# Comparison of the Metropolis and Wang Landau algorithms for computing the Ising model

Andrew Read

February 2013

**Abstract**

This Metropolis and Wang Landau algorithms represent two different approaches to solving statistical problems using Monte Carlo methods. The Metropolis algorithm directly models random fluctuations in the system, while the Wang Landau algorithm uses a random walk to determine the density of states as a function of system energy and therefore the partition function. This project compared these two different approaches in evaluationg the Ising model in 2, 3 and 4 dimensions. It was found that for large lattices both algorithms produce accurate estimations of the analytical solution, but for small lattices the two algorithms produce different solutions. In addition each approach has strengths and weaknesses in different applications. For modest size lattices the basic Wang Landau algorithm produced high quality results very efficiently, but scaling this algorithm to larger lattices requires a more sophisticed implementation. The Metropolis algorithm is less efficient overall, but the same implementation copes equally will with large lattices given sufficient computation time.

## 1 Introduction

The Ising model is a very simplifed model of intramolecular forces. In spite of the simplicity of the model, it has been found to contain the essential characteristics of cooperative phenomena such as phase transitions. It can be applied to a wide range of physical systems such as gas-liquid critical phenomena, magnetic Curie points, order-disorder transitions in alloys, and phase separation in liquid mixtures. In outline, the model assumes that the physical system can be represented by a regular lattice of nodes, and that each node exists in one of two possible configurations (Fig. 1). Interaction energies between neighbouring nodes depend on their alignment. The nodes could be domains in a ferromagnet oriented "up" or "down", mixtures of molecules, or mixtures of molecules and empty spaces. The Ising model was first investigated by Wilhelm Lenz and Ernst Ising in 1925 at Hamburg University and has been applied to a wide variety of problems since the 1960's [13].

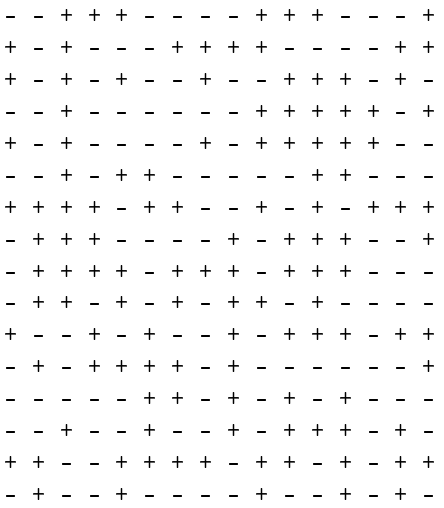

Figure 1: Rendering of a 16 x 16 node Ising model

The Ising model is ideally suited to investigation using computational algorithms. An early technique was the Metropolis algorithm[1], which directly simulates fluctuations in the lattice using a Monte-Carlo process. In successive steps, atoms in the lattice are selected at random and their spins can be flipped according to certain rules that take into account the potential change in lattice energy and the temperature. By operating the algorithm with suitable averaging over a range of temperatures, the characteristics of the Ising model can be measured. In addition, the Metropolis algorithm allows the lattice and its fluctuations to be visualized either as snapshots at certain temperatures or as a continuing animation.

The Metropolis algorithm is a very elegant and broadly used computational technique, but an alternative approach offering higher computational efficiency was proposed by Wang and Landau in 2001[2]. The Wang Landau algorithm is also based on a Monte-Carlo process, but this time the fluctuations of the Ising model are not simulated directly. Rather, a random walk technique is used to count how many alternative configurations of the lattice are available at each possible energy level, i.e. the density of states as a function of energy. Once the density of states has been determined, a numerical summation is performed over all possible energy levels in the parttition function to calculate the average magnetization and energy.

Since the Wang Landau algorithm was first published various studies have looked at its effectiveness and at potential improvements. Zhou and Bhatt[3] gave a proof of the convergence of the Wang Landau algorithm and suggested a optimization strategy. Schutz and Landau[4] investigated how the density of states for large systems could be established by conducting multiple random walks over adjacent restricted energy ranges without incurring boundary effects. Lee, Okabe and Landau[5] derived an expression for the residual error of the Wang Landau algorithm and as a result identified the central role of the histogram accumulated during the density of states calculation in the overall accuracy of the method. Recently, Caparica and Cunha-Netto[6] conducted an extensive study of the impact of various implementation adjustments on the accuracy and precision of the algorithm. A central element of their method was to run the algorithm multiple times and obtain the histogram of the location of the peak of the specific heat capacity.

This project aims to evaluate the Ising model for different lattices using both the Metropolis and Wang Landau algorithms and compare and contrast the results obtained with each. The results will demonstrate that the Metropolis and Wang Landau algorithms both produce the expected Ising model behaviour, but that specific quantitative results may differ.

