Assessment 2: Mini Project

BQ23603

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1. Introduction and Background Information

1.1. Context and Motivation

Statistical mechanics is a branch of physics that connects the microscopic properties of individual particles with the macroscopic behaviour of thermodynamic systems. By knowing the energy states of each particle, we can construct the partition function, $Z = \sum_k e^{-\beta E_k}$, which serves as a cornerstone for predicting macroscopic quantities such as temperature, pressure, and magnetisation. This framework reveals that at high temperatures (small β), all states are nearly equally probable, while at low temperatures (large β), the system favours low-energy configurations.

The Ising model is a prime example of applying these ideas. In this model, each atomic spin can be either +1 or -1, and the energy is determined by interactions with neighbouring spins, for example, in a 1D chain, $E = -J \sum_i s_i s_{i+1}$. Aligned spins contribute to lower energy, leading to macroscopic phenomena like ferromagnetism, where a net magnetisation $M = \sum_i s_i$ emerges.

This project leverages Monte Carlo methods, particularly the Metropolis algorithm, to simulate the Ising model in both one and two dimensions. By generating and sampling many configurations according to their Boltzmann probabilities, the simulation captures the transition from disordered states at high temperatures to ordered, low-energy states at low temperatures. This investigation provides the necessary theoretical and computational framework to understand how microscopic interactions give rise to macroscopic order.

1.2. The Problem

The objective of this project is to implement a Monte Carlo simulation of the Ising model in both one and two dimensions using C++ and object-oriented programming. By varying the temperature parameter (β), the simulation investigates the behaviour of spin systems, specifically focusing on energy and magnetisation distributions. The simulation results are then compared against theoretical predictions to validate the correctness of the model.

1.3. Theoretical Background

1.3.1 Partition Function and Boltzmann Distribution

A central concept in statistical mechanics is the partition function, defined as:

$$Z = \sum_k e^{-\beta E_k}$$

where E_k is the energy of the k^{th} configuration and $\beta = \frac{1}{k_B T}$ (with k_B being Boltzmann's constant and T the absolute temperature). The partition function encapsulates the contributions of all possible states to the thermodynamic behaviour of the system.

The probability of the system being in a state with energy E_k is given by:

$$P(E_k) = \frac{e^{-\beta E_k}}{Z}$$

At high temperatures (small β) all states are nearly equally probable. Conversely, at low temperatures (large β), states with lower energy dominate the probability distribution.

1.3.2 The Ising Model

The Ising model is a simplified representation of interacting spin systems where each spin s_i can take a value of +1 or −1. In the one-dimensional (1D) Ising model, the energy of the system is given by:

$$E = -J \sum_i s_i s_{i+1}$$

where T is the interaction strength (typically set to 1 for simplicity). The magnetisation M is defined as:

$$M = \sum_i s_i$$

For example, in a chain of three atoms, there are $2^3 = 8$ possible configurations. When all spins are aligned (all +1 or all −1), the system achieves the lowest energy, and the magnetisation reaches its maximum absolute value.

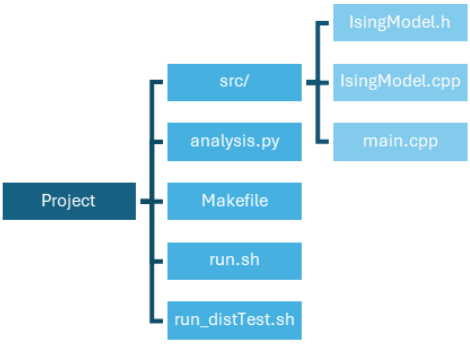
1.3.3 Monte Carlo Methods

For larger systems, the number of configurations grows exponentially, making direct enumeration of the partition function infeasible. Monte Carlo methods provide an efficient means to sample the configuration space. The procedure involves:

1. Randomly initializing the spin configuration.
2. Selecting a random spin and computing the energy change ΔE if that spin were flipped.
3. Accepting the spin flip with probability:$P = min\left(1, e^{-\beta \Delta E}\right)$, which favours lower-energy states while still permitting occasional moves to higher-energy states.
4. Repeating this process for many iterations to sample the ensemble of configurations.

2. Implementation

2.1. File Structure



2.2. Code Architecture

The project is divided into several components that promote clarity, maintainability, and ease of testing:

2.2.1 Header and Source Files

- **IsingModel.h**
  Defines two primary classes: one for the 1D Ising model (IsingModel) and one for the 2D variant (IsingModel2D). This header file is central to the project's object-oriented design and establishes the interface that the corresponding source file implements.
  - **Class IsingModel (1D):**
    - **Private Members:**
      - `int N` stores the number of spins in the one-dimensional chain.
      - `const double J = 1.0`
      - `double beta`: the temperature factor.
      - `std::vector<int> spins`: holds the spin configuration, where each element is either +1 or -1.
      - `std::mt19937 rng`: Random number generator.
      - `std::uniform_real_distribution<double>uniform_dist`: a distribution object that generates random real numbers in the interval [0,1].
      - A private member function `double delta_E(int i)const` computes the change in energy that would result from flipping the spin at index i.
    - **Public Members:**
      - The constructor `IsingModel(double beta,int n_spins=100)` initialises the model with a specified number of spins and a given beta value.
      - `void initSpins()`: initialises the spin configuration with random +1 or -1 values.
      - `Void simulate(int steps)`: implements the Monte Carlo simulation loop to update the spin configuration over a specified number of steps.
      - `Double totalEnergy()const`: calculates the total energy of the current spin configuration by summing over interactions between neighbouring spins.
      - `Double totalMagnetisation()const`: sums the spins to determine the overall magnetisation.
      - Utility functions like `void spins_print()` and `void spins_stats()` for outputting the configuration and its properties.

        - Accessor functions, including a const version and a non-const version of `getSpin()`, to retrieve the current spin configuration.
    - **Class IsingModel2D (2D):**
        - **Private Members:**
            - `int L`: represents the grid size for the two-dimensional model (resulting in an $L \times L$ grid).
            - `std::vector<std::vector<int>> spins`: a two-dimensional vector that holds the grid of spins.
            - The rest is the same as the 1D version.
            - A private function `double delta_E(int x, int y)const` computes the change in energy if the spin at position (x, y) were flipped, taking into account the contributions from the four nearest neighbours.
        - **Public Interface:**
            - The constructor `IsingModel2D(double beta, int grid_size=100)` sets up the 2D model with a specific grid size and bata value.
            - The rest is the same as the 1D mode.
- **IsingModel.cpp**
  Implements all member functions declared in IsingModel.h. These include:
    - `initSpins()`, which randomizes the spin configuration.
    - `simulate()`, which performs the Monte Carlo updates.
    - `totalEnergy()` and `totalMagnetisation()`, which compute key physical properties.
    - Utility methods such as `spins_print()` for debugging and `spins_stats()` for quick checks.

2.2.2. Main Program (main.cpp)

- Parses command line arguments to determine whether to run in 1D or 2D mode, the value of β, and the number of configurations to generate.
- Creates the output directories (data_1D/ or data_2D/) if they do not already exist.
- Instantiates either an IsingModel or an IsingModel2D object and repeats the simulation for the specified number of independent configurations.
- Writes the final energy and magnetisation of each configuration to a results.txt file for subsequent analysis.
- Has an embedded testing mode when the command line argument TEST is used
    - 1D testing
        - Tests for a 3-spin chain, enumerates all 8 possible configurations and prints their magnetisation and energy. These can be compared against the examples in the project specification.
    - 2D testing
        - Runs several predefined test cases. Each test explicitly sets the spin configuration and then prints the calculated energy and magnetisation, along with the expected results.

2.2.3. Analysis (analysis.py)

- A Python script that reads the simulation outputs from data_1D/ and data_2D/.
- Produces histograms of energy and magnetisation and trend plots of average energy and magnetisation vs β.
- Saves plots in visualisations_1D/ or visualisations_2D/ for easy inspection of how the system's behaviour changes with temperature.

2.2.4. Running

- Compile main.cpp and IsingModel.cpp then:
  - ***./IsingSim<mode><beta><n_configs>[n_spins|grid_size]***
    - Run 1D or 2D simulation
  - ***./IsingSim TEST***
    - Run tests

2.2.5. Build and Run Scripts

- **Makefile:** Defines compilation rules, linking instructions, and targets like make test for running embedded test routines.
- **run.sh:** Automates the process of cleaning, building, running simulations over a predefined range of β values, and then invoking analysis.py.
- **run_distTest.sh:** Automates specific test cases with specific parameters needed to test if the distribution matches the theoretical distribution.

2.3. Monte Carlo Steps Implementation

- **Random Spin Selection**
  On each iteration, a single spin is chosen at random. In 1D, this means picking an index in $[0, N-1]$, and in 2D, picking (x, y) in $[0, L-1] \times [0, L-1]$.
- **Energy Difference**
  The change in energy ΔE is calculated if that spin were flipped. Only the nearest neighbours contribute to the Ising model, making this step efficient.
- **Acceptance Criterion**
  - If $\Delta E \leq 0$, the flip is accepted unconditionally (the system moves to a lower or equal energy state).
  - If $\Delta E > 0$, the flip is accepted with probability $e^{-\beta \Delta E}$. This prevents the simulation from getting stuck at a local minimum and ensures correct sampling of higher energy states at finite temperatures.
- **Equilibration and Sampling**
  A user-specified number of spin-flip attempts is performed. After a sufficient number of iterations, the system typically reaches an equilibrium distribution from which energy and magnetisation can be measured

2.4. Parameter Selection

The following choices strike a balance between computational cost and capturing essential physics:

- **System Size (pre-specified)**
  - **1D**: 100 by default
  - **2D**: 100 x 100 grid by default
- **Monte Carlo Steps**
  - **1D**: 100,000 spin-flip allows for high statistical accuracy and reliable sampling.
  - **2D**: 1,000,000 attempts per configuration, this balances runtime with statistical accuracy on a 100×100 grid.
- **Number of Independent Configurations**
  Each run reinitialises the spins randomly, ensuring uncorrelated samples. The default is 1,000 configurations for 1D, this allows for a large number of configurations while also making sure the run time does not get too long. For 2D I use 100, this is

because it requires many more Monte Carlo steps so reducing the number of configurations helps to greatly reduce runtime

Range of β Values
The chosen set of β values {0.0, 0.1, 0.5, 1.0, 2.0, 5.0,10.0} spans from effectively infinite temperature (β =0), where all states are equally likely, to very low temperature (β =10), where the system heavily favours its ground states. Intermediate values allow for a gradual transition.

