Thermodynamic simulations using the Ising Model

Project B4 – Computational Physics

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Abstract

The behaviour of the Ising model over a 25x25 square array was investigated using a Monte Carlo method. Energy, magnetisation, specific heat capacity and magnetic susceptibility were measured for several cases: varying temperature with no field, low positive, and low negative field; and varying field with low and high temperature. In the case of varying temperature, a critical temperature T_c was found, indicating a phase transition. In the case of varying field, two critical fields B_c were found, depending on the direction of variation.

Theory

The Ising model aims to simulate the behaviour of a magnetic material. In the 2D case, a square array of spins is considered. The spins can either be up or down, and in the simple case, as this investigation, only interactions between directly neighbouring spins are counted. The energy of the system is given by these neighbouring interactions and the interaction between the spins and an external magnetic field:

$$E = -\frac{1}{2}\sum_{i,j} \boldsymbol{J}_{ij}\boldsymbol{S}_i \cdot \boldsymbol{S}_j - \mu \sum_k \boldsymbol{S}_k \cdot \boldsymbol{B}$$

$\boldsymbol{J}_{ij} = J$ for neighbouring spins, and 0 otherwise. The factor of $\frac{1}{2}$ is to avoid double-counting.

A system will always tend to minimise the total E, so for a ferromagnetic material (that is, one with $J > 0$), the most favourable state has all spins aligned.

Let us consider the calculation of an observable, say the average energy, from this model.

$$\langle E \rangle = \sum_n E(n) P(n)$$

It is the sum over every state of the energy of that state, multiplied by the probability of the system being in that state – the state's Boltzmann factor:

$$P_n = \frac{1}{Z} e^{-E(n)/k_b T}$$, where Z is the partition function.

The rest of this report will use the symbol β to mean $\frac{J}{k_B T}$.

If each spin has two states, a system of N spins has 2^N states – even a tiny 5-sided array has a total of 33,554,432 possible configurations. Hence it can be seen that the consideration of every state quickly becomes computationally intractable.

This problem is solved by taking a sampling of these states. One could sample many states and then weight them by their Boltzmann factors, but a great deal of time would be wasted on calculations for states contributing very little to the result. An alternative approach is to use the Metropolis algorithm.

The algorithm is well-described in Metropolis' original paper [1], but to give a short summary here: configurations are chosen according to their Boltzmann factors, and then weighted evenly. In order to do this for a array of spins:

1. A spin is randomly chosen to be flipped. ΔE, the change in total energy from pre- to post-flip, is calculated.
2. The flip is accepted if a random number $0 < n < 1$ is less than $e^{-\beta \Delta E}$, according to the Boltzmann factor. This represents the spin flipping by absorbing heat from the environment.
3. It can be seen that if ΔE is negative, i.e. the move is energetically favourable, this quantity will always be greater than one and hence the move is always accepted.
4. Whether or not the spin flipped, the system is now taken to be in a new configuration and the process starts anew.

If the process is repeated *ad infinitum*, it is ergodic: that is, it visits every possible configuration.

A further complication arises in the calculation of the specific heat capacity and magnetic susceptibility. Heat capacity in the thermodynamic sense is $C = \frac{\partial E}{\partial T}$. Calculating derivatives is difficult in the model, but the specific heat capacity can also be written in terms of the variance of the energy: $C = N^{-2} J^2 k_B \beta^2 (\langle E^2 \rangle - \langle E \rangle^2)$ (*for the derivation, refer to appendix A*). In this form the specific heat capacity is easy to calculate from the observables obtained from the model. In a similar way, the magnetic susceptibility can be derived to be $\chi = N^{-2} \beta \left(\langle S^2 \rangle - \langle S \rangle^2 \right)$.

Method

A 25x25 square array was used. In order to avoid any end effects, periodic boundary conditions were applied – that is, the first and last row were taken to be the same, and likewise for the first and last columns. Physically, this can be visualised as the array being on the surface of a three-dimensional torus.