# 2 Theory of the Ising Model

## 2.1 Description of the Ising model

A simple instance of the Ising model might be a two dimensional lattice of atoms, each of which can be in one of two possible states. There is an interaction energy between every atom and each of its nearest neighbours expressed by the following Hamiltonian

$$H = -J \sum_{\langle i,,j \rangle} S_i S_j - \sum_i h.S_i$$

where $S_i = \pm 1$ is the state of the atom at site $i$ , $\sum_{ij}$ indicates the sum over the four nearest neighbours, $J$ is a constant with units of energy, and $h$ is the contribution of an external field. The Ising model may describe a ferromagnetic system, in which case $S_i$ is the magnetization of atom $i$ , $J > 0$ , and consequently neighbouring spins are at a lower energy when aligned. If the lattice is allowed to equilibrate at some temperature then the total interaction energy and magnetization will, on average, reach steady values.

## 2.2 Analytical solution of the phase transition

In a ferromagnetic Ising model it is observed that at sufficiently low temperatures the atomic spins in a lattice are generally all aligned, resulting in overall lattice magnetization. At sufficiently high temperatures the spins are generally at random and the lattice has no overall magnetization. There is a crossover between the low temperature ordered state and the high temperature disordered state. In two or more dimensions this crossover occurs with a sharp boundary between the two regions of different magnetization. The sharp boundary indicates that a phase transition has occurred. The temperature at which the phase transition occurs is known as the critical temperature.

The Ising model in one dimension can be solved by expressing the Hamiltonian using a matrix, the *transfer matrix*, to sum the contributions between each pair of atoms in the array. The partition function is found to be the trace of the transfer matrix and is computed by determining the eigenvalues[12].

The Ising model in two dimensions was analytically solved by Lars Onsanger in 1944. The solution follows the same principal as the solution for the one dimensional case, but is highly complex mathematically. Onsanger showed that for an infinite lattice the phase transition occurs at a temperature given by[7]

$$k_B T/J \;=\; 2/\ln(1+\sqrt{2}) \;= 2.269185...$$

## 2.3 Critical exponents

Near the phase transition critical temperature, state variables such as average magnetization and heat capacity are found to vary with temperature according to power laws as follows:

$$t \;=\; \frac{T - Tc}{Tc}$$

$$f(t) \;=\; a * t^{\lambda}$$

$$\lambda \;=\; \lim_{t\to 0} \frac{\ln\, f(t)}{\ln\, t}$$

where $T$ is the temperature, $T_c$ is the critical temperature, $a$ is an amplitude factor, and $\lambda$ is one or other critical exponent. For the two dimensional Ising model, the first two critical exponents and their analytically determined values are as shown in Table 1:

| State variable, $f(t)$ | Critical exponent, $\lambda$ | Analytic value |
|---|---|---|
| Heat capacity, $C$ | $\alpha$ | 0 |
| Magnetization, $M$ | $\beta$ | $\frac{1}{8}$ |

Table 1: First two critical exponents of the the two dimensional Ising Model

These power laws and their critical exponents are important because they are believed to represent properties that apply across a wide range of systems exhibiting continuous phase transitions, and are independent of the most of the individual system details. Thus different physical systems may have identical physical exponents, a phenomenon known as universality[11].

## 2.4 Computational solutions

Although Onsanger's solution for critical temperature and critical exponents of the two dimensional Ising model is available, it may still be more straightforward to approach the problem using numerical techniques. In addition the Ising model in three dimensions or more can only be solved numerically.

The number of possible configurations of an Ising lattice is very large: $2^{L^D}$ for a $D$ dimensional lattice spanning $L$ atoms in each direction. For this reason it is not feasible for a computational method to evaluate each configuration directly (Table 2). Instead, the Metropolis and Wang Landau algorithms take a random walk through the space of alternative lattice configurations (the state space) and make measurements on a sample basis. Accurate determinations for the characteristics of the Ising model can be had once sufficient measurements have been accumulated. This general approach is called a Monte-Carlo method.

The key quantities that the algorithms should determine across the range of temperatures under investigation include the average magnetization, the average interaction energy, and the average heat capacity per atom. Magnetization and interaction energy can be measured directly from the lattice. The heat capacity is related to the energy, $E$, by

$$C = \frac{k_B}{T^2}\left(\langle E^2\rangle - \langle E\rangle^{\,2}\right)$$

The critical temperature is observed to occur at the point where the heat capacity reaches a maximum, so by evaluating the heat capacity at each temperature the algorithms can also determine the critical temperature.

## 2.5 The Metropolis algorithm

The Metropolis algorithm performs a direct simulation of the physical system. It sets up a lattice at a given temperature and follows its fluctuations in discrete time steps. The algorithm proceeds as follows:

1. Set the current temperature
2. Create a new lattice in the initial configuration. In a "hot start" the lattice spins are initially set at random. In a "cold start" the lattice spins are initially aligned
3. Select one candidate spin in the lattice at random and calculate the energy change, $\triangle E$ , that would result from flipping that spin
4. Apply the following rules to determine whether to flip the candidate spin. If $\triangle E \leq 0$ , then flip. If $\triangle E > 0$ , then flip with probability $p = e^{-\triangle E/k_B T}$
5. Periodically measure the average magnetization, $\langle m \rangle$, the average energy, $\langle E \rangle$, and the average energy squared, $\langle E^2 \rangle$, for the lattice
6. Return to step 3 until sufficient measurements have been accumulated for the current temperature
7. Return to step 1 and increment the temperature for the relevant range of temperatures

