Investigating the Ising model through object-oriented programming and Monte Carlo methods.

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The investigation aimed to use Object-Oriented Programming and Monte Carlo methods on C++ to simulate the 1D and 2D Ising Model for particle spins. The effect of temperature on energy and magnetisation was explored. The program was initially tested for a small system consisting of either a 3-spin chain or a 3-by-3 grid. The simulation produced results that aligned well with theory, with average energy increasing with temperature and average magnetisation displaying a decreasing trend. The program was then extended to a 100-spin chain and a 100-by-100 grid, producing trends similar to those for the smaller systems. The main source of limitations was the number of iterations used for the Monte Carlo simulation.

INTRODUCTION

In statistical mechanics, the aim is to describe the macroscopic properties of a system by considering the possible configurations of the particles within that system. These individual configurations, or microstates, contribute to the system's overall behaviour. For large systems, the number of possible microstates is extremely large, and analysing each one becomes impractical. Thus, numerical methods become a useful tool for sampling microstates and performing statistical analysis to yield macroscopic quantities.

One system in which numerical methods become particularly useful is the Ising model. This model provides insight into the ferromagnetic-to-paramagnetic phase transition, and it consists of a configuration of particle spins, each with a state of +1 or -1. The energy of the system is determined by interactions between spins (the bonds between atoms), and the magnetisation is the sum of the spins. These interactions affect the overall macroscopic properties of the system.

The Monte Carlo algorithm is suitable for simulating the Ising model. This algorithm works on a reject/accept basis, where a microstate's probability, determined by its energy and temperature, is compared to a randomly generated value. By generating a large set of configurations, the system is more likely to sample microstates with higher probabilities. This allows the simulation to approximate the system's behaviour by analysing averages (ie. energy or magnetisation) and distributions, rather than relying on individual microstates.

In this investigation, the Ising model was simulated through a Monte Carlo algorithm in C++, using object-oriented programming (OOP), for both 1D and 2D systems. By changing the temperature of the system, its behaviour was explored, and the changes in energy and magnetisation were studied.

BACKGROUND INFORMATION

In the 1D Ising model, the energy of an interaction between a spin and its neighbours is given by:

$$E_{ij} = -J\sigma_i\sigma_j, \tag{1}$$

where σ_i and σ_j are the spins of the selected atom's neighbours. J is a constant, that was set to 1 in this investigation. If the spins are aligned, the system will be in a lower energy state than if they were opposing. For a system of three spins, the possible configurations, along with their total energy and magnetisation are shown on Table 1, as an example.

Configuration	Total Energy	Magnetisation
↑↑↑	$-2J$	$+3$
↑↑↓	$0J$	$+1$
↑↓↑	$2J$	$+1$
↑↓↓	$0J$	-1
↓↑↑	$0J$	$+1$
↓↑↓	$2J$	-1
↓↓↑	$0J$	-1
↓↓↓	$-2J$	-3

TABLE I. Possible configurations, energy, and magnetization for a 3-spin Ising model.

To calculate the total energy of a system, the individual energies of each spin are added (given by Equation 1), and the final result is divided by two, to avoid double counting of the bond energies. The equation used is:

$$E_{\text{total}} = -\frac{J}{2}\sum_{\langle i,j\rangle}\sigma_i\sigma_j \tag{2}$$

Additionally, the total magnetisation is obtained by adding the spins:

$$M_{\text{total}} = \sum_i \sigma_i. \tag{3}$$

Similar equations are used for the 2D case, except that the spin now has left, right, top and bottom neighbours. Depending on a spin's position in the grid, some of its neighbours might be assigned values of 0.

The probability of a system being in a given microstate of total energy E is given by:

$$P \propto exp(-E/k_bT). \tag{4}$$

From Equation 4, it is possible to consider the likelihood that a system is in a given microstate based on the values of energy and temperature. For low temperatures, the probability will be maximised for lower energies, as higher energy microstates are not accessible due to the exponential nature of the Boltzmann factor. At higher temperatures, higher energy states become accessible, so the system is able to explore a wider range of energies.

