temperatures compared to at high temperatures?

Your task: Provide a code which meets the above outlined requirements; to provide figures of the initial and final states of the system at 3 different temperatures; and to comment on the size of the 'chunks' you see at low vs. high temperatures.

(b) For a sufficiently large 1D Ising model, the partition function can be computed exactly. We present the result without proof:[2]

$$Z = \big(2\cosh(\beta\epsilon)\big)^N \tag{11}$$

Using Equation 11, derive equations for internal energy per dipole, $u = U/N$, free energy per dipole, $f = F/N$, entropy per dipole, $\mathcal{S} = S/(N)$, and specific heat capacity, $c = C/N$. Note that you should be using relations for a canonical ensemble. You should obtain the following results:

$$u = -\epsilon\tanh(\beta\epsilon), \tag{12}$$

$$f = -\epsilon - kT\ln\Big(1 + e^{-2\epsilon\beta}\Big), \tag{13}$$

$$\mathcal{S} = \frac{\epsilon}{T}(1 - \tanh(\beta\epsilon)) + k\ln\Big(1 + e^{-2\epsilon\beta}\Big), \tag{14}$$

$$c = \frac{\epsilon^2\beta}{T\cosh^2(\beta\epsilon)}. \tag{15}$$

Your task: Provide derivations, starting from Equation 11, for $u, f, \mathcal{S}$, and c.

[2] A relatively simple proof can be found in Schroeder, *An Introduction to Thermal Physics* (3rd ed.), pg. 343.

(c) Compute and plot figures for u, f, $\mathcal{S}$, c and the reduced magnetisation per dipole, $m = M/(\mu_B N) = \overline{s}$, of the 1D Ising model against temperature, T, using your simulation with $N = 100$ (don't forget to include error bars for your simulated values). Obtain values for at least ten different temperatures (including temperatures near, but not at, 0 K). You should compute time-averages of these values to obtain the best results. You should also make sure that you give your system enough time at each temperature to be in (roughly) thermodynamic equilibrium before you start making measurements of these variables. For each of these values (except m), also plot the exact solutions from part (b). The choice of presentation format is up to you; we are just looking for you to present all of the data in a clear and comprehensible way.

Your task: Provide plots for $u, f, \mathcal{S}, c$ and m against T for at least 10 T values (including error bars); plot the exact solutions for $u, f, \mathcal{S}$ and c.

(d) Explain what the high and low temperature values from your plots indicate about the finite 1D Ising model (i.e., are the spins parallel at low/high temperatures? Are there larger 'chunks' of parallel spins at lower or higher temperatures? How can you tell, based on your data?). Compare your data against the exact results; are there any differences? If so, suggest why there might be differences.

Your task: Explain what your plots indicated about the finite 1D Ising model at low and high temperatures; compare this to the exact results and explain any differences.

(e) An infinite 1D Ising model should have a time-average m value equal to 0 at $T = 0$; does this agree with your results? Explain why there might be a difference. In doing so, create a histogram of the m values you obtain using the `hist` function in MATLAB by running your simulation at least 100 times at temperatures $T = 2.0$, $T = 1.0$ and $T = 0.5\ \epsilon/k$ with $N = 100$. Then produce three identical histograms, except with $N = 500$. You should notice that the magnetisation for $N = 500$ sets in at lower temperatures than for $N = 100$. What does this suggest about whether the infinite 1D Ising model has a phase transition (i.e., what does this suggest about whether there is a spontaneous magnetisation for $T \geq 0$)?

Your task: Explain differences in m between your simulation and the expected values; create histograms of m values at 3 different temperatures for 2 different N values; explain whether the infinite 1D Ising model has a phase transition based on these histograms.

Question 2

(Core project. Five pages maximum. Questions 1 & 2 graded together out of 70%.)

In this question, you will be extending your simulation of a 1D Ising model into a 2D Ising model. You will also be plotting relevant data on thermodynamic properties at a variety of N values, and discussing the implications of these data for the behaviours of both finite and infinite 2D Ising models. There are five parts in this question.