## 2.6 The Wang Landau algorithm

In effect, the Wang Landau algorithm determines the partition function of the system via the density of states and then uses it in a numerical summation of the partition function to calculate the lattice characteristics. Consider two expressions for the partition function, $Z$, as follows

$$Z = \sum_{\sigma} e^{-E(\sigma)/k_B T} = \sum_{E} g(E)\, e^{-E/k_B T}$$

In the first case the partition function is computed over each available state, $\sigma$. As previously mentioned, the total number of available states will be $2^{L^D}$, which is too many to evaluate. In the second case the partition function is computed over each available energy, $E$ , and makes use of the density of states, $g(E)$. It can be shown by considering the configurations of a lattice that the total number of available energy levels is

$$1 + \frac{1}{2} D.L^D$$

which is a much smaller quantity than the total number of states (Table 2).

| **Dimensions,** $D$ | **Lattice span,** $L$ | **Available states** | **Available energy levels** |
|---|---|---|---|
| 2 | 8 | $1.8 \times 10^{19}$ | 65 |
| 2 | 16 | $1.1 \times 10^{77}$ | 257 |
| 2 | 32 | $1.8 \times 10^{308}$ | 1025 |
| 3 | 8 | $1.3 \times 10^{154}$ | 769 |
| 4 | 8 | $1.0 \times 10^{1233}$ | 8193 |

Table 2: Total number of available energy levels for different Ising lattices

The Wang Landau algorithm determines the density of states through a random walk process. At each step the probability of moving from the current configuration to a new candidate configuration is *inversely proportional* to the relative density of states of their lattice enrgies. A histogram is calculated to track the number of visits to states at each energy level. When the histogram become flat it indicates that the density of states has been properly determined to within the given level of accuracy. Since the density of states is not

initially known, the starting condition for all $E$ is $g(E) = 1$ . An adjustment factor is added to increase each density of states each time a certain energy is visited.

The algorithm proceeds as follows:

1. Set $g(E) = 1$ for all $E$ and set the initial value of the adjustment factor, $f$
2. Create a new lattice in the initial configuration with lattice energy $E_1$ . Hotstart and coldstart are as for the Metropolis algorithm
3. Select one candidate spin in the lattice at random and calculate the lattice energy, $E_2$,that would result from flipping that spin
4. Flip the spin with probability, $p = \min(g(E_1)/g(E_2), 1)$
5. The current energy of the lattice is labelled $E_1$
6. Update the density of the current state with $g(E_1) = g(E_1) * f$
7. Update the histogram that records visits to the available energy levels with $H(E) = H(E) + 1$
8. Periodically test the histogram for flatness using a certain flatness criterion, say 80%
9. Return to step 3 until the histogram satisfies the flatness criterion
10. Reduce the adjustment factor, $f$ , and zero the histogram with $H(E) = 0$ , for all $E$
11. Return to step 3 until the adjustment factor is below a predefined final value
12. Normalize the density of states by recognizing that the lowest energy configuration has a density of states of 2, (i.e. all spins aligned in either one of two ways)
13. Use a numerical summation with the partition function and the calculated density of states to determine the average values of energy, magnetization, and heat capacity. For example the average energy of the lattice at a certain temperature is given by$\langle E \rangle = \sum_E E.g(E) e^{-E/k_B T}$

# 3 Computational implementation

The algorithms were implemented in ANSI C and run on a desktop PC with an Intel i7 processor. Functions for lattice manipulation, such as initialization, flipping a spin, or taking measurements were identically implemented between both the Metropolis and Wang Landau algorithms. Data analysis and chart preparation was done with Wolfram Mathematica. The source code and results are available as open source files[9].

Some implementation specifics are as follows:

- Lattices of all sizes and dimensions were structured in memory as a one dimensional array with periodic boundary conditions. Using this data structure, the nearest neighbours to a particular cell at memory address, $A$ , are referenced using the lattice span, $L$, and dimensions, $D$, at memory addresses $A \pm 1$ , $A \pm L$ , $A \pm L^2$, ... , $A \pm L^D$. In each case a modulus function is used to ensure that the reference is always within range of the array, thus representing the periodic boundary conditions.
- In the Wang Landau algorithm, rather than computing $g(E)$ directly, $ln\, g(E)$ is computed. The adjustment factor, $f$ , is maintained as $ln\, f$ and step 6 of the Wang Landau algorithm is rewritten as $ln\, g(E_1) = ln\, g(E_1) + ln\, f$ . This avoids the potential for overflow or diminished accuracy with a very large range of floating point values, as suggested by Robin Landau[10].
- To avoid the uncertain effectiveness of library random number routines[8], a random number generator was implemented directly based on a method suggested by Knuth, as follows[8]

$$X_{n+1} \leftarrow (3141592621 * X_n)\, mod\, 2^{64}$$

# 4 Results

## 4.1 State variables as a function of temperature

Lattices of 2, 3 and 4 dimensions with sizes 32 x 32, 8 x 8 x 8, and 8 x 8 x 8 x 8, were evaluated by both the Metropolis and Wang Langdau algorithms. Charts were generated for average magnetization, energy and heat capacity per site for each lattice size and algorithm (Figs. 2-7). The results of the Metropolis and Wang Landau algorithms are very similar. For all of the lattices, the average magnetization per size is equal to unity at low temperatures but tends to zero at high temperatures after a phase transition. The phase transition occurs at higher temperatures but is less pronounced with the higher dimensional lattices. The average energy per site at low temperatures tends to a limit that scales linearly with the number of dimensions, while at high temperatures all lattices show zero average energy per site. The average heat capacity per site tends to zero at both low and high temperatures but rises to a maximum at the temperature of the phase transition, the critical temperature.