- **Parameters for distribution tests**
  - 1D Model
    - ***Beta*** = {0, 10}: two extreme values
    - ***num_configs*** = 10,000: high number of configs to have enough samples to check the theoretical distributions.
    - ***n_spins*** = 3: this is the number of spins provided in the example.
  - 2D Model
    - ***Beta*** = {0, 10}: two extreme values
    - ***num_configs*** = 10,000: high number of configs to have enough samples to check the theoretical distributions.
    - ***grid_size*** = 2: A small grid allows for an easier time calculating the theoretical distribution.

2.5 Version Control

2.5.1. Commits

The commit history is meticulously structured, each message has a summary line/title that gives an overview of what the commit includes. After this, the message includes all the details of what changes were made. Commits were made when some part of the project was completed or updated.

2.5.2. Branches

Branches were used strategically to manage different features and phases of development:

- **Feature Branches:** Separate branches were dedicated to the 1D and 2D implementations (feature/1D and feature/2D). This allowed isolated development and testing of each model without interference.
- **Integration Branch:** A branch named feature/integration was created to merge the separate implementations into a unified codebase. This branch was used to combine the unified main file, the consolidated analysis script, and to reorganise the file structure into a more maintainable format.

2.5.3. Tags

Tagging was employed to mark significant milestones and stable releases in the project:

- **Version Tags:** For example, tags such as v1.0, v0.2-2D, and v0.1-1D were applied to commits that represented major integration points or stable versions of either the 1D or 2D simulation code. These tags indicate that a particular commit meets the criteria for a complete, tested, and functional version.
- **Release Identification:** The use of tags allows for easy identification of which commit corresponds to a particular release or milestone, facilitating future reference and rollback if necessary.

3. Testing

3.1. 1D Testing

3.1.1. Theoretical Distribution

For a 1D chain of three spins ($s_1, s_2, s_3 \in \{+1, -1\}$) with nearest neighbour interactions and $J = 1$, the energy is given by:

$$E = -J(s_1 s_2 + s_2 s_3)$$

Where:

$$P(E_k) = \frac{e^{E\beta J}}{Z}$$

There are $2^3 = 8$ possible configurations:

Configuration	*Calculation*	*E*	*M*
(+1, +1, +1)	−[(+1)(+1)+(+1)(+1)]=−[1+1]=−2	-2	3
(+1, +1, -1)	−[(+1)(+1)+(+1)(−1)]=−[1−1]=0	0	1
(+1, -1, +1)	−[(+1)(−1)+(−1)(+1)]=−[−1−1]=+2	2	1
(+1, -1, -1)	−[(+1)(−1)+(−1)(−1)]=−[−1+1]=0	0	-1
(-1, +1, +1)	−[(−1)(+1)+(+1)(+1)]=−[−1+1]=0	0	1
(-1, +1, -1)	−[(−1)(+1)+(+1)(−1)]=−[−1−1]=+2	2	-1
(-1, -1, +1)	−[(−1)(−1)+(−1)(+1)]=−[+1−1]=0	0	-1
(-1, -1, -1)	−[(−1)(−1)+(−1)(−1)]=−[+1+1]=−2	-2	-3

When β = 0, all states and configurations are equally likely hence:

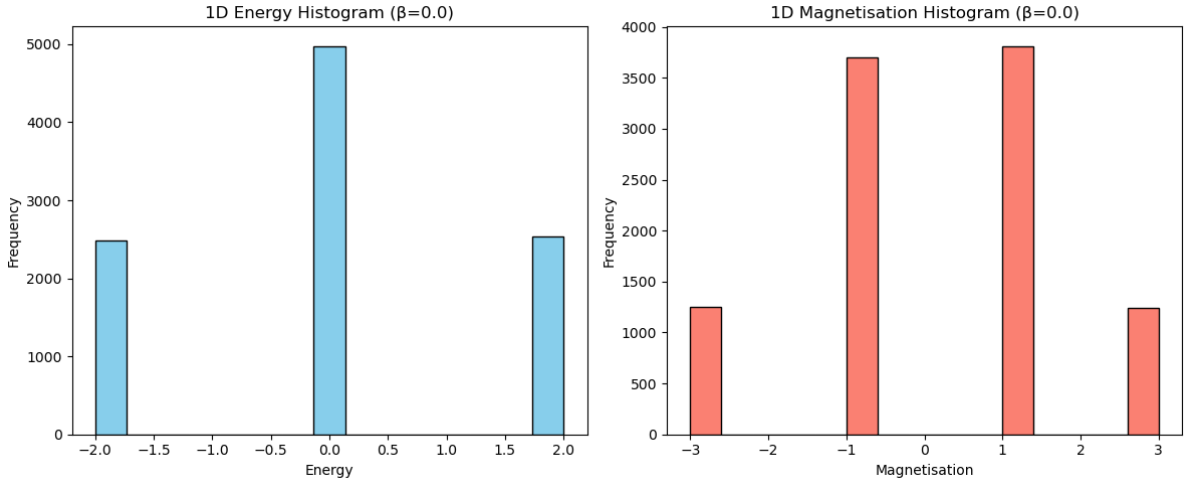
- $P(E = -2) = \frac{2}{8}$ = 25%
- $P(E = -2) = \frac{4}{8}$ = 50%
- $P(E = -2) = \frac{2}{8}$ = 25%

When β = 10 (low temperature):

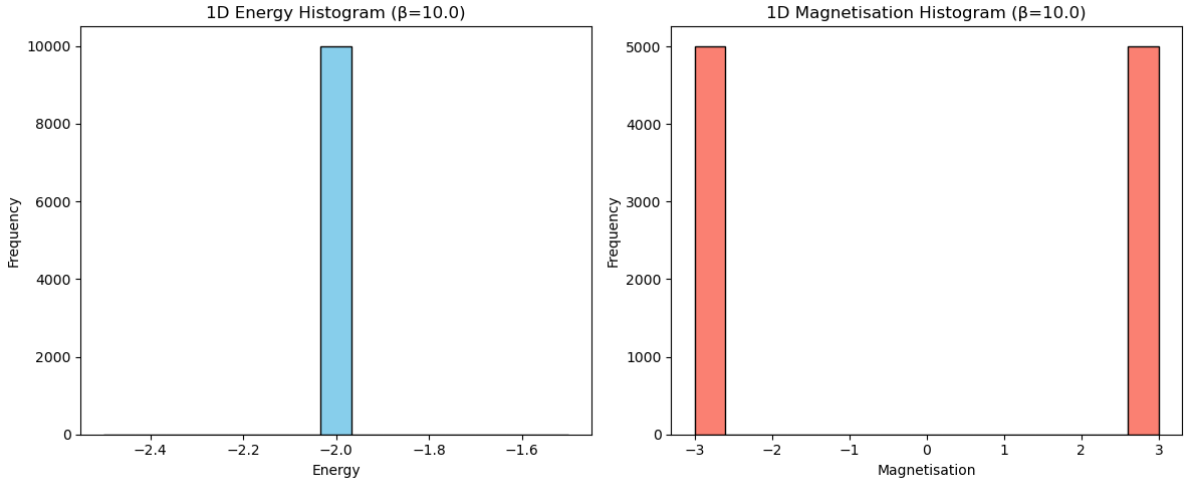
- For $E = -2$: $e^{-10(-2)} = e^{20}$ (very large)
- For $E = 0$: e^0 = 1
- For $E = 2$: $e^{-10(2)} = e^{-20}$ (very small)

Here we see its very concentrated around -2

3.1.2. Distribution from Results



- We can see here that -2 and 2 have a frequency of around 2500 and 0 has a frequency of 5000. This follows the theoretical distribution.



- We can see here that -2 has a frequency of around 10,000 (total number of configurations) this is in line with the theoretical distribution.

3.2. 2D Testing

3.2.1. Theoretical Distribution

For a 2×2 grid with open boundaries, the energy is computed by summing interactions over horizontal and vertical bonds. There are 4 bonds in total (2 horizontal and 2 vertical). The energy is given by:

$$E = -J\left(s_{11}s_{12} + s_{21}s_{22} + s_{11}s_{21} + s_{12}s_{22}\right)$$

With $J = 1$.

By enumerating all $2^4 = 16$ configurations, one finds:

- $\boldsymbol{E = -4}$**:** Occurs when all spins are aligned (all +1+1+1 or all −1-1−1), there are 2 configurations.
- $\boldsymbol{E = +4}$**:** Occurs in 2 configurations (when spins are arranged diagonally, leading to all bonds contributing unfavourably).
- $\boldsymbol{E = 0}$**:** Occurs in 12 configurations.

Hence, at β = 0:

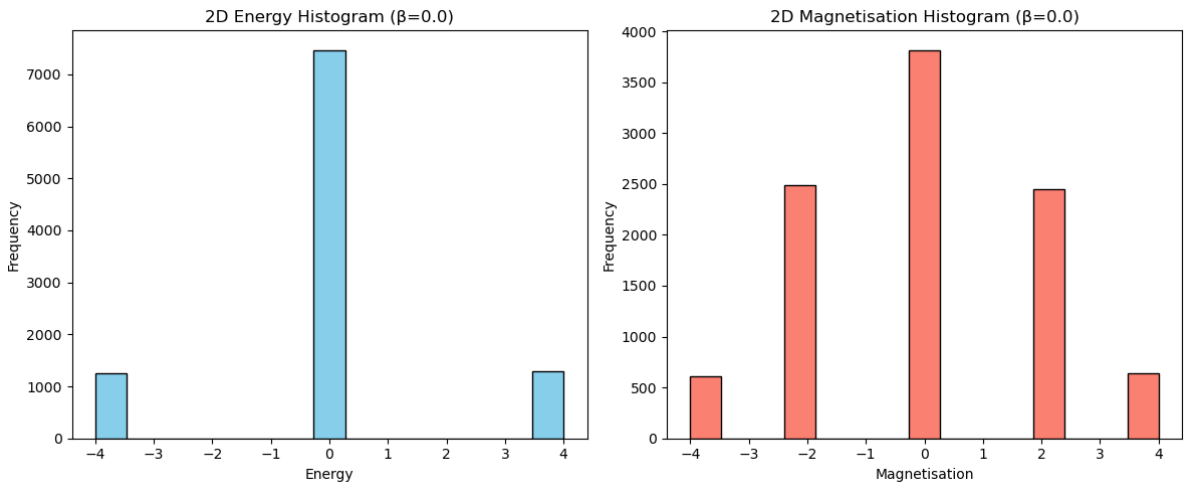
- $P(E = -4) = \frac{2}{16} = 12.5\%$
- $P(E = 0) = \frac{12}{16} = 75\%$
- $P(E = +4) = \frac{2}{16} = 12.5\%$