Measurements are taken once the system has achieved equilibrium – the steps taken to get to that stage are not of interest. In order to determine when the system has achieved equilibrium, the average energy of a moving block of 100,000 steps was chosen, after some experimentation. If the energy of one block was within 1% of the energy of the previous block, the system was taken to be in equilibrium. A cut-off point of 1 million steps was also implemented, after it was seen that at high temperatures even the large-sized blocks chosen did not produce a settled average energy. Once at equilibrium, 100,000 steps were used to take measurements for the 4 observables of interest.

In order to shorten the time required to achieve equilibrium, the array was initialised either at an aligned configuration – all spins up – for low temperatures, or a random configuration for high temperatures. This is because it is expected for low temperatures that the system will find its way to the most energetically favourable state, with all spins aligned, whereas for high temperatures it is expected that the thermal energy will cause randomly fluctuating spins.

As seen above, the Metropolis algorithm is ergodic only if it is of an infinite duration. In a practical application with limited time, probable states may not be counted if they are separated from the current configuration by improbable states. To solve this problem, the simulation is re-run several times with different random number seeds, in order that all probable states may be counted. It was decided to average the results obtained for 20 runs.

Measurements were taken over varying temperature and field. Instead of varying the value of T over a large range, it was decided to vary the value of β between 0 and 1. Steps of 0.01 were taken. Also, instead of varying B, the value of μB was varied between -1 and 1, again in steps of 0.01.

Because my program was written in Python, by this point it was running quite slowly. In order to speed things up I split the code into three files: one to read eventual results, one called 'getresults' to set conditions and save results, and a final file, 'iterator', that implemented the metropolis algorithm and averaged observables. The iterator file was converted to plain C code using Cython, and this was compiled with -Ofast to a shared object that could be called from getresults. A quick trial revealed a speed improvement of over 20%.

Results

1) Varying β, no field

Energy

Figure 1 shows how the energy of the system varies with β. On this scale, and with no field,

$$E = -\frac{1}{2}\sum_{i,j} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

between neighbouring i and j.

With $\beta = 0$, i.e. infinite temperature, energy $= 0$. This fits with theory: at high temperature, spin orientation is completely random. Hence a site will, on average, be connected to two up and two down spins, giving $E = 0$.

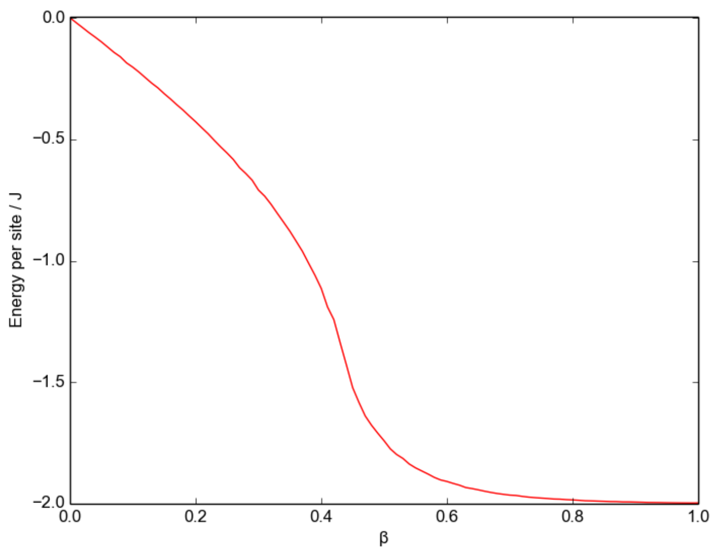

Fig. 1: Energy against β, no field

With $\beta = 1$, i.e. low temperature, energy $= -2$. This likewise fits with theory: at a low temperature, the most favourable state has all spins aligned, so a site will generally be connected to four equal spins. After applying the factor of 0.5 for double counting, $E = -2$, as obtained.

The sharpest drop in energy – where the second derivative changes sign – occurs at around $\beta = 0.45$, indicating a phase transition. Below this critical temperature T_c, it is much easier for the system to maintain an aligned state, and therefore energy quickly approaches -2.