## 4.2 Measurement of the critical temperature

The critical temperature can be estimated by measuring the temperature at which the average heat capacity per site reaches its maximum. Two dimensional lattices with sizes 8 x 8, 16 x 16, and 24 x 24 were evaluated with both the Wang Landau and Metropolis algorithms, and further lattices with sizes 32 x 32 and 64 x 64 were evaluated with the Metropolis algorithm. In each evaluation 10,000 measurements were made of the critical temperature. These measurements were averaged and a Gaussian distribution fitted (Figs. 8-15). The fitting of a Gaussian distribution is justified by the Central Limit Theorem and by the observed correspondence of the Gaussian to the histogram of critical temperature measurements. The coefficient of variation is calculated as the standard deviation of the critical temperature measurements divided by the mean. Calculation of a coefficient of variation is justified by the fact that the critical temperature is always positive and non-zero. It gives a comparable indication of the spread of critical temperature measurements about the mean.

The analytically determined value of the critical temperature for an infinite two dimensional lattice is given by the Onsanger solution and is, to 4 significant figures, $k_B T/J = 2.269$ . The results of the Metropolis and Wang Landau algorithms are notably different from this value and from each other for smaller lattices but very close for larger lattices, as summarized in Table 3.

| **Lattice size** | **Metropolis** | **Wang Landau** | **Analytical** |
|---|---|---|---|
| 8 x 8 | 2.353 | 2.361 | - |
| 16 x 16 | 2.287 | 2.317 | - |
| 24 x 24 | 2.256 | 2.299 | - |
| 32 x 32 | 2.267 | - | - |
| 64 x 64 | 2.268 | - | - |
| Infinite | - | - | 2.269 |

Table 3: The measured and theoretical values of the critical temperature express in units of $k_B T/J$

### 4.3 Critical exponents

The fit of the theoretically expected behaviour of the average magnetization of the lattice near the critical point given by the critical power law with the computed results was examined by superimposing the theoretical and computed results in a chart. Figs. 16 and 17 show the results for a 32 x 32 lattice evaluated with both the Metropolis and Wang Landau algorithms. In each case the approximate behaviour of the phase transition can be seen, but the fit to the critical power law is not particularly good. This is because of the effect of the relatively small lattice in broadening the phase transition. In Fig. 18, a 128 x 128 lattice has been evaluated with the Metropolis algorithm and the theoretically expected power law chart of average magnetization has been superimposed. Although the experimental chart itself is much rougher due to constraints on the allotted computational time, the fit with the theoretical chart is much better because the larger lattice permits a more pronounced phase transition to occur.