For β = 10:

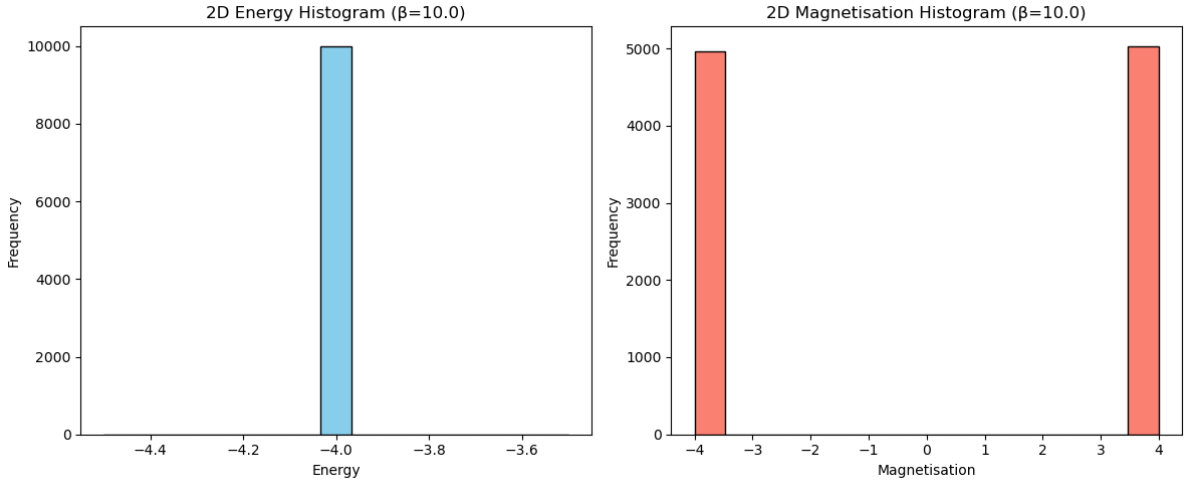
- For $E = -4$: $e^{-10(-4)} = e^{40}$ (very large)
- For $E = 0$: e^0 = 1
- For $E = 4$: $e^{-10(4)} = e^{-40}$ (very small)

At low temperatures, the system is overwhelmingly driven to the lowest energy state $(E = -4)$. As a result, nearly all samples will have $E = -4$, corresponding to either the all up or all down configuration.

3.2.2. Distribution from Results



- We can see here that -4 and 4 have a frequency of around 1250 and 0 has a frequency of 7500. This follows the theoretical distribution.



- We can see here that -4 has a frequency of around 10,000 (total number of configurations) this is in line with the theoretical distribution.

3.3. Other Testing

```
=== 1D TESTING MODE ===
State: +++
Energy: -2  Magnetisation: 3
------------------
State: ++-
Energy: 0  Magnetisation: 1
------------------
State: +-+
Energy: 2  Magnetisation: 1
------------------
State: +--
Energy: 0  Magnetisation: -1
------------------
State: -++
Energy: 0  Magnetisation: 1
------------------
State: -+-
Energy: 2  Magnetisation: -1
------------------
State: --+
Energy: 0  Magnetisation: -1
------------------
State: ---
Energy: -2  Magnetisation: -3
------------------
```

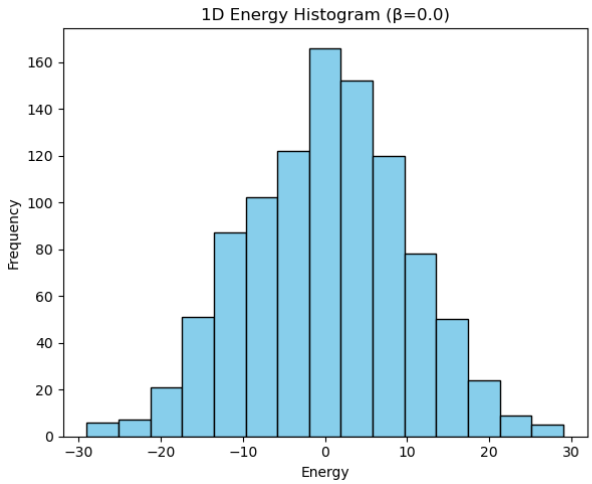
```
=== 2D TESTING MODE ===
+ +
+ +
Expected Energy: -4
Energy: -4  Magnetisation: 4
------------------
+ -
- +
Expected Energy: 4
Energy: 4  Magnetisation: 0
------------------
+ +
+ -
Expected Energy: 0
Energy: 0  Magnetisation: 2
------------------
+ + +
+ + -
+ + +
Expected Energy: -6
Energy: -6  Magnetisation: 7
------------------
+ + +
+ + +
+ + +
Expected Energy: -12
Energy: -12  Magnetisation: 9
------------------
+ - +
- + -
+ - +
Expected Energy: 12
Energy: 12  Magnetisation: 1
------------------
```

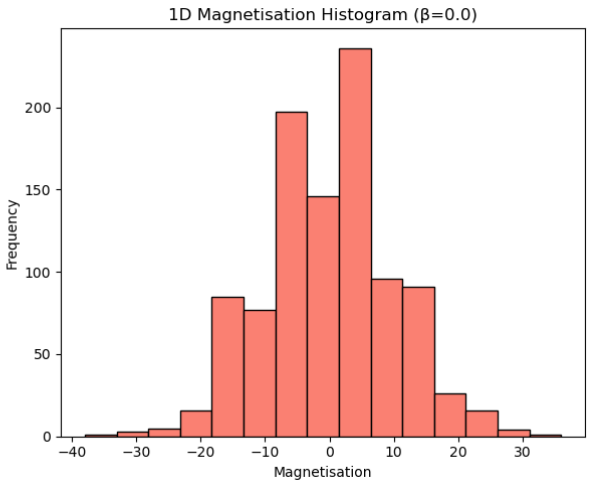
- We can see here that the energy and magnetisation calculations for all tests are correct.

4. Results and Analysis

4.1. 1D

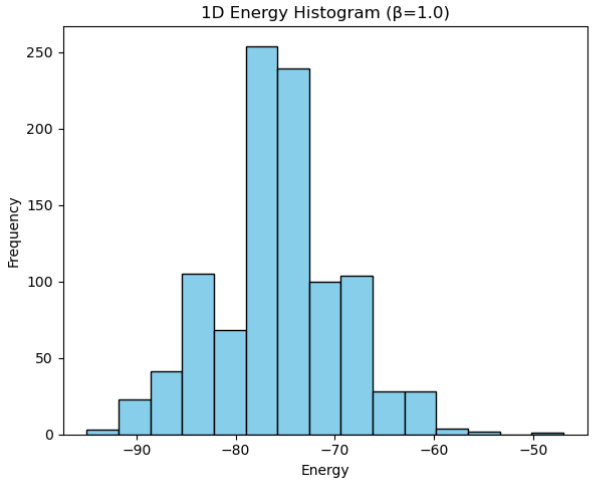
4.1.1 Analysing Histograms[1]

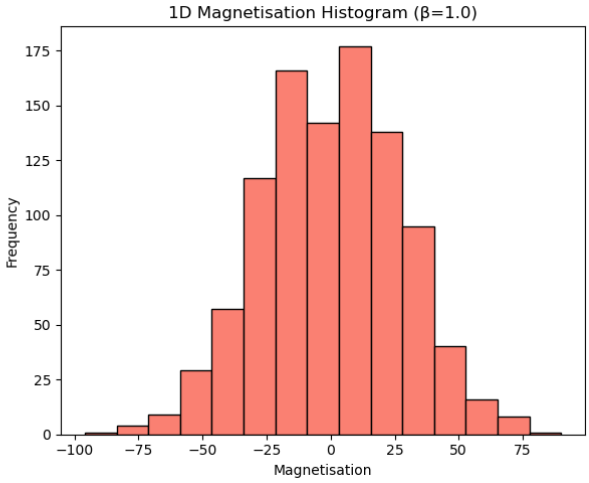




β=0.0 (High Temperature)

- **Energy:** The histogram is relatively broad and centred at higher (less negative) energies, reflecting the fact that all spin configurations are equally likely.
- **Magnetisation:** The distribution is centred near zero, indicating that spins are roughly as likely to be up as down. No strong bias toward alignment is press.