METHODOLOGY

The core of this investigation was based around the C++ programming language, with an emphasis on OOP and numerical methods (Monte Carlo algorithm). Git was used to create separate branches for different stages of development (separating the 1D Ising model from the 2D Ising model). Four branches were created: main, 2D, 1DAnalysis, and 2DAnalysis.

The main branch encompassed the basic code for a one-dimensional chain of atoms. An Atom class and an AtomChain class were created for the purpose of this project. The Atom class' purpose was to randomly assign values of either -1 or 1 to the created object. The class also contained functions to allow the user to obtain an atom's state (getState()), and to flip the state of the atom (ie. 1 becomes -1). The AtomChain class created an N sized vector of Atom objects, and contained functions to print the chain, select an atom, and calculate the total energy and magnetisation. Thus, an object of class AtomChain is composed of a given number of spins, each with a randomly assigned value.

A montecarlo.cpp file was created to encompass the algorithm. The algorithm requires an object of class AtomChain. The MonteCarlo file is composed of two functions: the computeEnergyChange function and the MonteCarlo function. To compute the energy change, boundary conditions had to be considered, setting a neighbour to 0 if the selected atom was at the beginning or end of the chain. For a random chain of atoms, the steps of the simulation are the following:

1. Selecting a random atom from the chain using a randomly generated index and the getAtom member function.
2. Calculating the energy change for the system if the selected atom were to flip, applying Equation 1 (with $J = 1$). This was done through the computeEnergyChange function and the getAtom function (to obtain the selected atom's neighbours).
3. Computing the probability (Equation 4) using a the calculated change in energy.
4. Generating a random decimal between 0 and 1, and comparing it to the calculated probability on step 3. If the random decimal was smaller than the probability, then the selected atom was flipped using the flip function.

The process detailed above was repeated for a selected number of Monte Carlo iterations, producing a configuration. The number of iterations that was deemed suitable for this investigation depended on the size of the system. For a chain of 3 spins or a 3-by-3 grid, 10000 iterations was appropriate. This number of iterations ensured that the system was able to explore sufficient microstates, settling into a final more stable configuration. The total energy and magnetisation of a configuration were obtained through the totalEnergy and totalMagnetisation functions. For every 10000 Monte Carlo iterations, one configuration was produced. In order to understand the average behaviour of the system, 10000 configurations were produced for a selected temperature. The energy and magnetisation of each configuration were written on a text file, and plotted as a histogram using Python (Pandas and MatPlotLib). For larger systems, the number of Monte Carlo iterations had to be increased.

The same process was extended to 2D in its corresponding branch. Instead of a vector of atoms, a vector of vectors was produced in order to form a grid, with randomly assigned values of spin. The AtomChain class was replaced by an AtomGrid class, and the code was adapted for the appropriate boundary conditions for energy calculations.

The last two branches, 1DAnalysis and 2DAnalysis, did not modify the workings of the code, but did modify the final output in main.cpp. These two branches were produced to illustrate the relationship between average energy and magnetisation with temperature. In both branches, the code in the main branch and in the 2D branch was looped over for a range of temperatures, and the average energy and magnetisation of 10000 configurations was calculated for each temperatures. This data was written on a text file, which was then used to create a scatter plot using Python. For the 2D system, the number of Monte Carlo iterations was increased to 100000, due to the size of the system. Using a smaller value for iterations in the 100-by-100 grid yielded inaccurate results, despite it working for 3-by-3.

For all branches, the parameters (number of spins, temperature, number of configurations, and number of iterations) could be modified directly in the main.cpp file.

The code was bundled using git. It must be noted though, that when the bundle is cloned, all branches except the main one become remote. This means that all branches need to be individually checked out in the clone to create a local copy.

PRELIMINARY TESTING

Before applying the program to 100 spins, it was first tested for a chain of three spins to ensure expected behaviour. The possible states of a 3-spin chain are shown on Table 1. The resulting histograms from the Monte Carlo algorithm were displayed on Figure 1, for low and high temperatures. The average energy and average magnetisation graphs with respect to temperature are shown on Figure 2.