(a) Extend your simulation code to a 2D Ising model with $N = 100^2$ (i.e., a 100×100 lattice). Provide plots of the initial and final states for at least three different temperatures (we recommend $T = 3$, $T = 2$ and $T = 1$ ϵ/k). Make sure to change the `set` command from Question 1 so your lattice looks like a square (if you are using that command). Plot (but don't provide!) snapshots every time all dipoles have had a chance to flip (it will help to use MATLAB's `drawnow` command for this). What do you notice about the lattice as time progresses at these three different temperatures?

Your task: Provide code for a 2D Ising model; provide plots of the initial and final states of this model at 3 different temperatures; describe how the lattice changes as time progresses at these different temperatures.

(b) What happens to the size of the 'crystals' as the temperature decreases? Does there appear to be some critical temperature below which the crystals can be as large as the lattice? Estimate this temperature. What does this suggest about whether a phase transition exists for the 2D Ising model?

Your task: Comment on the size of the crystals as T decreases; comment on whether T_c exists, and if so estimate it; comment on whether this suggests a phase transition for the 2D Ising model.

(c) Provide plots of values for u, f, $\mathcal{S}$, c and $|m|$ (note the absolute value bars here) against T at $N = 20^2$, $N = 50^2$ and $N = 100^2$ (with error bars). What do you notice about the values for c as N increases? What behaviour appears to happen around T_c? What does this suggest about the heat capacity of an infinite 2D Ising lattice at T_c?

Your task: Provide plots for $u, f, \mathcal{S}, c$ and $|m|$ against T at 3 different N values (with error bars); comment on how c changes with N, particularly around T_c; based on this, comment on the heat capacity of an infinite 2D Ising lattice at T_c.

(d) Provide a plot of the mean positive and negative values of m against T for $N = 5^2$, $N = 10^2$ and $N = 20^2$ (we recommend you average the m values from at least 100 runs of your simulation for each temperature and N value) (include error bars). At what temperatures do these mean m values begin to significantly diverge? What does this suggest about the critical temperatures T_c at each of these N values? How do you expect the critical temperature to change as N increases (say, in the limit of an infinitely big lattice)?

Your task: Provide plots of mean positive and negative m values against T for 3 different N values (with error bars); estimate the temperature that these m values diverge; comment on what this suggests about T_c for these N values; comment on how T_c will change as N increases.

(e) Starting with a lattice at $T = 1\ \epsilon/k$ in thermodynamic equilibrium (with at least $N = 20^2$), slowly increase the temperature up to $T = 3\ \epsilon/k$, then slowly decrease the temperature back to $T = 1\ \epsilon/k$. Provide plots at each of these temperatures (so 3 in total). What happens to the spontaneous magnetisation as you increase the temperature? Is the magnetisation after cooling always the same as the initial magnetisation? Use these observations to argue that T_c is analogous to the Curie temperature for real ferromagnetic materials. Given that the Curie temperature of iron is about 1043 K, determine what the ϵ value is for iron if you were modelling it as a 2D Ising lattice (you will need to determine what T_c is in terms of ϵ/k; state this value when computing iron's ϵ value).

Your task: Provide at least 3 plots as you increase and decrease the temperature of a 2D Ising lattice; comment on the spontaneous magnetisation as T increases; comment on whether m can change after this heating/cooling process has finished; argue that T_c is the Curie temperature for a 2D Ising lattice; estimate ϵ if the 2D Ising lattice was being used to model iron.

Additional Tips for the Core Project

Find below a list of tips to help you in simulating an Ising model and obtaining the data necessary to do well in the core project.

First, you should avoid undesirable 'metastable' states for the 2D Ising model (where multiple domains exist which are infinitely long due to our periodic boundary conditions; these look like 'rivers' surrounded by 'riverbanks'; see Figure 1 for clarification). By keeping your lattice sufficiently small ($N = 100^2$ or less) and slowly cooling your lattice, this prevents almost all such states appearing.