To illustrate this, figures 2, 3, and 4 indicate the system at high temperature, T_c, and low temperature respectively. Black areas indicate spin up, and white spin down. The system recorded was the last one obtained from the 20 runs.

At high temperature, the array has randomly oriented spins, as expected. At T_c, large areas of equal down spins are observed, with some islands of positive spin still present. At low temperature, the array consists entirely of up spins. At that temperature the array always consisted of up spins in the model, because it was initialised that way. If the array had been randomly initialised each time, it would take far longer to reach equilibrium but would also consist of down spins half the time.

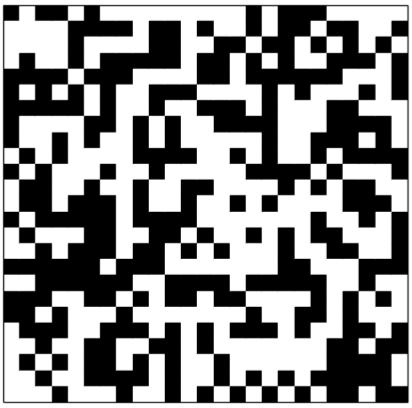

Fig. 2: Array at high temp.

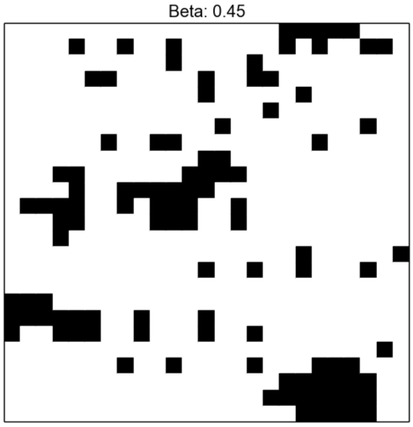

Fig. 3: Array at T_c

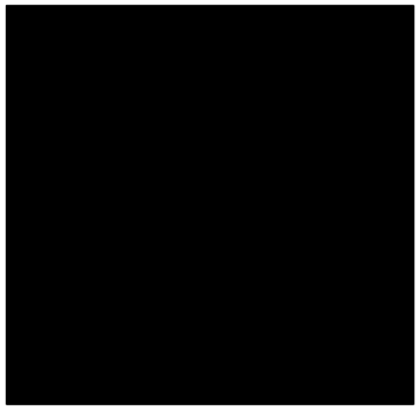

Fig. 4: Array at low temp.

Magnetisation

Figure 5 shows how the magnetisation of the system varies with β. This data does not agree well with theory: at low beta the magnetisation should be close to 0. In addition, the averages for magnetisation were made regardless of sign, which is probably why there are poor results that do not show a trend on the left of the figure.