Observing the low-temperature histograms for a 3-spin

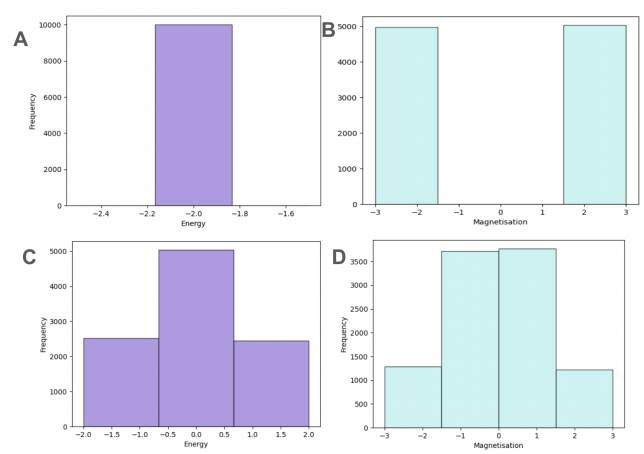

FIG. 1. Histograms for a 3-spin chain of atoms. (A) Energy distribution at a low temperature (0.1). (B) Magnetisation distribution at a low temperature. (C) Energy distribution for a temperature of 3.5. (D) Magnetisation distribution for a temperature of 3.5.

chain, the distributions match what was expected from Table 1. At lower temperatures, the system occupies the lowest energy states, where all the spins are aligned. This energy corresponds to -2. Observing the distribution for the magnetisation, the frequency peaks at 3 and -3. The two peaks in the magnetisation graph correspond to the spins being all either up or down. These further corroborate the idea that at lower temperatures, the system finds itself in its lowest energy state, thus having all spins aligned.

When the temperature was increased to 3.5, the distributions broadened, reflecting the fact that the system can now access higher energy states. At this temperature, most configurations have a total energy of 0, as indicated by the main peak in the distribution. This occurs because, at higher temperatures, configurations with balanced spin alignments become more probable. This is also illustrated by the magnetisation histogram for a temperature of 3.5. Smaller peaks at energies of -2 and 2 correspond to configurations where the system occupies lower or higher energy states, as a result of fluctuations. For the majority of configurations, the magnetisation was mostly +1 or -1. Since magnetisation can be either positive or negative, the values are symmetrically distributed around 0.

As for the average energy and magnetisation against temperature graphs, a clear trend is observed. For the energy graph, increasing the temperature results in the average energy increasing (approaching 0). For low temperatures, the energy remains fairly stable at around -2, but increasing the temperature causes a rapid increase in the average energy, settling again at 0. The magnetisation had an opposing trend, with the average magnetisation decreasing as the temperature increased. At low temperatures, the system occupies the ground state, with all spins aligned, with an average absolute magnetisation of 3. As the temperature increases, the average magnetisation sharply drops, reaching around 1.

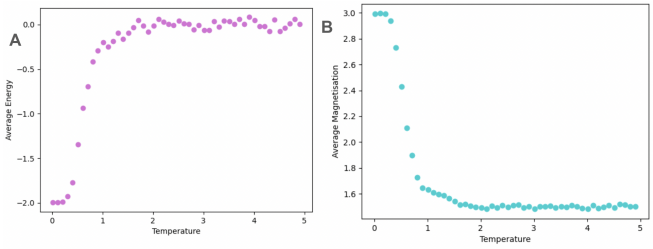

FIG. 2. Scatter plots for average energy (A) and average magnetisation (B) against temperature for a 3-spin chain. Absolute values were used for the average magnetisation.

Therefore, the data obtained from the Monte Carlo simulation aligns with the expectations from the Ising model for a chain of 3 spins. The investigation was then extended to 2D using a square grid of spins, and tested for a 3-by-3 grid, with results shown on Figures 3 and 4.