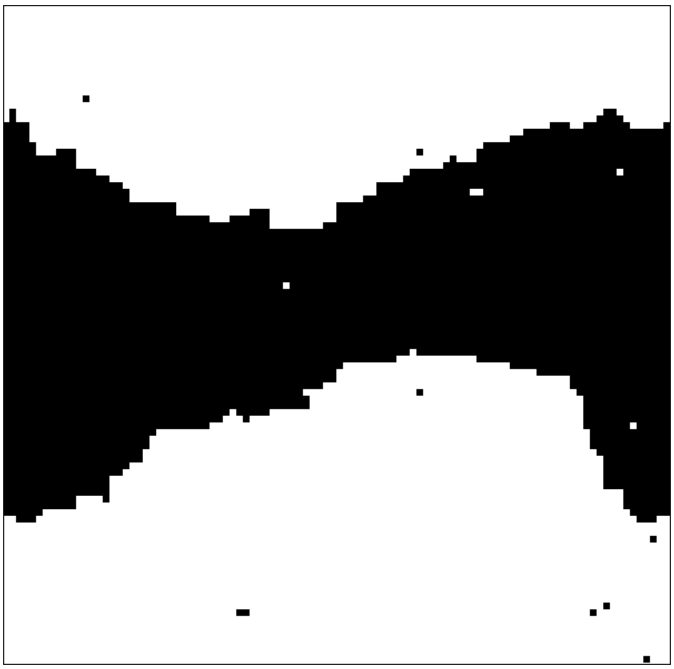

Figure 1: An example of an undesirable metastable state. Notice that the spin-down segment (in black) extends infinitely across the periodic boundaries, as do the spin-up segments (in white). Such a state is only stable for finite 2D Ising lattices with periodic boundaries, and not infinite lattices (which, at low T, have only one spontaneous magnetisation at equilibrium).

Secondly, you should make sure your states are at (rough) thermodynamic equilibrium before you begin measuring any data. This typically means letting the dipoles 'flip' more times for larger lattices so that the effects of neighbouring spins can transfer 'through' the entire lattice. Importantly, lattices take more 'flips' to reach thermodynamic equilibrium at lower temperatures if starting from a random state. So, when 'cooling' or 'heating' a lattice, there are two viable options: either you let the dipoles flip many times before you begin measuring data (with the number of flips increasing as the temperature decreases), or you can use the previous end-state at the higher temperature as your initial state at your lower temperature. Either option is fine, however if you choose the latter make sure you run multiple 'cooling'/'heating' runs to capture the variability in the phase transition (since otherwise you lock in the spontaneous magnetisation chosen at higher temperatures in your lower temperature lattices).

Thirdly, when estimating your error values, use the `std` function in MATLAB (or otherwise

compute the standard deviation of your data), since we can assume the errors are Gaussian distributed in our simulation.

Fourthly, make sure you preallocate the memory of all your variables to prevent your code from running slower than it needs to.

Finally, it is often easier to visualise and operate our simulations when using a "natural" system of units. We recommend you try this here. These natural units would be such that your relevant constants are set to 1 (this would make $\mu_B = \epsilon = 1$). Boltzmann's constant is also set to 1. This converts our units into, e.g., energy, ϵ; temperature, ϵ/k; etc.. Although not absolutely necessary, we're sure that if you adopt this system of units, you'll appreciate how much easier it is to work with your simulation!

Question 3

(Extension: open-ended investigation. Ten pages maximum. Graded out of 30%, for a total project grade out of 100%.)

In the previous two questions, you developed computational methods to model 1D and 2D Ising models, and used these to explore some of the thermodynamics of these systems in a guided way. One of the powerful aspects of computational modelling is that it allows you to perform "experiments" quickly and in regimes that may be difficult to access in the laboratory. With computational modelling, you are limited mainly by your own creativity. In this sense, computational work allows you to experience what is involved in physics research, more so than undergraduate learning activities such as labs and assignments.