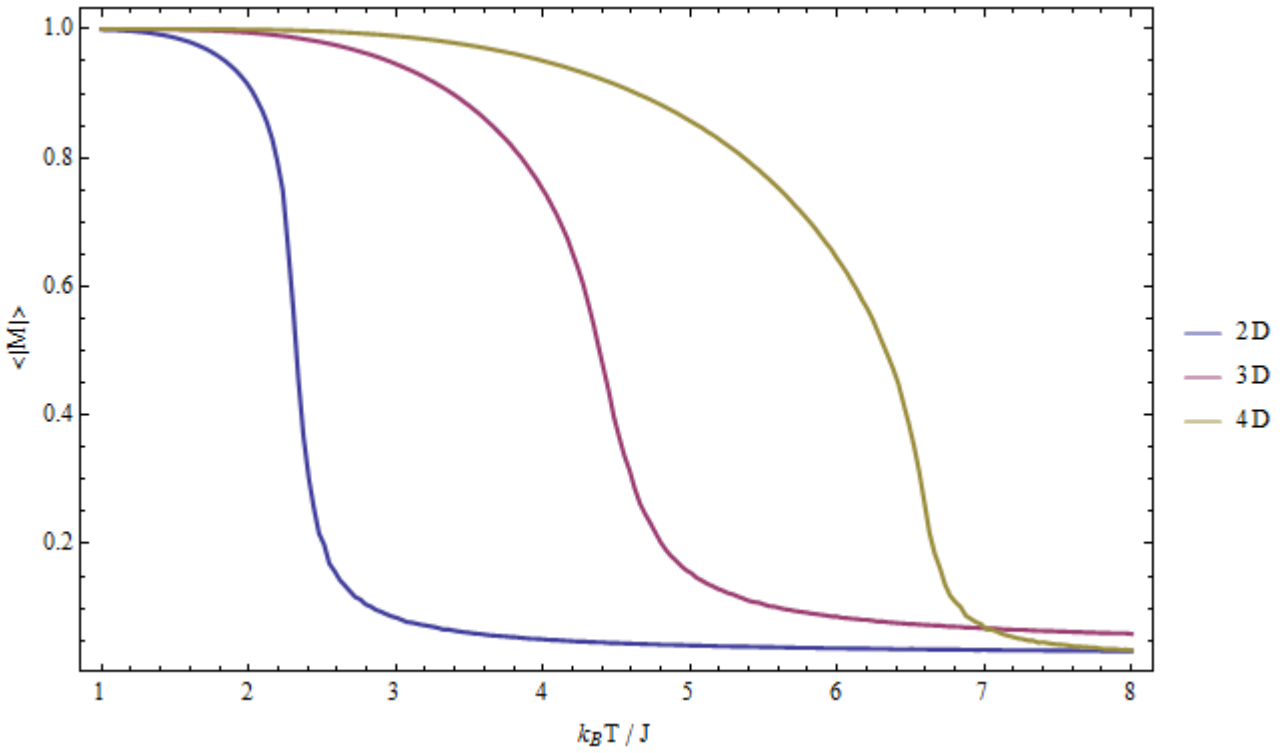


Figure 2: Lattice magnetization per site as a function of temperature generated for 2, 3, and 4 dimensional lattices by the Metropolis algorithm

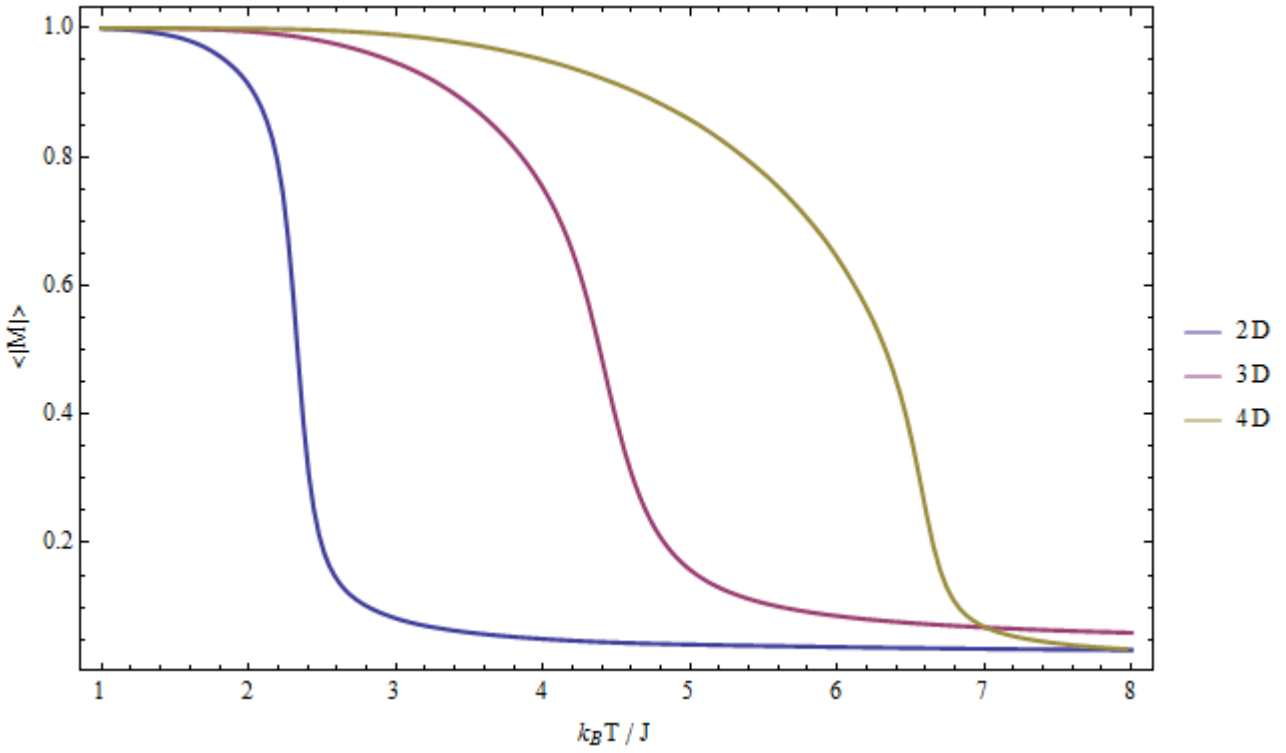


Figure 3: Lattice magnetization per site as a function of temperature generated for 2, 3, and 4 dimensional lattices by the Wang Landau algorithm