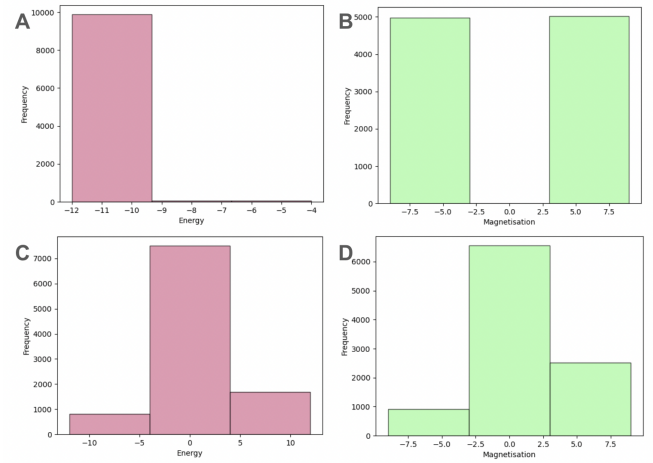

FIG. 3. Histograms for a 3 x 3 grid of spins. (A) Energy distribution at a low temperature (0.1). (B) Magnetisation distribution at a low temperature. (C) Energy distribution for a temperature of 3.5. (D) Magnetisation distribution for a temperature of 3.5.

Observing the low-temperature energy and magnetisation histograms, the general behaviour of the system is consistent with the 3-spin chain. For the energy graph, most of the configurations had a total energy ranging between -12 and -10, with very few configurations having slightly higher energies. Due to the number of bins selected for the magnetisation, it is observed that there are two peaks for magnetisation: one ranging between -9 and -3 and one ranging from 3 to 9. This does not fully provide information on the average value, but the graphs in Figure 4 provide further information that demonstrates the accuracy of the model. Values of -9 and 9 are expected for low temperatures, as the spins are aligned. For higher temperatures, both the magnetisation and the energy are distributed about 0, as the system has stabilised at a higher energy and reached a more disordered state.

Considering Figure 4, the results are as expected. Due to

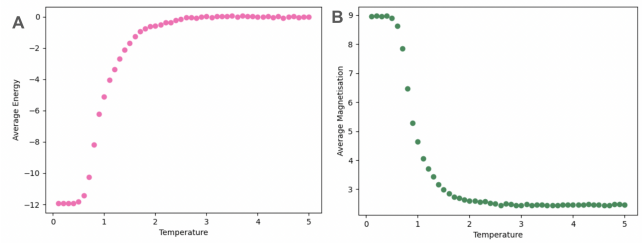

FIG. 4. Scatter plots for average energy (A) and average magnetisation (B) against temperature for a 3 x 3 grid. Absolute values were used for the average magnetisation.

the small size of the grid, a total of 10000 Monte Carlo iterations was sufficient to produce accurate results, with the peak magnetisation being 9, when all spins are aligned. As for the energy graph, the system starts out in its lowest energy configuration and settles at 0 as the temperature increases. Having checked the model for appropriate behaviour for smaller systems, it was then tested for larger systems, with a 100-spin chain and a 100-by-100 grid.

RESULTS FOR N = 100 AND DISCUSSION

1-dimension

Due to the large size of the system, the number of Monte Carlo iterations used had to be increased to 100000 to obtain accurate results. Nevertheless, despite the number of iterations and limited accuracy, the overall behaviour of the system matches what was theoretically expected from the smaller systems.

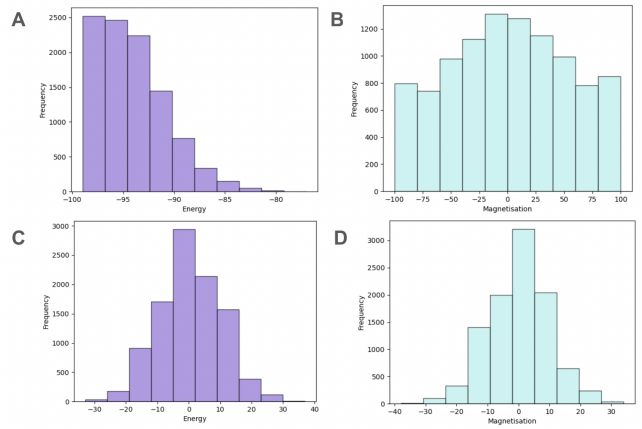

FIG. 5. Histograms for a 100-spin chain. (A) Energy distribution at a low temperature (0.1). (B) Magnetisation distribution at a low temperature. (C) Energy distribution for a temperature of 3.5. (D) Magnetisation distribution for a temperature of 3.5.