This final question in your computational project is open-ended—you get to decide what thermodynamics you explore and what questions you answer. We strongly recommend that you use the code you have developed in Questions 1 and 2 as a basis. However, it is up to you. As always, when you write up your project, you should include any new sections of code as snippets in your report, along with sufficient details of your complete code such that your tutor can follow what you've done (perhaps in an Appendix).

In answering this question you should:

- Form a specific hypothesis that you can test.
- Include theoretical modelling, to allow quantitative tests of your hypothesis.
- Extend your code, or build new code, to address your hypothesis.
- Perform simulations, and quantitatively compare the results to your theoretical model. Include uncertainties where appropriate.
- Conclude and discuss any insights you have gained.

Your hypothesis and simulations should extend significantly beyond the thermodynamics you have already explored in Questions 1 and 2. In grading, you will be rewarded for showing originality, for the depth with which you describe the physics involved, and for the robustness of your analysis and conclusions. You should be careful to clearly state any approximations you make. If you are unsure about what physics to explore, or how to proceed with testing it, it may be a good idea to discuss with your tutor.

Some examples that you could focus on are:

- *The 3D Ising Model.* Extend your 2D Ising model into a 3D one. Then, using this 3D model, produce plots of data for u, f, $\mathcal{S}$, c and $|m|$. In whatever way you can, estimate the critical temperature of your model. Compare your results to those in published literature on the topic.
- *The Effects of an External Magnetic Field.* Include an external magnetic field B in your 2D Ising model. Can you change the spontaneous magnetisation of your lattice

(once it's below T_c) by applying a strong enough magnetic field? Can you magnetise your system when $T > T_c$? Plot both $|m|$ and u against B at $T < T_c$, $T = T_c$ and $T > T_c$. You should vary B by both decreasing it and increasing it; do your results differ at all, and are there any discontinuities? If so, does this suggest a first order or a second order phase transition in your model at these different temperatures? Make sure to justify your conclusions.

- *Correlation Function and Length.* The correlation function for an Ising model is a measure of the tendency for spins to align themselves at different temperatures and distances from some fixed lattice point (labelled r here):

$$\mathcal{C}(r,T) = \overline{s_i s_j} - \overline{s_i}^2, \tag{16}$$

(here the overline represents the average values). Determine this correlation function for a variety of r and T values (specifically, consider at least three temperatures: $T < T_c$, $T = T_c$ and $T > T_c$). Also determine the correlation length, $\sigma(T)$, i.e., the r value which reduces the value of $\mathcal{C}(r,T)$ by a factor of e, for different T values. Provide a plot of σ against T. You should use a lattice of at least $N = 20^2$, and let r vary from 1 to half the lattice length. Also apply an external magnetic field and, for at least three temperatures $T < T_c$, $T = T_c$ and $T > T_c$, produce plots for σ against B.

- *Critical Exponents for the 2D Ising Model.* It is known that, for the 2D Ising model, $m \propto (T_c - T)^\beta$ (here β is the critical exponent, **not** the inverse temperature). Estimate what the value of β is. In whatever way you can, also determine values of the magnetic susceptibility:

$$\chi \propto \left(\frac{\partial m}{\partial B}\right)_T \tag{17}$$

(you can, e.g., use numerical differentiation, or differentiate an equation obtained through curve-fitting to do this). It is also known that $\chi \propto (T - T_c)^{-\gamma}$. Estimate the value of γ, and show that it does not depend on what direction T approaches T_c (note that T_c will shift slightly due to your applied magnetic field on a finite-sized lattice).

- *2D Lattice Gas.* An Ising model in an external magnetic field is equivalent to a 2D lattice gas, a lattice where each point is either occupied or unoccupied by a particle (you should research how to convert your Ising model into one for a lattice gas; some coordinate transformations will be necessary). In this case, low density states imply a gas phase, and high density states imply a liquid phase. Provide plots for u, f, $\mathcal{S}$, c, ρ and P for this lattice gas. For simplicity, you can compute P using the following equation (which applies equally well to ideal gases!):

$$P = \frac{kT}{v_Q} e^{\mu\beta}, \; v_Q = \left(\frac{h}{\sqrt{2\pi m k T}}\right)^3, \tag{18}$$

where v_Q is the quantum volume, μ is the chemical potential of the lattice gas, h is Planck's constant, and m here is the mass of each particle. Construct a gas-liquid phase diagram on a $P - T$ plot, and determine the functional form of the gas-liquid phase boundary on this diagram.