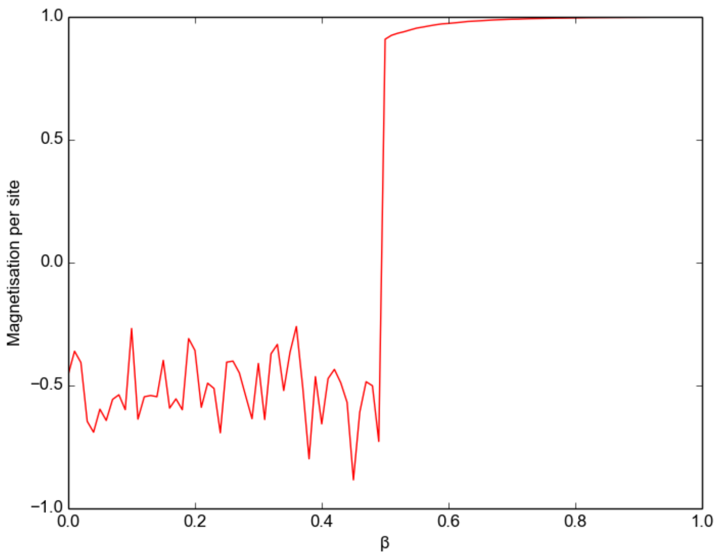

Fig. 5: Magnetisation against β, no field

The main jump in the figure does not occur at the T_c of $\beta = 0.45$ found from the energy, but at $\beta = 0.5$, and only because it was at that temperature that the model started initialising the array with equal up spins. After that temperature the data agrees with theory – approaching low temperature, magnetisation approaches 1, seeing as the spins are all up. The right of the figure does not suffer from the problem of neglecting the signs, because is is highly unlikely at low temperatures for the model to enter into negative magnetisation from being entirely positive.

Specific heat capacity and magnetic susceptibility

Figures 6 and 7 show how the specific heat capacity and magnetic susceptibility vary with β. Because they are derivatives of energy and magnetisation respectively, they should have peaks corresponding to the jumps in figures 1 and 4.

The specific heat capacity behaves exactly as expected: there is a peak corresponding to the phase transition, at the T_c of $\beta = 0.45$. The magnetic susceptibility seems to give much better data that the magnetisation, probably because it was calculated from the variance of the sum of spins, and not magnetisation, thus avoiding the averaging problem. However, the peak is found at a lower β of around 0.4.

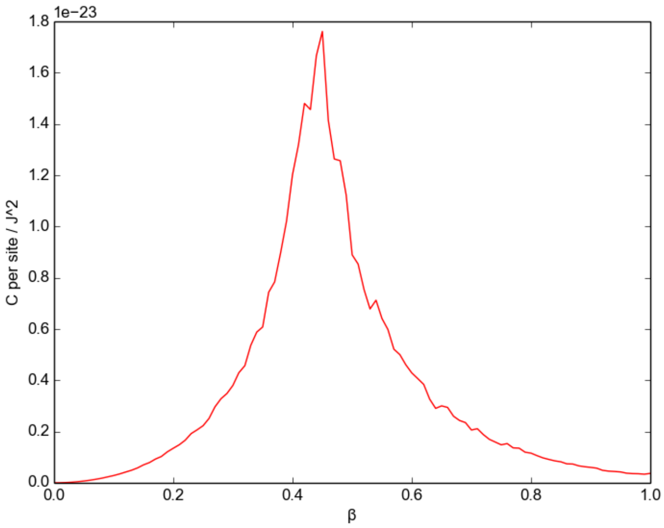

Fig. 6: Specific heat capacity against β, no field

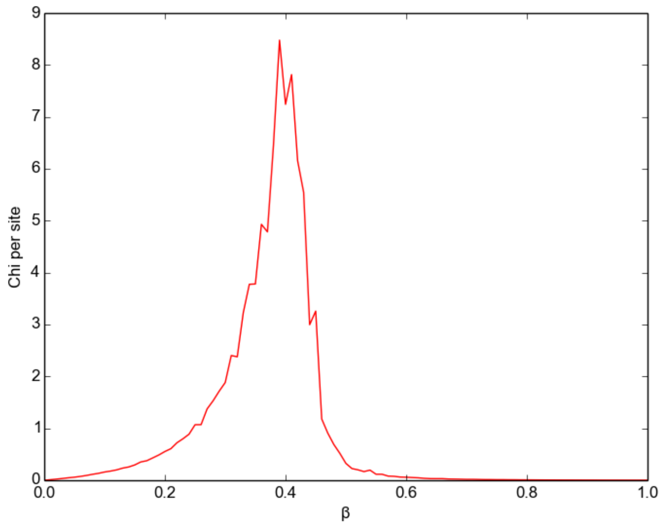

Fig. 7: Magnetic susceptibility against β, no field

2) Varying β, low positive field.

Energy

Figure 8 shows how the energy of the system varies with β, with an external field of 0.5J. The shape is roughly similar to that of figure 1, with some expected changes.