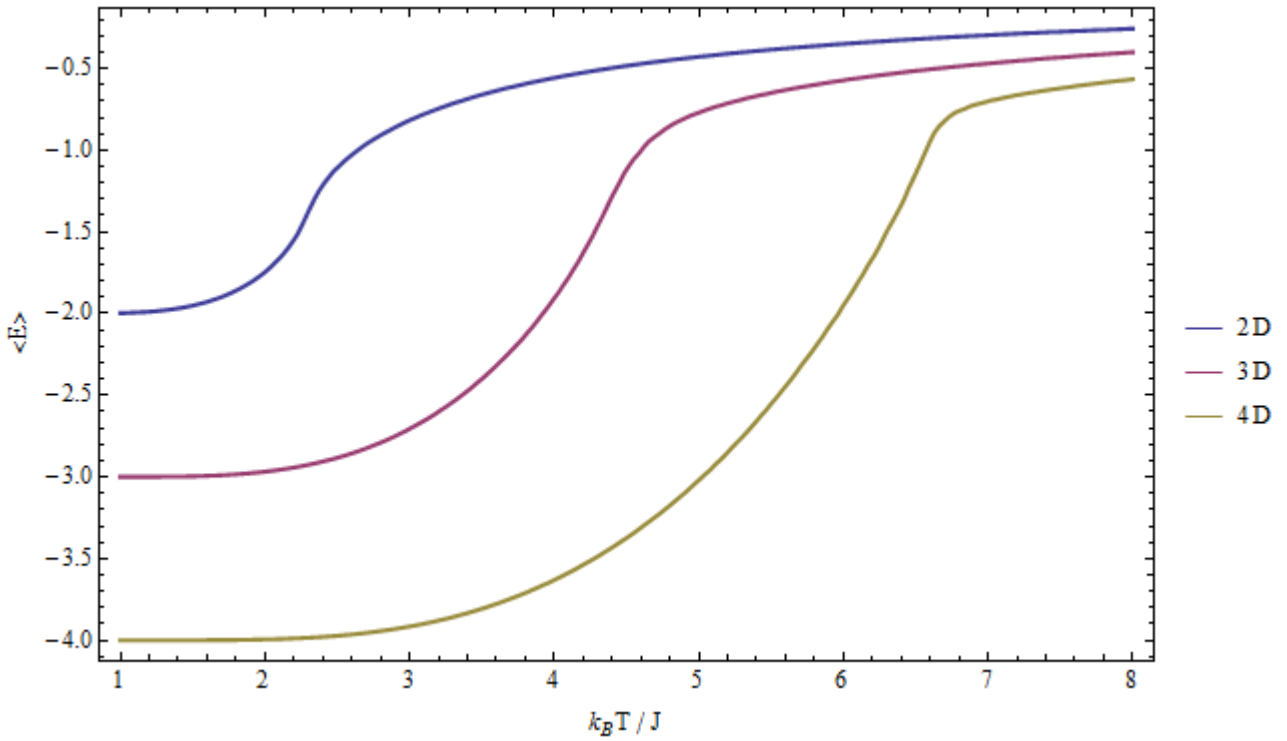


Figure 4: Lattice energy per site as a function of temperature generated for 2, 3, and 4 dimensional lattices by the Metropolis algorithm.

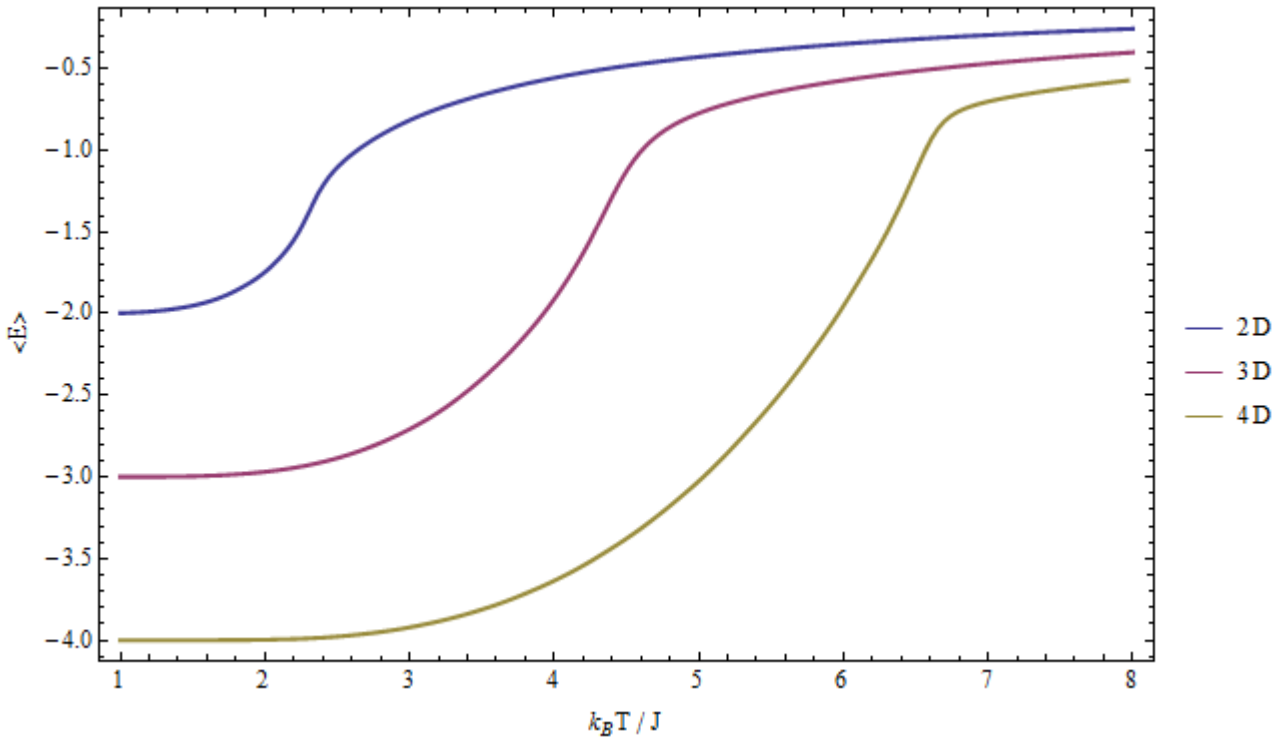


Figure 5: Lattice energy per site as a function of temperature generated for 2, 3, and 4 dimensional lattices by the Wang Landau algorithm.