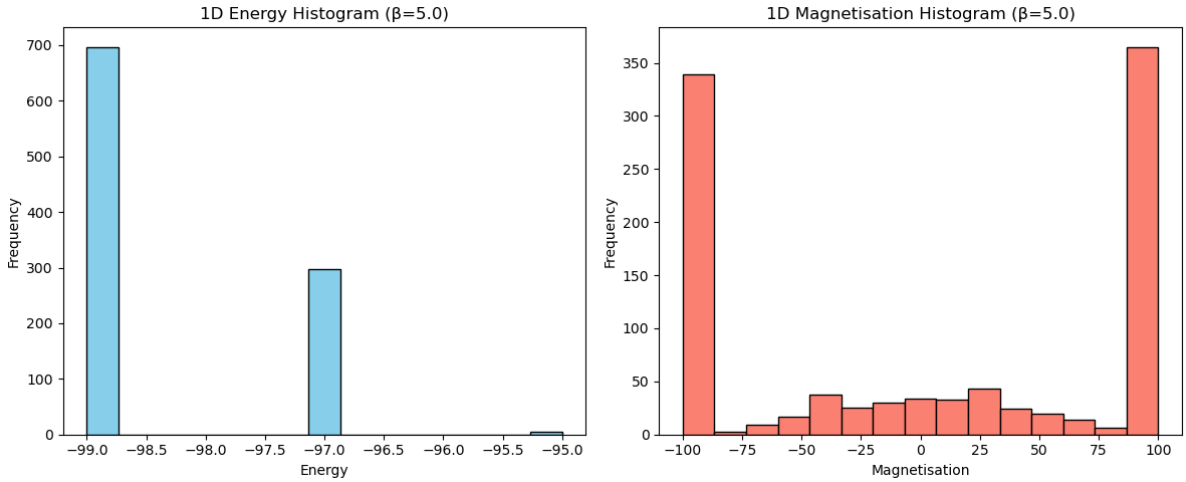




β = 1.0

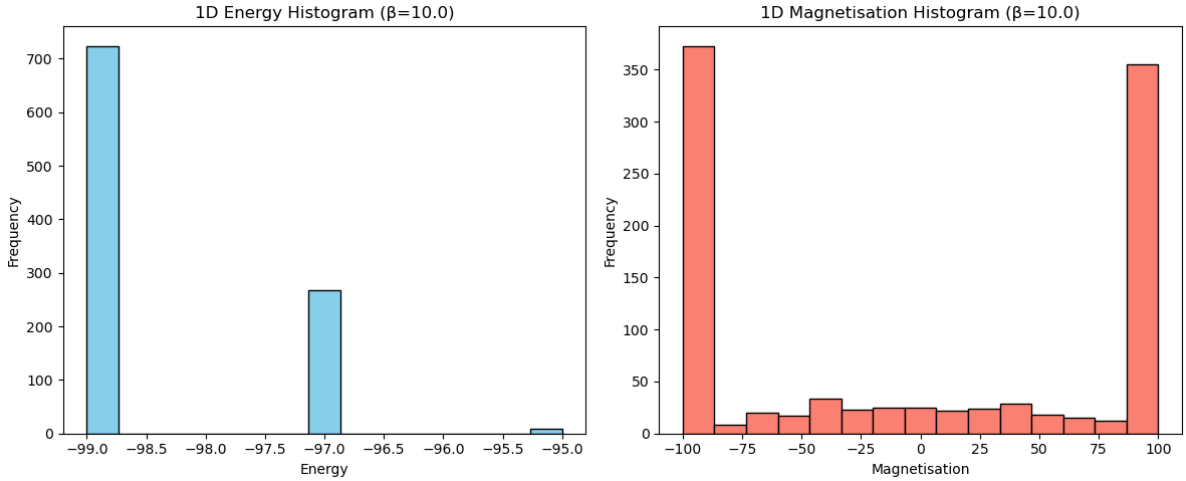
- **Energy:** The distribution shifts further into negative territory. You can see a more pronounced peak, indicating that many spins are aligning, but the system still samples a range of energies.
- **Magnetisation:** The histogram remains somewhat broad but begins showing more weight at nonzero magnetisations.

[1] I know these are not necessary, but I have included them as I believe they nicely show the effect of temperature on the values of energy and magnetisation. Also note that both 1D and 2D have more histograms that are shown in the appendix as adding all of them would have added unnecessary complexity and length to the main analysis.



β = 5.0

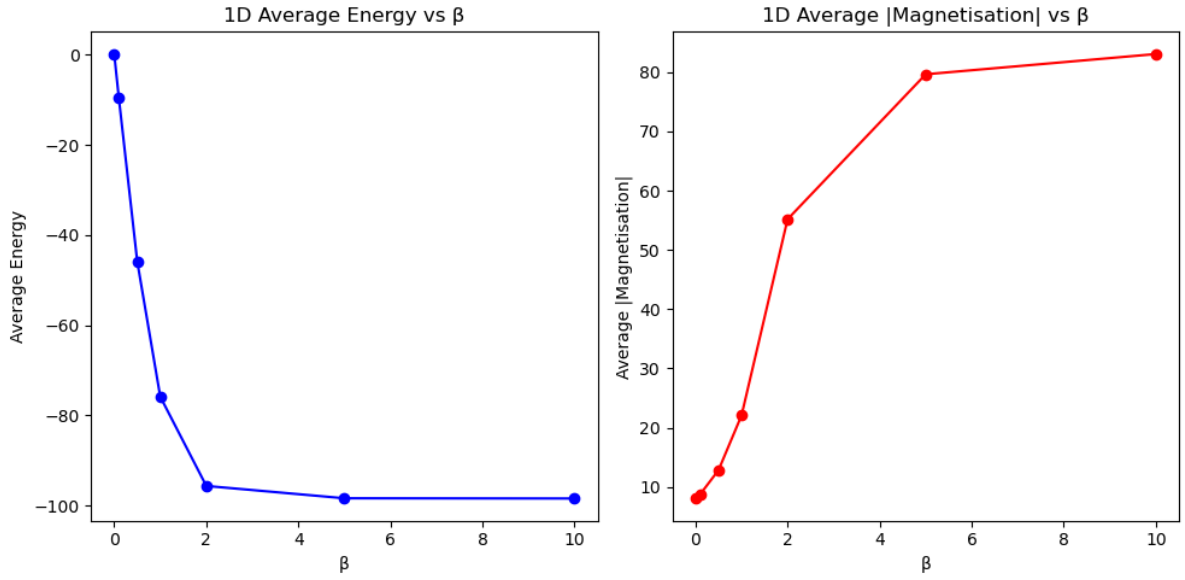
- **Energy:** Only a couple of bins dominate, suggesting the system is now almost locked into near-ground-state configurations.
- **Magnetisation:** A large fraction of states cluster around ±100, meaning the chain is often fully (or almost fully) magnetised.



β = 10.0 (Low Temperature)

- **Energy:** The histogram is almost entirely concentrated in a couple bins at the lowest energies. The system is effectively in a ground state with minimal energy.
- **Magnetisation:** Correspondingly, you see large peaks near ±100. If the chain falls into all up or all down, it typically remains there. Very small amount of not fully aligned spins.

4.1.2. Average Energy and Magnetisation vs β



Average Energy vs. $\boldsymbol{\beta}$:

- Starts at a relatively high value near $\boldsymbol{\beta}$ =0.
- Decreases sharply from $\boldsymbol{\beta}$ = 0 to $\boldsymbol{\beta} = \mathbf{1}$, indicating a growing tendency for spins to align. Decreases more gradually from 1 to 5
- Approaches a minimum near $\boldsymbol{\beta} = \mathbf{5}$ as there Is not much change from this point onwards, indicating the system has effectively settled into a ground state.

Average |Magnetisation| vs. $\boldsymbol{\beta}$:

- Near zero at $\boldsymbol{\beta} = \mathbf{0}$, reflecting the random, disordered phase.
- Sharp increase from 0 to 2.
- From $\boldsymbol{\beta}$ = 2 to $\boldsymbol{\beta} = \mathbf{10}$ the increase is very gradual. From 5 to 10 is where the chain seems to be almost fully aligned with either +1 or -1 spins as the increase here is fairly minimal

4.1.3. Linking to Theoretical Distribution

High Temperature ($\boldsymbol{\beta} = \mathbf{0}$)

- Observed Behaviour:
  - Average Energy is around 0, reflecting the random distribution of spins.
  - Average |M| is near zero, indicating no net alignment.
- Theoretical Expectation:
  - All states are equally likely at infinite temperature, producing broad energy histograms cantered around intermediate values and magnetisation histograms peaking near zero.

Intermediate $\boldsymbol{\beta}$ (0.1 to 2.0)

- Observed Behaviour:
  - Average Energy drops sharply from $\boldsymbol{\beta}$ = 0 to $\boldsymbol{\beta}$ = 1, then more gradually toward $\boldsymbol{\beta}$ = 5.
  - Average |M| rises quickly from near zero up to moderate values.
- Theoretical Expectation:
  As temperature decreases, flips that lower energy are increasingly favoured. Energy

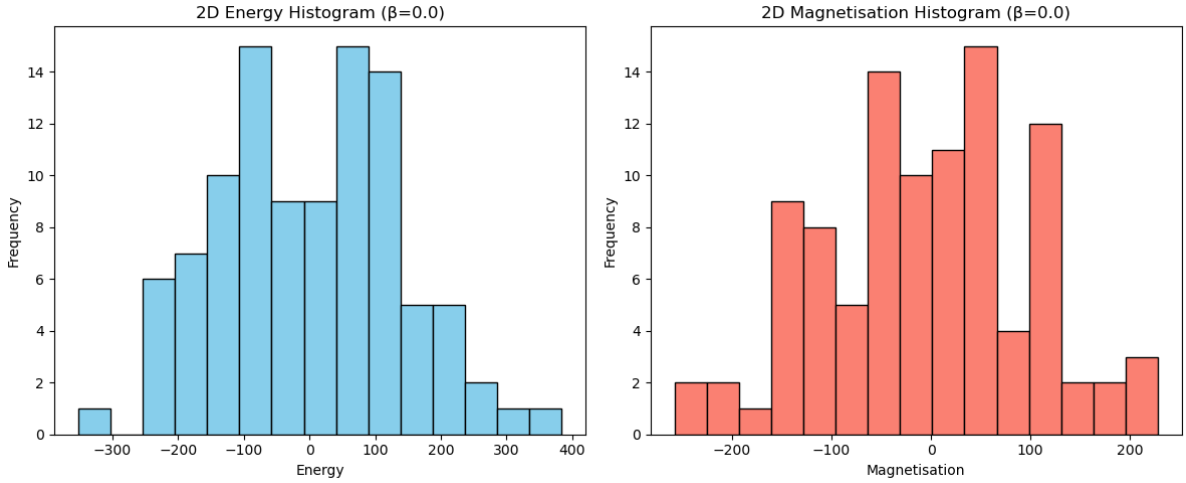
histograms become more skewed toward negative values, and magnetisation histograms shift away from zero, indicating partial alignment of spins.

Low Temperature ($\beta \geq 5$)

- Observed Behaviour:
  - Average Energy levels out near its minimum, showing that the system is close to a ground state.
  - Average |M| approaches its maximum (near ±100 for a 100-spin chain), signifying near-complete alignment.
- Theoretical Expectation:
  At low temperatures, thermal fluctuations are minimal. The energy histogram collapses around the ground state, and the magnetisation histogram shows peaks at ±N, confirming that spins are locked into fully aligned configurations.