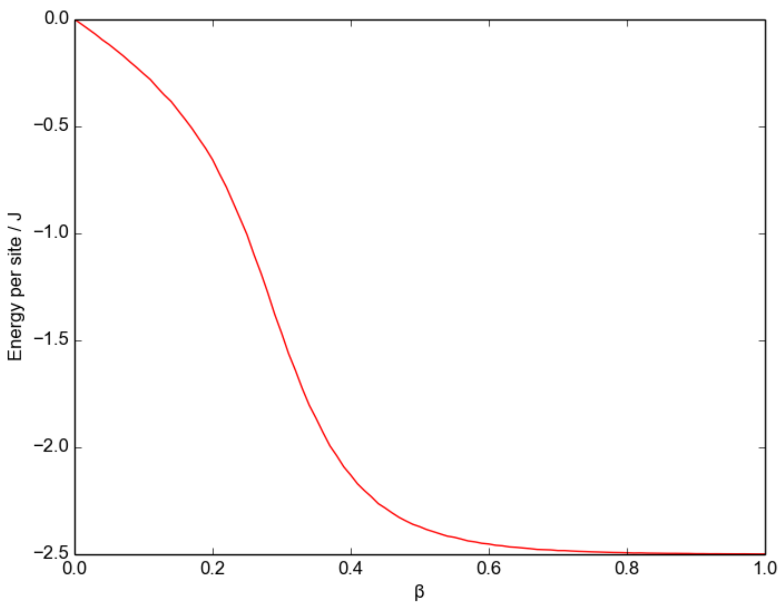

Fig. 8: Energy against β, field = 0.5J

The energy at high temperature is 0 as expected, because the effect of the field is negligible compared to the spin fluctuations due to temperature. At low temperature, the energy is -2.5, also as expected. The interaction energy gives an energy of -2 as previously discussed, and the field of 0.5J gets subtracted to produce -2.5.

Also of note is that the T_c is higher, at a lower β of around 0.3. This is because the external magnetic field helps to impose spin direction, and thus the system can resist a greater temperature before losing alignment.

Magnetisation

Figure 9 shows how the magnetisation of the system varies with β, with an external field of 0.5J.

Once again, the data is not ideal. The same artificial jump can be seen at β = 0.5, as in figure 4, but another feature is present: the magnetisation increases with lower temperature, due to the field helping to impose a spin direction. No phase transition is observed however.

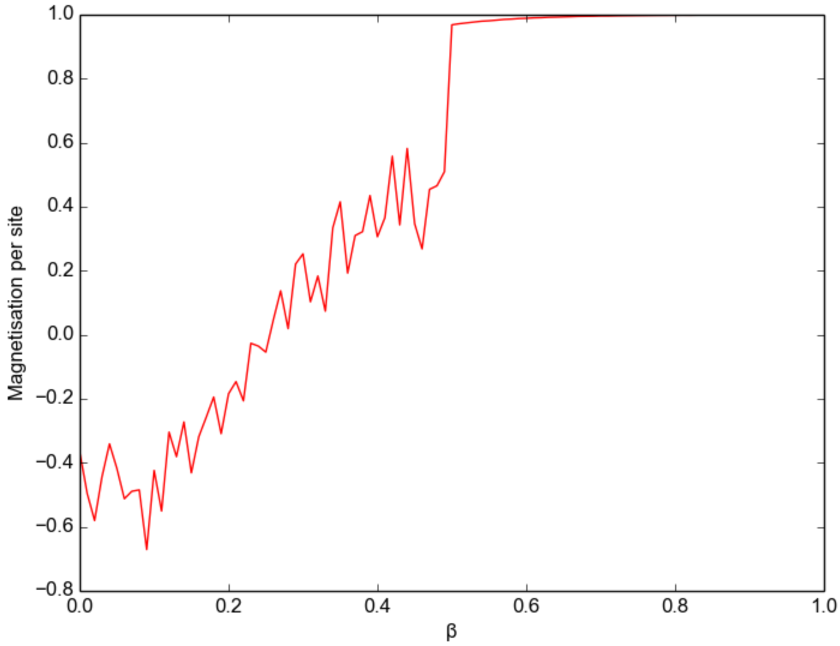

Fig. 9: Magnetisation against β, field = 0.5J

Specific heat capacity and magnetic susceptibility

Figures 10 and 11 show how the specific heat capacity and magnetic susceptibility vary with β, with an external field of 0.5J.