From Figure 5, the temperature-dependent behaviour of the 100-spin chain can be observed. At low temperatures, the chain is in its lowest energy state due to an overall alignment of spins. In terms of magnetisation, the distribution is more spread out, indicating that the system can access a broader range of magnetisation values compared to energy values. This suggests that while the energy remains tightly concentrated around its minimum value, the magnetisation exhibits greater variability. This reflects the fact that vastly different degrees of spin alignment are available for similar energies. For the magnetisation graph, it can also be observed how there are secondary peaks in the -100 and 100 regions, indicating a complete alignment of the system.

When the temperature was increased, the values of both energy and magnetisation became more sharply centered around 0, indicating a more disordered state and that the system is now able to access more higher energy states. The spins exhibit an overall cancellation of magnetisation. This behaviour was expected from the Ising model. Although the low-temperature magnetisation histogram was also centered around 0, the spread for higher temperatures is clearly more sharply defined, whereas the low temperature spread exhibited a larger variance.

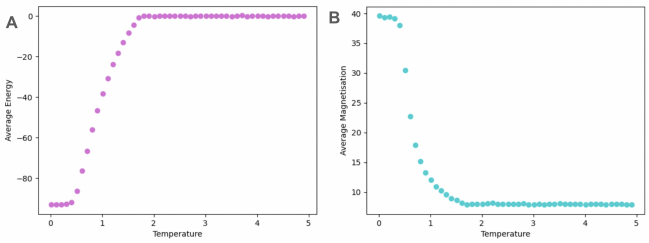

FIG. 6. Scatter plots for average energy (A) and average magnetisation (B) against temperature for a 100-spin chain. Absolute values were used for the average magnetisation.

The average trends for the chain with temperature are observed on Figure 6. The behaviour of the system is similar to that observed for the 3-spin chain on Figure 2. While the average energy increases sharply with temperature, the average magnetisation decreases with temperature. For magnetisation, the maximum value of average magnetisation lies around 40, which is lower than the expected maximum of 100, where all spins are aligned. This can be considered to be a result of the Monte Carlo algorithm used. Increasing the number of iterations could have resulted in more configurations being in a more aligned state. It is also important to consider that the value plotted is an average, and due to the large spread seen on Figure 5.B, there are many values that the magnetisation adopted. In both cases, increasing both the number of iterations and number of configurations would have provided a more accurate view of the macroscopic behaviour of the system, but this was limited due to computational constraints.

2-dimension

The number of Monte Carlo Iterations was also increased for a 2D square grid, as 10000 did not appear to be sufficient as it was for the 3-by-3 grid. The iterations were increased to 100000. Similarly to the 100-spin chain, the results for a 100-by-100 grid also aligned with the preliminary investigation.

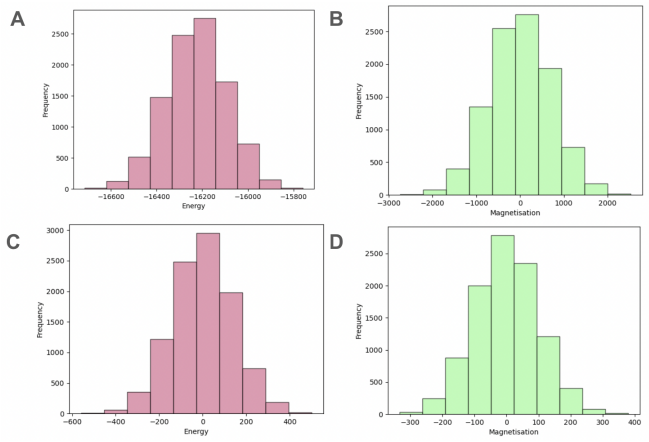

FIG. 7. Histograms for a 100 x 100 grid of spins. (A) Energy distribution at a low temperature (0.1). (B) Magnetisation distribution at a low temperature. (C) Energy distribution for a temperature of 3.5. (D) Magnetisation distribution for a temperature of 3.5.