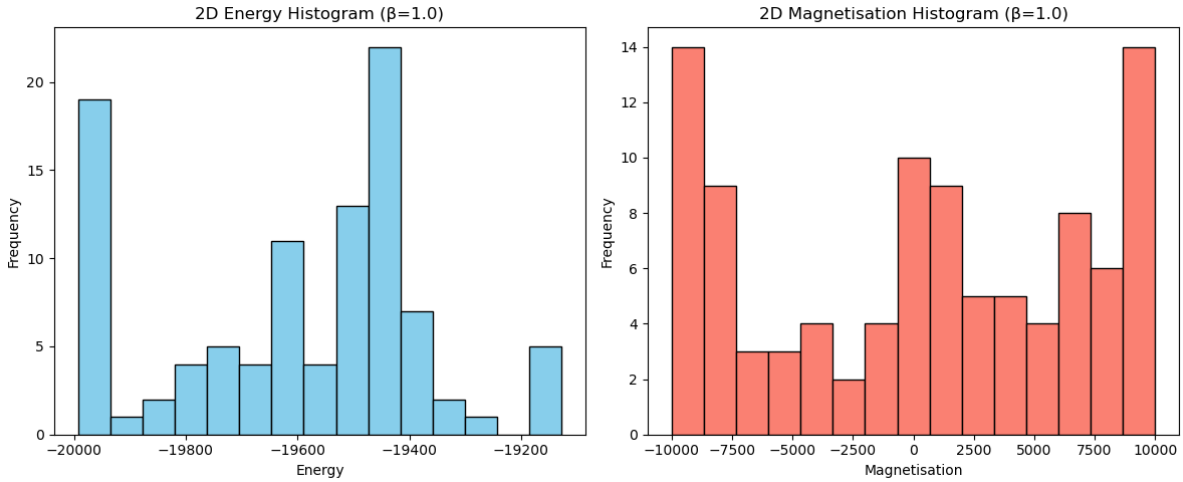
4.2. 2D

4.2.1 Analysing Histograms



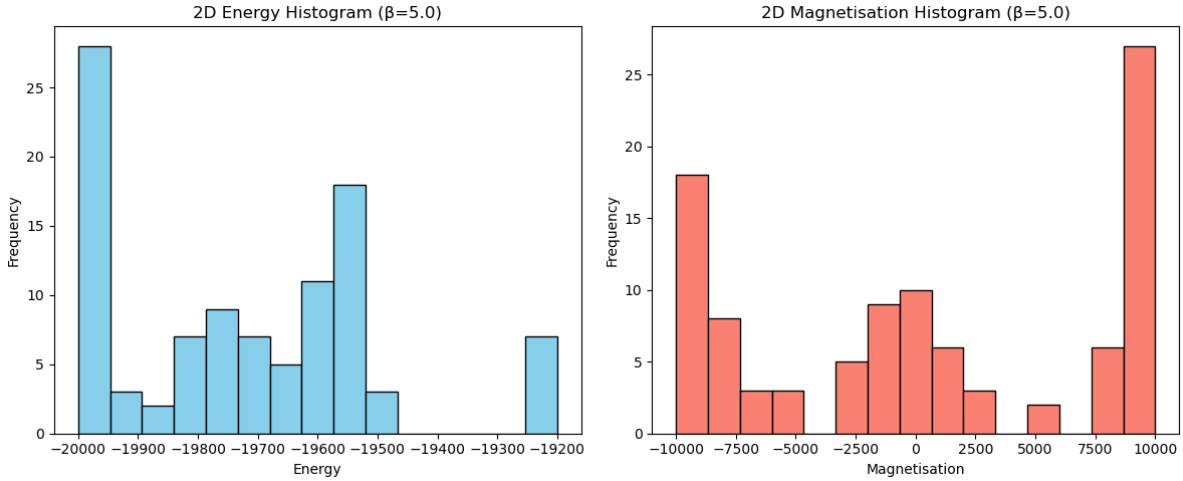
β =0.0 (High Temperature)

- **Energy:** The histogram is relatively broad and centred at around 0. β = 0 corresponds to infinite temperature in theory, all configurations are nearly equally likely, so the system's energy distribution reflects that randomness.
- **Magnetisation:** The distribution is wide and centred close to zero, consistent with the idea that there is no preference for up or down spins when all states are equally likely. In a large 2D grid, random fluctuations still average out to near zero net magnetisation.



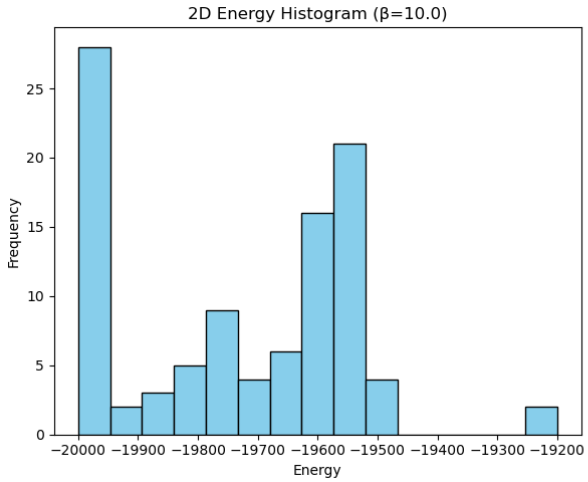
β =1.0

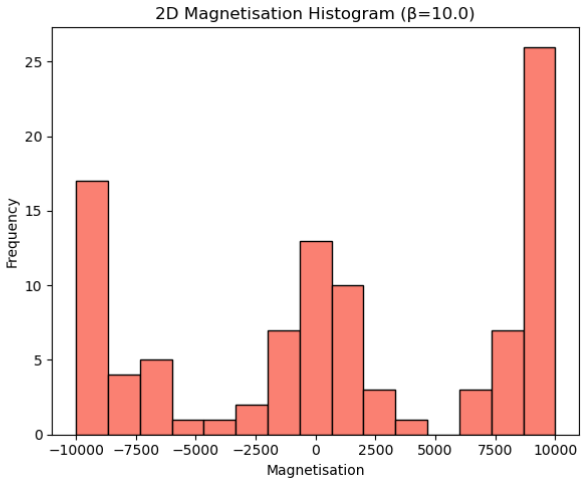
- **Energy:** The peak moves far left, indicating that the system is adopting more energetically favourable (aligned) configurations. While not fully locked into a single ground state, there is a clear preference for lower energy states.
- **Magnetisation:** The distribution becomes less bell shaped and more concentrated around the extremities.



β = 5.0

- **Energy:** The histogram has stayed within the same range however more configurations have clustered at the extremity indicating more systems are favouring full alignment.
- **Magnetisation:** There are more configurations clustering at the extremities, there also seems to be some asymmetry between the extremities likely due to the small number of configurations.

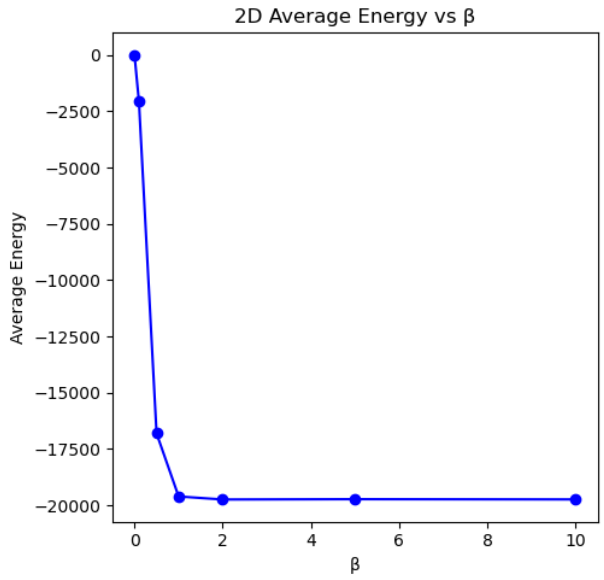


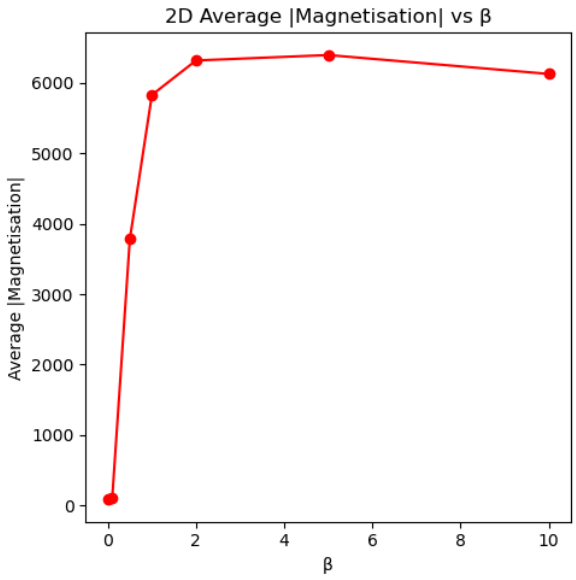


β = 10.0

- **Energy:** Little change from before.
- **Magnetisation:** Again, very little change from before.

4.2.2. Average Energy and Magnetisation vs β





- **Average Energy:**
  - Starts at 0 for $\boldsymbol{\beta}$ =0.
  - Plummets rapidly by $\boldsymbol{\beta} = \mathbf{1}$, reflecting the system's transition to more ordered configurations.
  - Levels off around $\boldsymbol{\beta}$ = 2 in a very negative range, indicating that almost all spins are aligned, minimising energy. This trend is far more pronounced than 1D.
- **Average |Magnetisation|:**
  - Begins near zero at $\boldsymbol{\beta}$ =0, consistent with a disordered state.
  - Rises sharply until $\boldsymbol{\beta} = \mathbf{1}$ showing that a large amount of spin alignment occurs early.
  - Seems to be about level from $\boldsymbol{\beta}$ = 2 onwards. Again, this is similar to 1D just far more dramatic.

4.2.3. Linking to Theoretical Distribution

High Temperature ($\beta = 0$)

- **Observed Behaviour**
    - Average energy is around 0, reflecting the random arrangement of spins.
    - Average |M| is also around 0, indicating no net alignment in a disordered phase.
- **Theoretical Expectation:**
  At infinite temperature, the system freely samples many configurations, resulting in near-zero magnetisation and broad energy histograms.

Moderate Temperatures to Low Temperatures ($\beta \geq 1$)

- **Observed Behaviour:**
    - The average energy plummets, showing that the grid quickly tends to lower-energy (more aligned) states, from the histograms we can also see we cluster around the most negative values.
    - |M| rises sharply, signalling that spins favour alignment rather than remaining random, from the histogram we can also see we cluster around the extremities.
- **Theoretical Expectation:**
  As β grows, thermal fluctuations become less dominant, favouring configurations that minimise energy. The system transitions rapidly toward a partially ordered state. The histograms are also in line with the theoretical expectation.

Comparison to 1D

The transition from disordered to ordered is **more pronounced** in 2D because each spin has more neighbours. Once the system starts to favour aligned configurations, energy and magnetisation shift dramatically over a relatively small range of β. In contrast, the 1D chain shows a somewhat smoother change. Both 1D and 2D models follow the same trend: at high temperature, spins are disordered, while at low temperature, spins align, minimising energy and maximising magnetisation.