The curve for specific heat capacity is not as neat as that of figure 6, but the main features are the same: a peak is seen around the same T_c as figure 8. Similarly, the peak for magnetic susceptibility is found at a lower β of around 0.25.

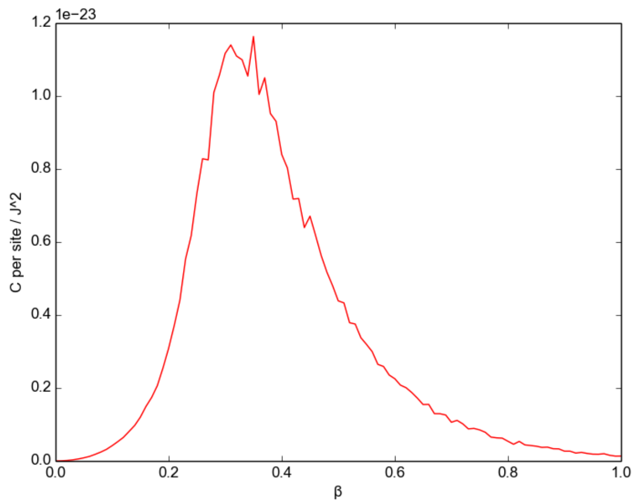

Fig. 10: Specific heat capacity against β, field = 0.5J

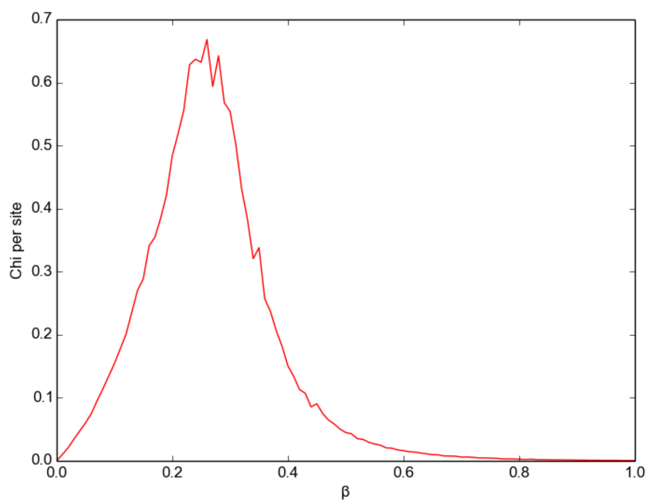

Fig. 11: Magnetic susceptibility against β, field = 0.5J

3) Varying μB, low temperature.

Energy and magnetisation

Figures 12 and 13 show how the energy and magnetisation vary with field, with a low temperature of β = 1.