- *Paramagnetic and Antiferromagnetic Materials.* When $\epsilon = 0$, your Ising model mimics paramagnetic materials. When $\epsilon < 0$, your Ising model mimics antiferromagnetic

materials (where spins tend to align antiparallel to their neighbours). Investigate thermodynamic properties of these types of materials, and provide plots of u, f, $\mathcal{S}$, c and $|m|$. Also investigate how these materials respond to external magnetic fields. Finally, for the antiferromagnetic material, estimate the value of the Néel temperature (an analogous concept to the Curie temperature, except for antiferromagnets).

- *Ising Models of Neural Networks.* Ising models can be used to create very simple neural networks (models that can, for example, determine the particular type of letter meant by someone's handwriting). Create your own such neural network by modifying your 2D Ising model code.[3] How robust is your neural network?

- *Ising Models of Binary Alloys.* Model a binary alloy (i.e., a lattice composed of two metal atoms) using the Ising model.[4] Provide plots of u, f, $\mathcal{S}$ and c against T, alongside any other relevant thermodynamic properties. Determine a phase diagram of the crystal types for such a binary alloy (you should see at least two: a periodic (ordered) and random (disordered) crystal).

- *Block Spin Transformations.* Take a 2D Ising lattice and divide every position into 3×3 'blocks' by assigning a single dipole whose direction depends on those of the other 9 dipoles. If more than half point up, the single dipole points up; likewise, if more than half point down, the single dipole points down. If you apply this transformation to the entire lattice, we reduce it to one whose width is 1/3 the original. This transformation is an example of a renormalisation group transformation, a powerful technique for studying the behaviour of systems near their critical points. Modify your code to apply such a block spin transformation to an original lattice, and observe and comment on how both the original and transformed lattices evolve over time. Provide plots of u, f, $\mathcal{S}$, c and $|m|$ against T for both the original lattice and the transformed one. You should find that, once both systems have equilibriated, the transformed lattice should generally represent a lattice at a *different* temperature. Call this the 'transformed' temperature; when is the transformed temperature greater that the original, and when is it less? Argue that, based on this answer and other observations, there should be three critical points upon successively applying block-spin transformations: either $T = 0$, $T \to \infty$, or $T = T_c$. For which initial temperatures will you end up at each fixed point? Comment on the implications of the critical temperature being a fixed point of the block spin transformation. For example, what does this imply about the effect that specific microscopic behaviours have on the large-scale dynamics of physical systems such as fluids, magnets, alloys, etc.?

- *Ising Models of Spin Glass.* A glass is a non-crystalline amorphous solid, i.e., one where there are no periodic crystalline structures. A spin glass is therefore a system of spins where the direction is frozen in place, and 'randomly' directed. Read the following paper by Edwards and Anderson about a model of spin glasses implementable in a 2D Ising model.[5] Modify your code to model a spin glass system, and investigate and produce plots for relevant thermodynamic properties of the system. Discuss your observations.

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[3] For more information on how to do this, see, e.g., `https://courses.physics.illinois.edu/phys466/sp2013/projects/2010/Bjaalie-Kelkhoff-Tegnered/HTML/NeuralNetworks.html`.

[4] For some help on how to do this, see, e.g., `https://en.wikitolearn.org/Course:Statistical_Mechanics/Statistical_mechanics_of_phase_transitions/Ising_model_and_binary_alloys`.

[5] You will have to log in via UQ to access the paper, which can be accessed here: `http://iopscience.iop.org/article/10.1088/0305-4608/5/5/017`.