On Figure 7, it is observed that the histograms for both low and high temperatures look different than those for the 1D investigation. For the low-temperature histograms, the distributions appear to be a lot more symmetrical than those for the 100-spin chain. The energy histogram for the low-temperature chain was skewed toward -100, whereas the energy histogram for the low-temperature grid was symmetrically distributed about -16200. This difference occurs as a result of the dimensions of the system. For 1D, there are fewer possible configurations as a spin can only interact with its immediate neighbours (left and right). The lower configuration number causes the energy values to cluster around the ground state. For the 2D system, a spin interacts with its left, right, top and bottom neighbours, yielding a higher number of possible configurations at a specified energy level. This means that there are multiple configurations that can yield the same total energy, hence resulting in a more symmetrical histogram. The energy values are distributed about the most probable energy.

In the chain system, it was observed that the low-temperature magnetisation histogram was more spread out than the high-temperature one. This was also observed in the grid system, except that due to the scale of the histograms, it is not as evident. Both magnetisation distributions are centered at 0, but the low-temperature one has a range between -3000 and 3000, while the high-temperature one has a range from -400 to 400. The smaller range in the high-temperature system reflects the more unaligned state of the spins, where there are more overall cancellations.

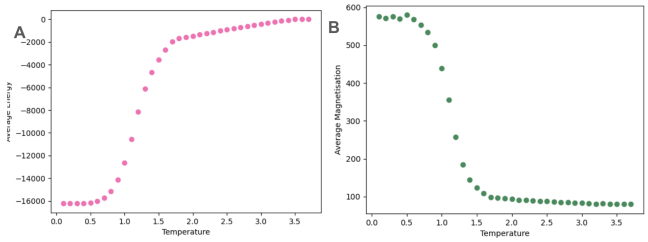

FIG. 8. Scatter plots for average energy (A) and average magnetisation (B) against temperature for a 100-by-100 grid. Absolute values were used for the average magnetisation.

The scatter plots on Figure 8 provide further information on the behaviour of both the system and the accuracy of the Monte Carlo algorithm. The trends exhibited by the graphs on Figure 8 are the same as those followed by the preliminary testing graphs and the chain graphs. However, due to the large number of objects in a 100-by-100 grid, it is possible that 100000 iterations were not sufficient to produce greatly accurate results. This is evidenced by the fact that the maximum value for average magnetisation of the system corresponds to 600, where the expected maximum would be somewhere close to 10000. This is likely a result of insufficient sampling, as modifying the value of iterations changed the results. Reducing iterations to 10000 caused the maximum value to be only 180, so the number of iterations can be considered to be a source of error. Overall, the general trends are correct, as the average energy starts at a minimum and increases with temperature to an average of 0 (also demonstrated by the histograms on Figure 7). The magnetisation also drops from a maximum value due to the lack of alignment in the spins.

CONCLUSION

Overall, the program used to simulate the Ising model was effective and accurate to a high degree. After performing a preliminary test on a smaller system, the model demonstrated a behaviour consistent with theory. The Monte Carlo algorithm successfully simulated the temperature dependent behaviour of energy and magnetisation, approximating the macroscopic properties of an N-sized system.

For the preliminary test case of an N = 3 system, the model was accurate, as the number of Monte Carlo iterations used was sufficient to access a wide range of configurations and reach equilibrium. The results matched expectations, with average total energy increasing with temperature and average magnetisation decreasing with temperature. As the system size increased to N = 100, the simulation continued to reflect the same trends, but computational constraints, such as the number of iterations, affected the accuracy of the results. This was evidenced by the magnetisation not reaching an average closer to the maximum value,indicating that further iterations would be needed to fully equilibrate the system. Therefore, although the correct trends were produced for both small and

large systems, the Monte Carlo algorithm proved to provide higher accuracy for the smaller system.

REFERENCES

[1] S.J. Blundell and K.M. Blundell. *Concepts in Thermal Physics.* Oxford University Press. pp. 199-273 (2006).