5. Conclusion

This project developed a Monte Carlo simulation of the Ising model in both one and two dimensions, using object-oriented C++ to investigate how the inverse temperature ($\boldsymbol{\beta}$) influences the system's energy (E) and magnetisation (M). At high temperatures ($\boldsymbol{\beta} \approx 0$), random spin orientations dominate, leading to broad energy distributions and near-zero net magnetisation. As $\boldsymbol{\beta}$ grows, spins increasingly align, driving the energy distribution toward more negative values and shifting magnetisation away from zero.

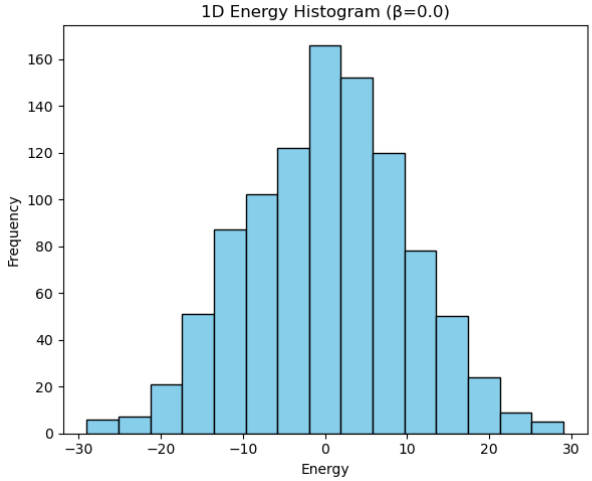
In the **1D** case, this ordering occurs relatively fast: once $\boldsymbol{\beta}$ reaches moderate values (around 2–5), the chain already shows substantial alignment, and by $\boldsymbol{\beta}$ =10, it is almost fully ordered. The energy histogram collapses near the ground state, and magnetisation peaks at ±N, matching the theoretical expectation that low-temperature fluctuations are negligible and the system locks into either the all-up or all-down state.

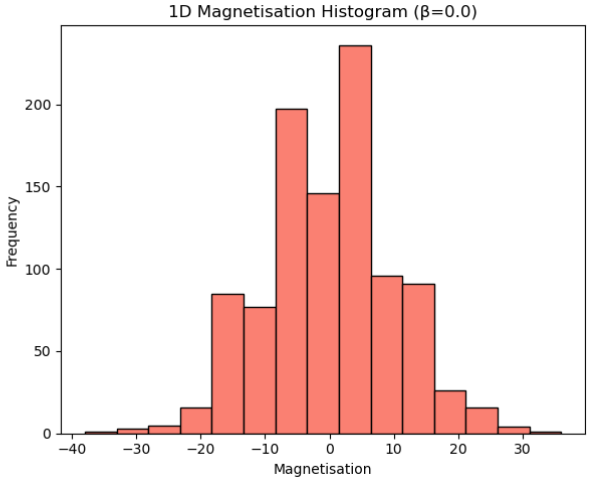
In **2D**, a similar progression is observed but with more dramatic changes over a slightly broader range of $\boldsymbol{\beta}$. The additional nearest-neighbour interactions speed up the shift toward aligned configurations. By $\boldsymbol{\beta}$ = 2 there is little change going forward in the average magnetisation. If it were possible to run more Monte Carlo steps we would likely see the histogram look exactly the same as the 1D.

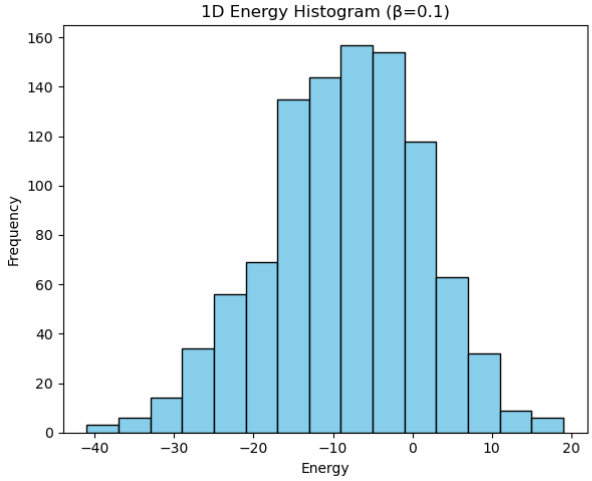
Overall, these results confirm that increasing $\boldsymbol{\beta}$ (decreasing temperature) systematically lowers the system's energy and raises its net magnetisation in both 1D and 2D, in agreement with theoretical expectations for the Ising model.