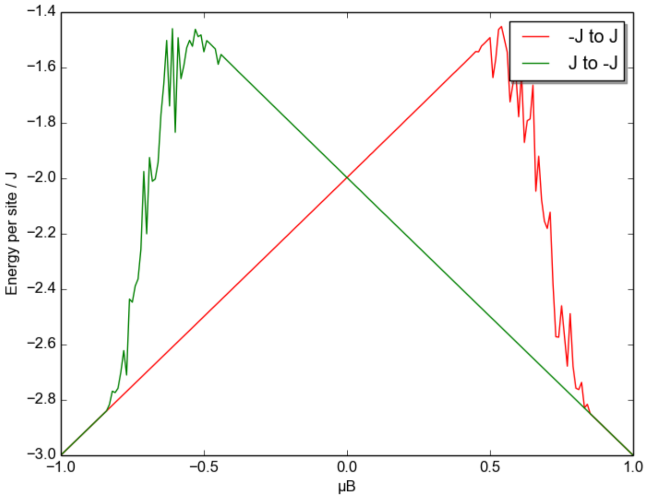

Fig. 12: Energy against field, $\beta = 1$

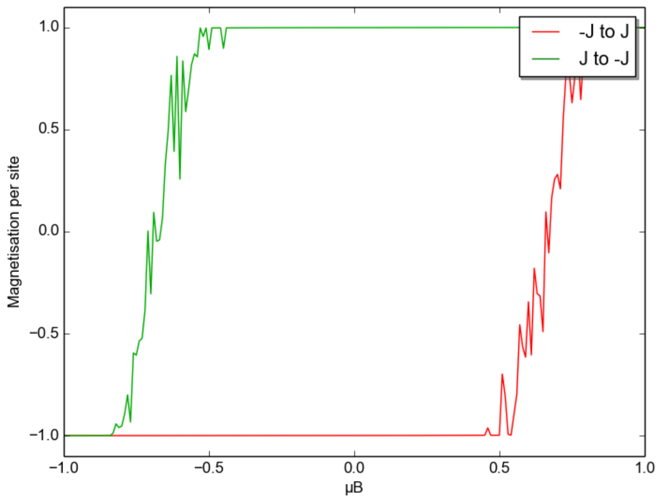

Fig. 13: Magnetisation against field, $\beta = 1$

For -J to J (the red lines), the initial magnetic field is large and negative. Hence the magnetisation is negative. The energy is -3 as all spins are equal (contributing -2) and aligned with the magnetisation (contributing -1). The magnetisation remains constant at -1, but the energy linearly increases as the field increases. This is because the increasingly positive field acts contrary to the magnetisation. The linearity of the increase fits with theory, as the field appears as a linear term in the energy of the system.

At a critical value B_c of the magnetic field, around $\mu B = 0.6$, the magnetisation sharply changes sign, as the field is enough to flip the spins. The energy starts to linearly decrease back to -3 as the field now grows in the same directions as the spins.

The opposite occurs for J to -J (the green lines). The magnetisation starts off positive, and at a B_c of around $\mu B = -0.6$ starts to sharply changes sign. The energy thus behaves in a mirror fashion to -J to J, as expected.

Specific heat capacity and magnetic susceptibility

Figures 14 and 15 show how the specific heat capacity and magnetic susceptibility vary with field, with a low temperature of $\beta = 1$.

The peaks for both graphs, and both directions of variation of the field, occur at the respective discontinuities for energy and magnetisation, confirming the behaviour of those discontinuities.