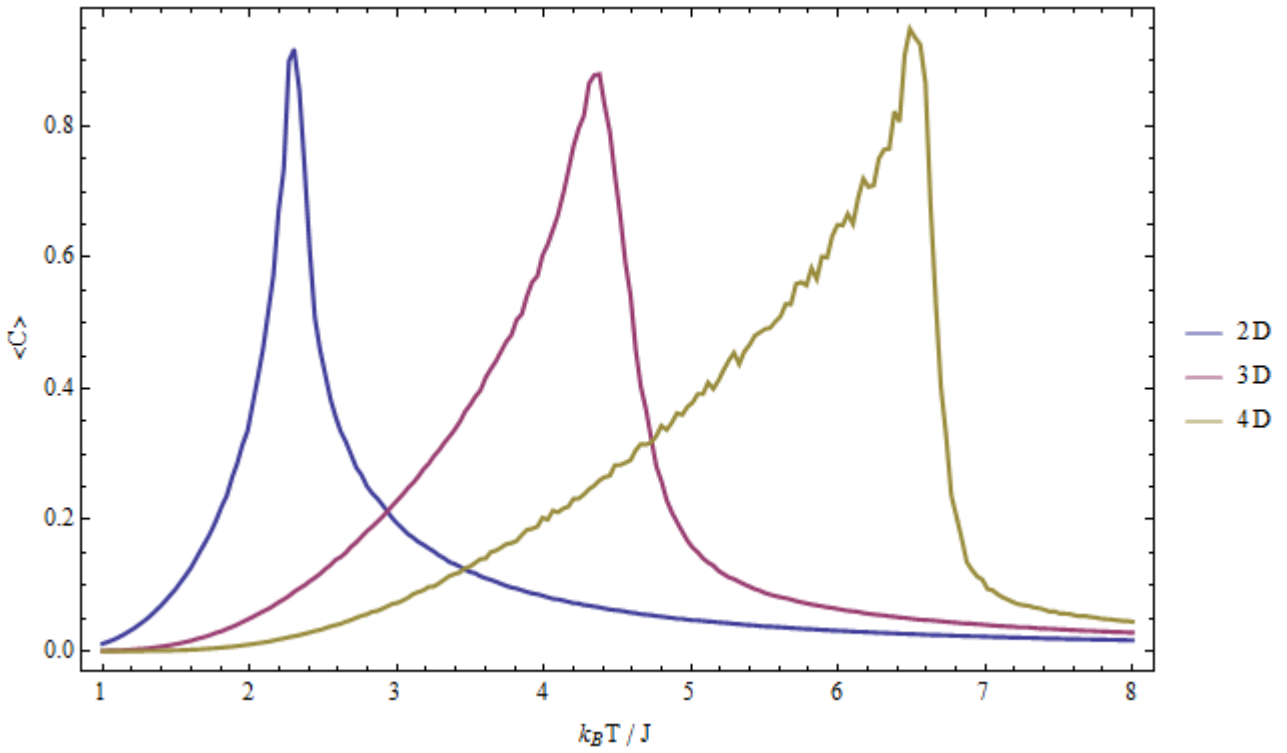


Figure 6: Lattice heat capacity per site as a function of temperature generated for 2, 3, and 4 dimensional lattices by the Metropolis algorithm.