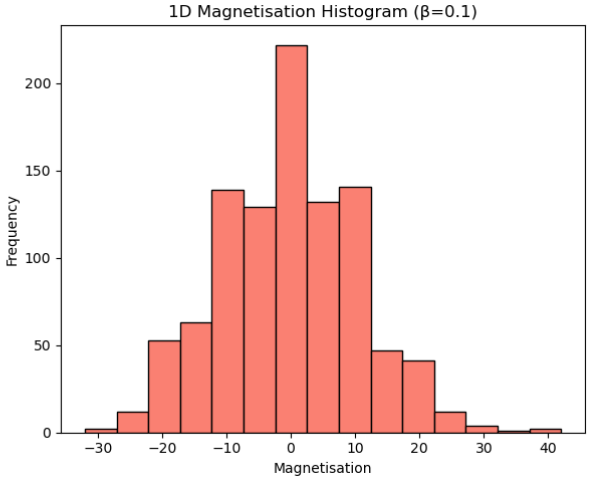
Appendix

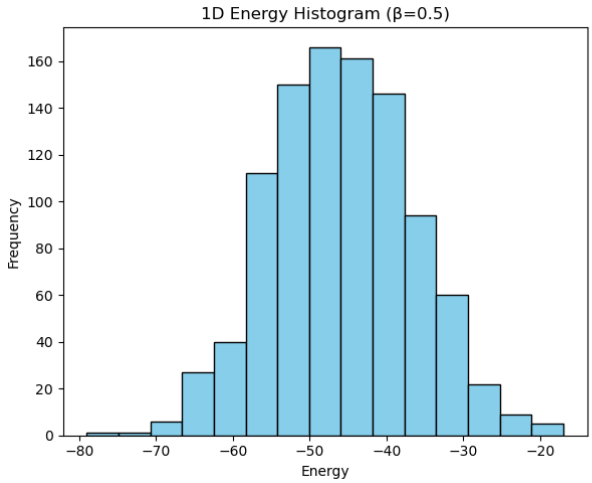
1D Histograms

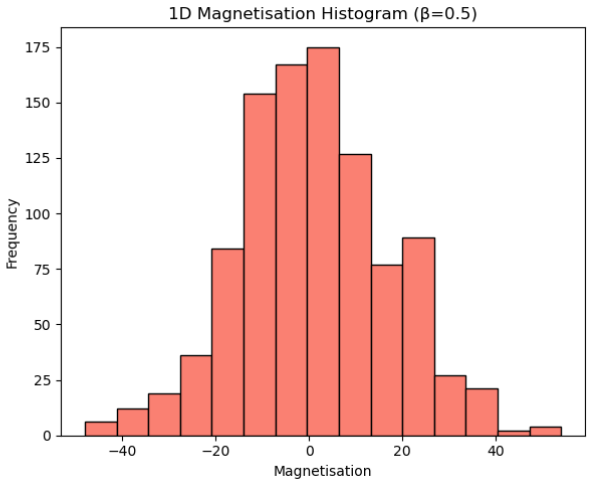


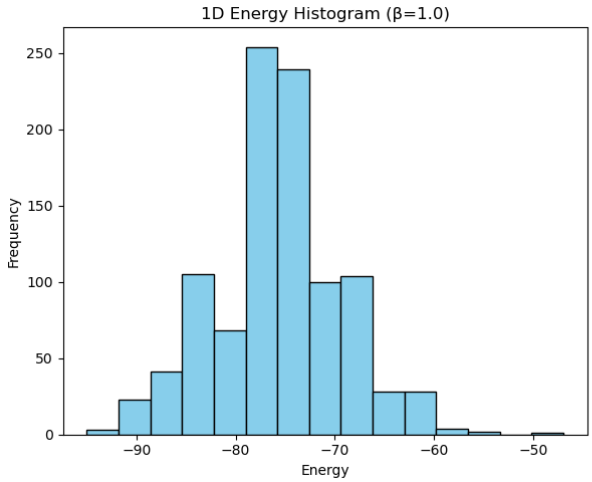


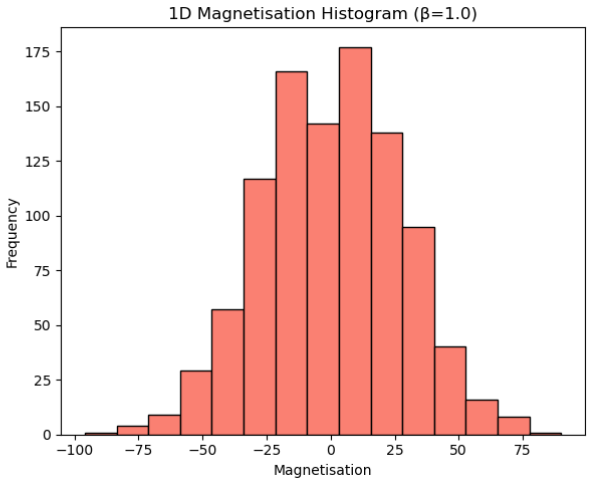


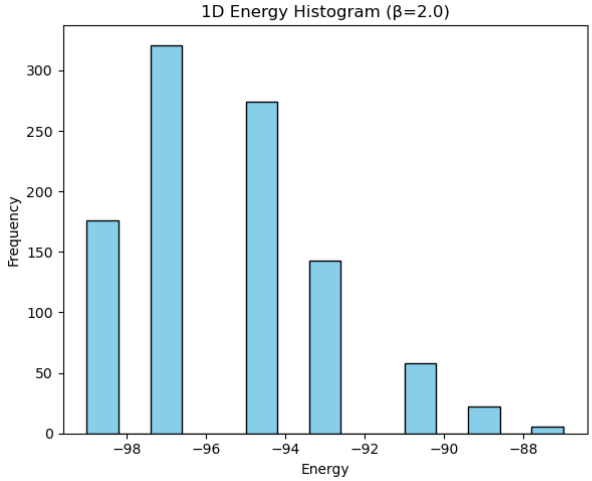


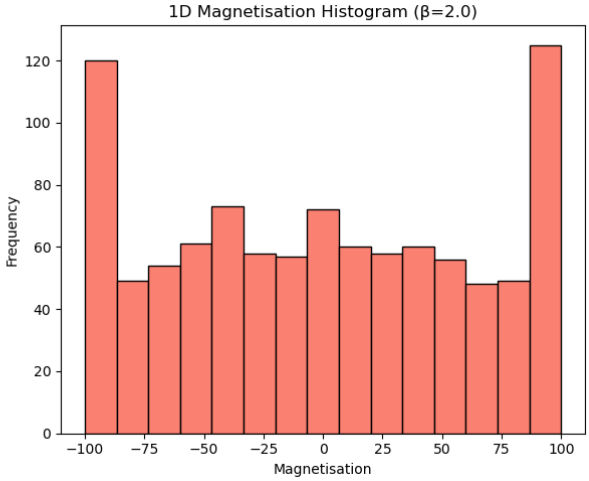


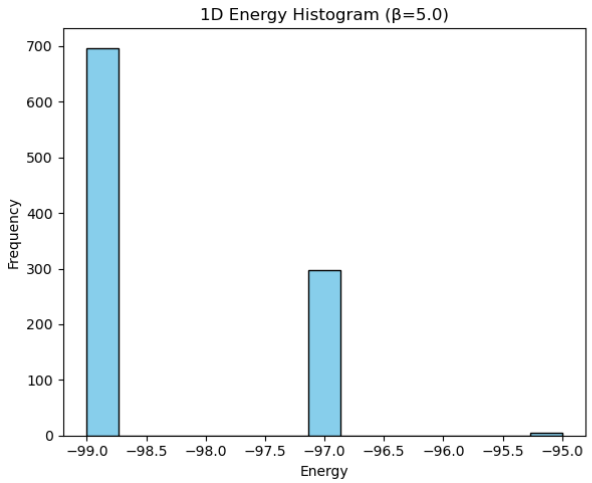


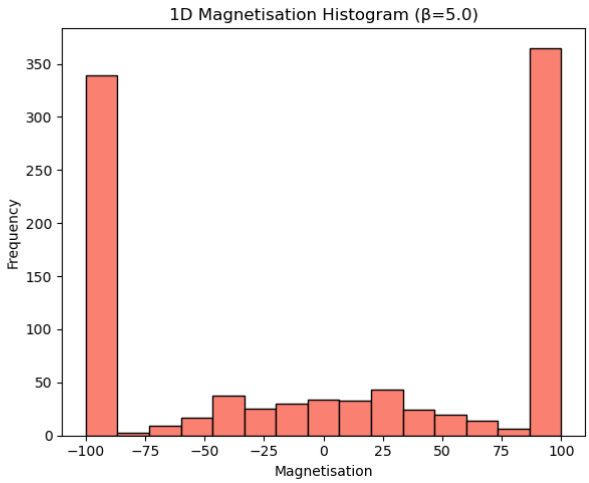

1D Energy Histogram (β=1.0)
Frequency
Energy
250
200
150
100
50
0
−90
−80
−70
−60
−50

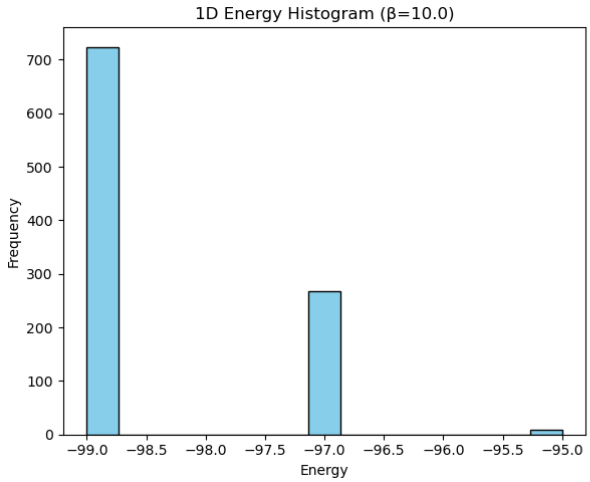

1D Magnetisation Histogram (β=1.0)
Frequency
Magnetisation
175
150
125
100
75
50
25
0
−100
−75
−50
−25
0
25
50
75

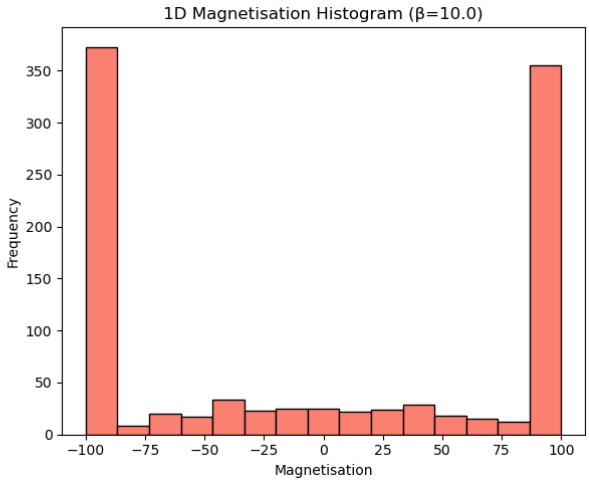

1D Energy Histogram (β=2.0)
Frequency
Energy
300
250
200
150
100
50
0
−98
−96
−94
−92
−90
−88


1D Magnetisation Histogram (β=2.0)
Frequency
Magnetisation
120
100
80
60
40
20
0
−100
−75
−50
−25
0
25
50
75
100

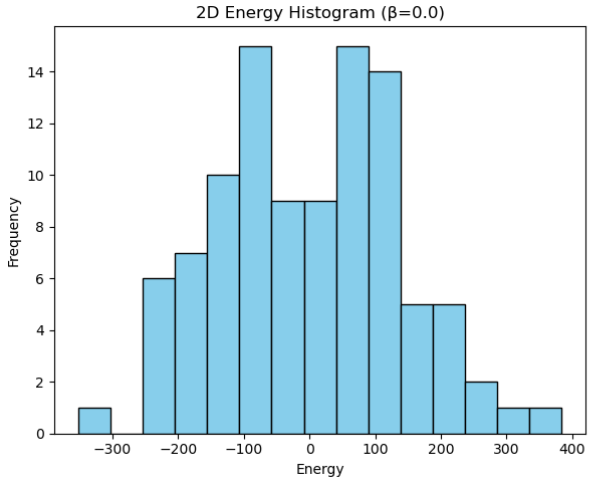

1D Energy Histogram (β=5.0)
Frequency
Energy
700
600
500
400
300
200
100
0
−99.0
−98.5
−98.0
−97.5
−97.0
−96.5
−96.0
−95.5
−95.0

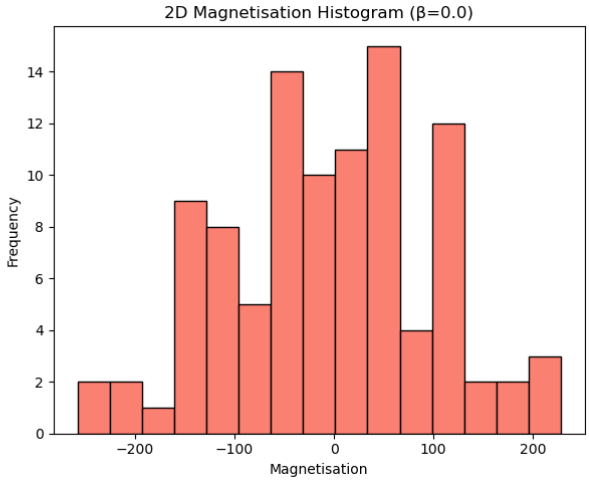

1D Magnetisation Histogram (β=5.0)
Frequency
Magnetisation
350
300
250
200
150
100
50
0
−100
−75
−50
−25
0
25
50
75
100