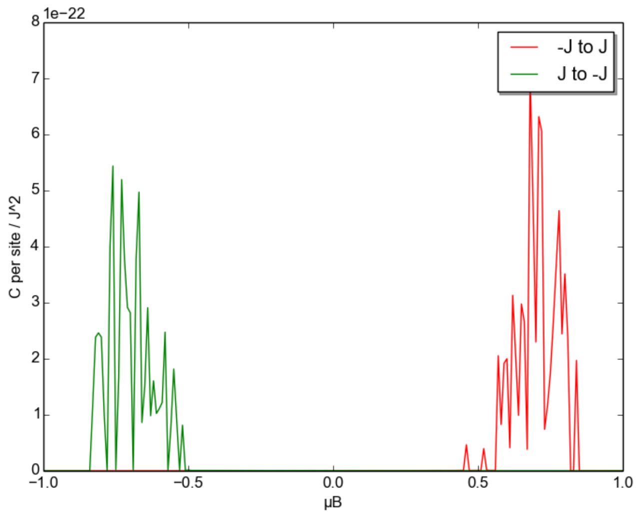

Fig. 14: Specific heat capacity against field, $\beta = 1$

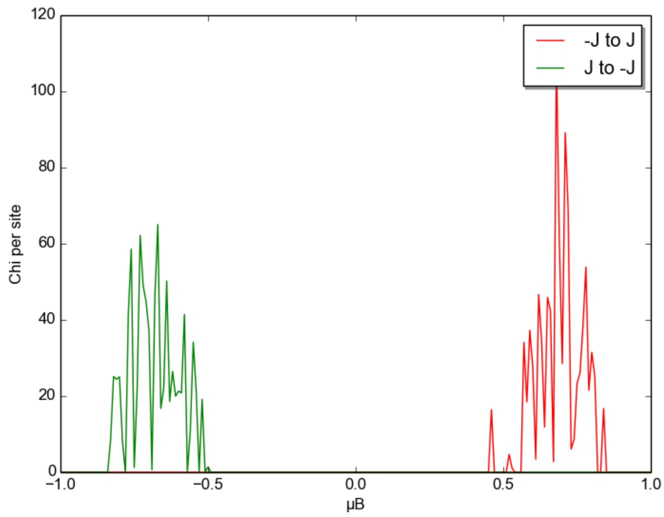

Fig. 15: Magnetic susceptibility against field, $\beta = 1$

Conclusions

This report has illustrated how finding exact calculations for the Ising model is computationally infeasible, and why the Metropolis algorithm using a Monte Carlo method is more appropriate.

Onsager's exact solution of the Ising model puts T_c in the case of no field at $\beta = 0.44$.[2] The results for energy and specific heat capacity agree very well with this value. However, the magnetisation produced poor results, and the phase transition on the graph was determined to be an artefact from the way the model was coded. The magnetic susceptibility did indicate a phase variation, but the position was lower than $\beta = 0.44$, and could not be verified from magnetisation results.

In the case for varying field at low temperature, a critical field of μB around ± 0.6 was found, at which the strength of the field was able to overcome the magnetisation, and flip the spins of the entire array. The effect of this behaviour on the energy was explained, and the positions of the peaks on the graphs of specific heat capacity and magnetic susceptibility confirmed the location of the critical field.

The model could have been sped up by taking the equilibrium configuration of the array as the initial configuration for the next step in temperature or field. It was decided not to do this because the multiple runs in order to average quantities were calculated for each step in temperature or field. However, multiple continuous runs could have been performed, and the averages calculated afterwards.

In addition, as discussed previously, the magnetisation results for varying β leave a lot to be desired. Either magnetisation calculations should have been done mindful of sign, or absolute values for magnetisation should have been used all the way through.

The phase transitions are not as sharp as they could be. In the thermodynamic limit, where the transitions are best observed, the lattice is of infinite size. Obviously this is computationally intractable, so a finite size has to be applied. The larger the size, the better defined the phase transitions, but the longer the system takes to reach equilibrium. A 25x25 square lattice was decided to be a balance between a good illustration of the phase changes and code run time.

Word count, excluding captions and titles = 2455

References

[1]: N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, et al. (1953), *Equation of state calculations by fast computing machines,* DOI: 10.1063/1.1699114

[2]: L. Onsager, *Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition*, DOI: 10.1103/PhysRev.65.117

Appendix A

Let $\beta = \frac{1}{k_B T}$. Heat capacity $C = \frac{\partial E}{\partial T} = -\frac{\beta}{T}\frac{\partial E}{\partial \beta} = \frac{\beta}{T}\frac{\partial^2 \ln Z}{\partial \beta^2} = \frac{\beta}{T}\frac{\partial}{\partial \beta}\left(\frac{1}{Z}\frac{\partial Z}{\partial \beta}\right)$

$$= \frac{\beta}{T}\left[\frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2} - \frac{1}{Z^2}\left(\frac{\partial Z}{\partial \beta}\right)^2\right] = \frac{\beta}{T}\left[\langle E^2\rangle - \langle E\rangle^2\right] = \beta^2 k_B\left[\langle E^2\rangle - \langle E\rangle^2\right]$$

Then in the case where $\beta = J/k_B T$, s.h.c for an $N \times N$ array: $N^{-2} C = N^{-2} J^2 k_B \beta^2\left[\langle E^2\rangle - \langle E\rangle^2\right]$.