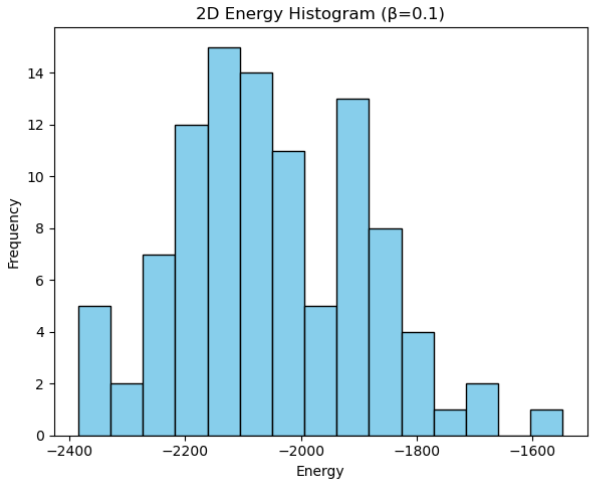


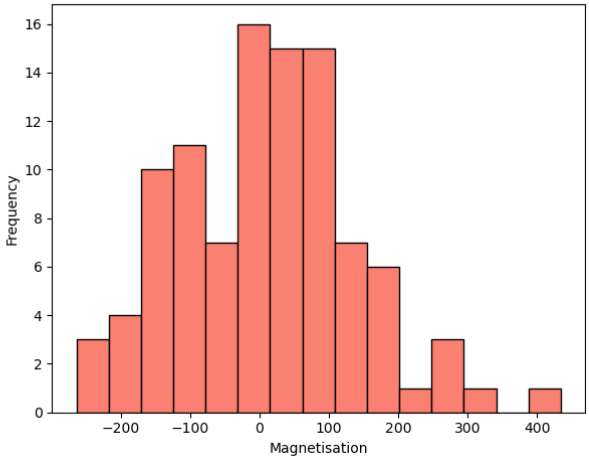


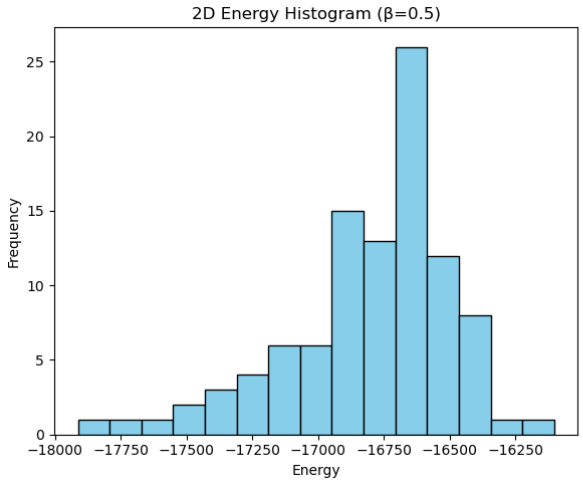
2D Histograms

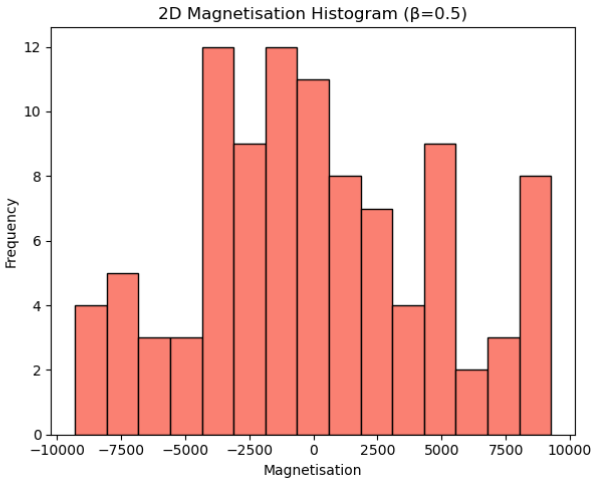


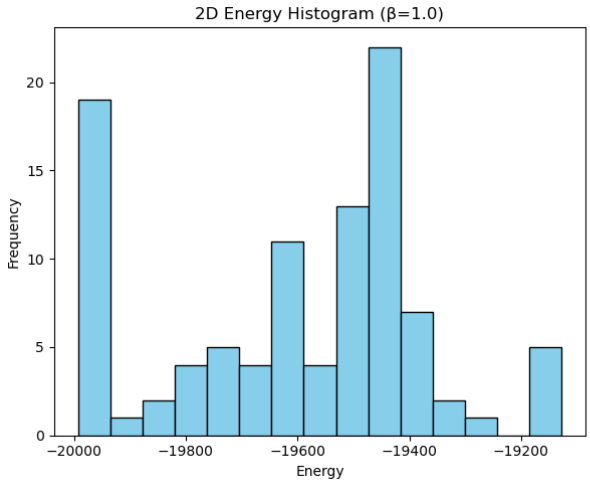


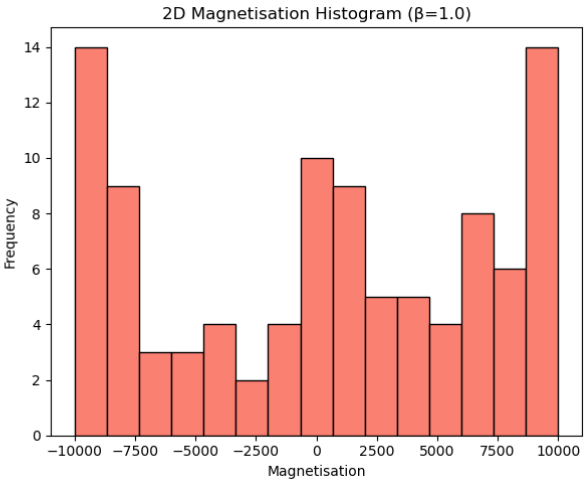


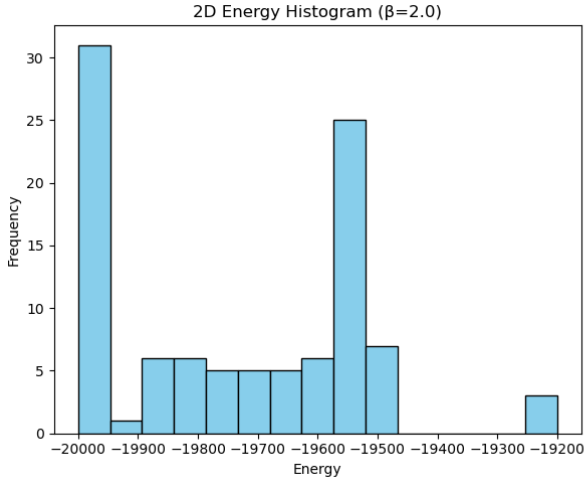


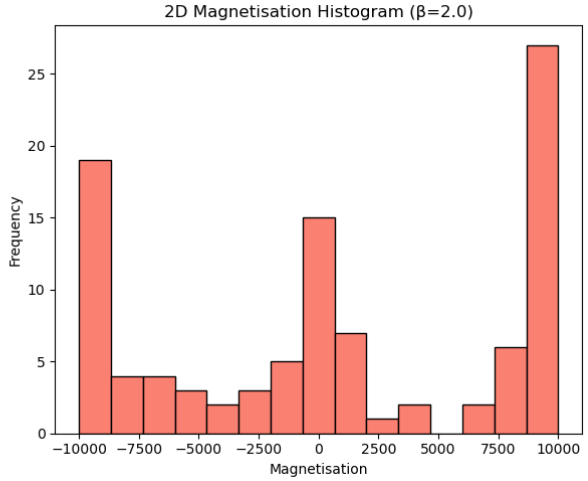

2D Energy Histogram (β=0.5)
Frequency
Energy
0
5
10
15
20
25
−18000
−17750
−17500
−17250
−17000
−16750
−16500
−16250

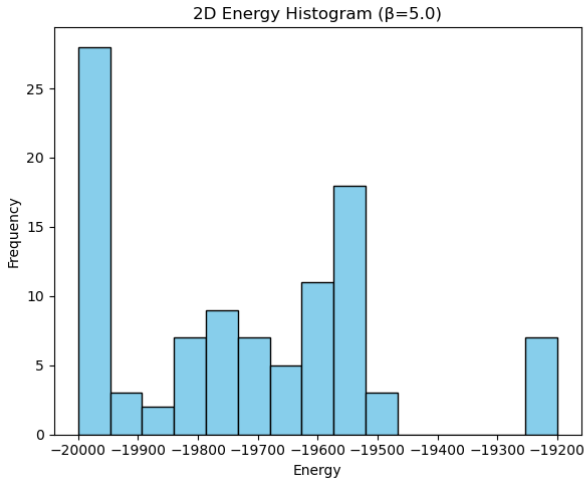

2D Magnetisation Histogram (β=0.5)
Frequency
Magnetisation
0
2
4
6
8
10
12
−10000
−7500
−5000
−2500
0
2500
5000
7500
10000

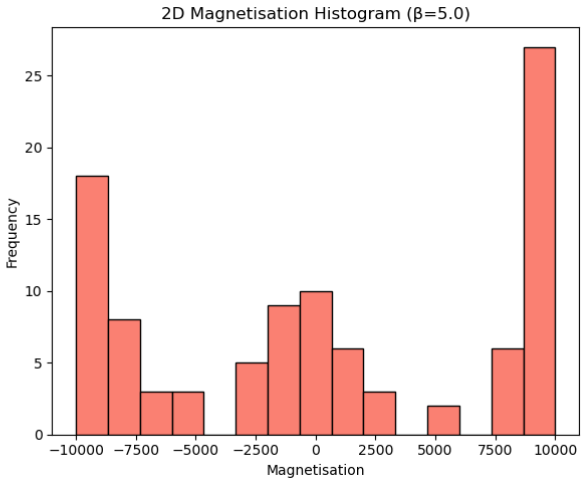

2D Energy Histogram (β=1.0)
Frequency
Energy
0
5
10
15
20
−20000
−19800
−19600
−19400
−19200

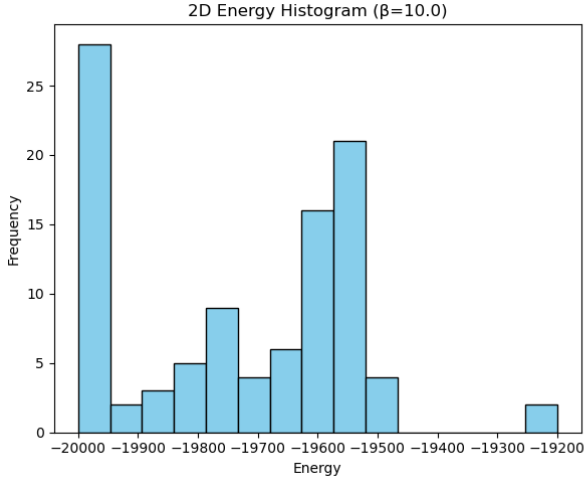

2D Magnetisation Histogram (β=1.0)
Frequency
Magnetisation
0
2
4
6
8
10
12
14
−10000
−7500
−5000
−2500
0
2500
5000
7500
10000

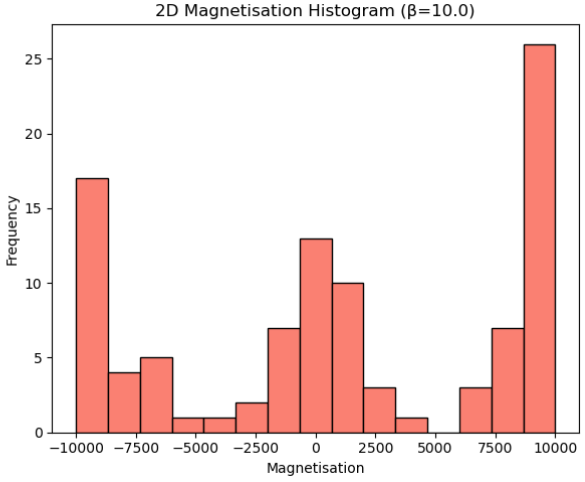

2D Energy Histogram (β=2.0)
Frequency
Energy
0
5
10
15
20
25
30
−20000
−19900
−19800
−19700
−19600
−19500
−19400
−19300
−19200


2D Magnetisation Histogram (β=2.0)
Frequency
Magnetisation
0
5
10
15
20
25
−10000
−7500
−5000
−2500
0
2500
5000
7500
10000


2D Energy Histogram (β=5.0)
Frequency
Energy
0
5
10
15
20
25
−20000
−19900
−19800
−19700
−19600
−19500
−19400
−19300
−19200


2D Magnetisation Histogram (β=5.0)
Frequency
Magnetisation
0
5
10
15
20
25
−10000
−7500
−5000
−2500
0
2500
5000
7500
10000


2D Energy Histogram (β=10.0)
Frequency
Energy
0
5
10
15
20
25
−20000
−19900
−19800
−19700
−19600
−19500
−19400
−19300
−19200


2D Magnetisation Histogram (β=10.0)
Frequency
Magnetisation
0
5
10
15
20
25
−10000
−7500
−5000
−2500
0
2500
5000
7500
10000