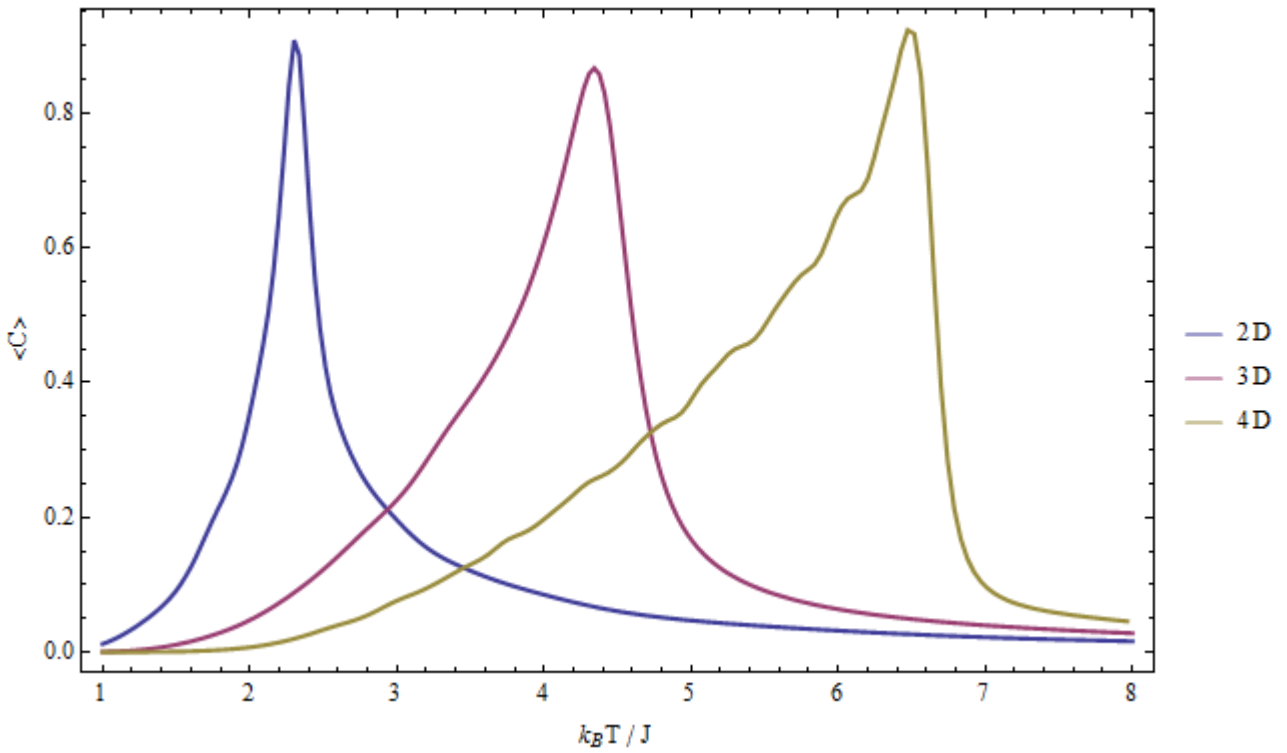


Figure 7: Lattice heat capacity per site as a function of temperature generated for 2, 3, and 4 dimensional lattices by the Wang Landau algorithm.

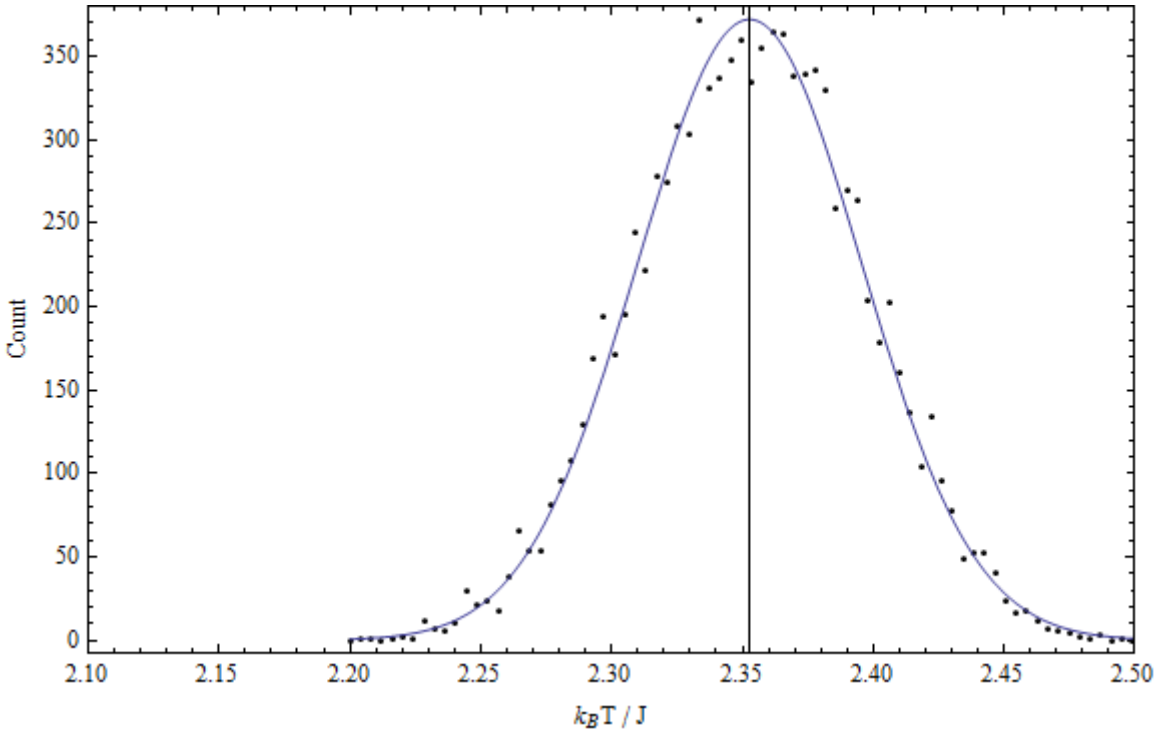


Figure 8: Histogram of 10,000 critical temperature measurements for an 8 x 8 lattice calculated by the Metropolis algorithm and the fitted Gaussian distribution. The mean is at $k_BT/J = 2.353$ and the coefficient of variation is 1.82%

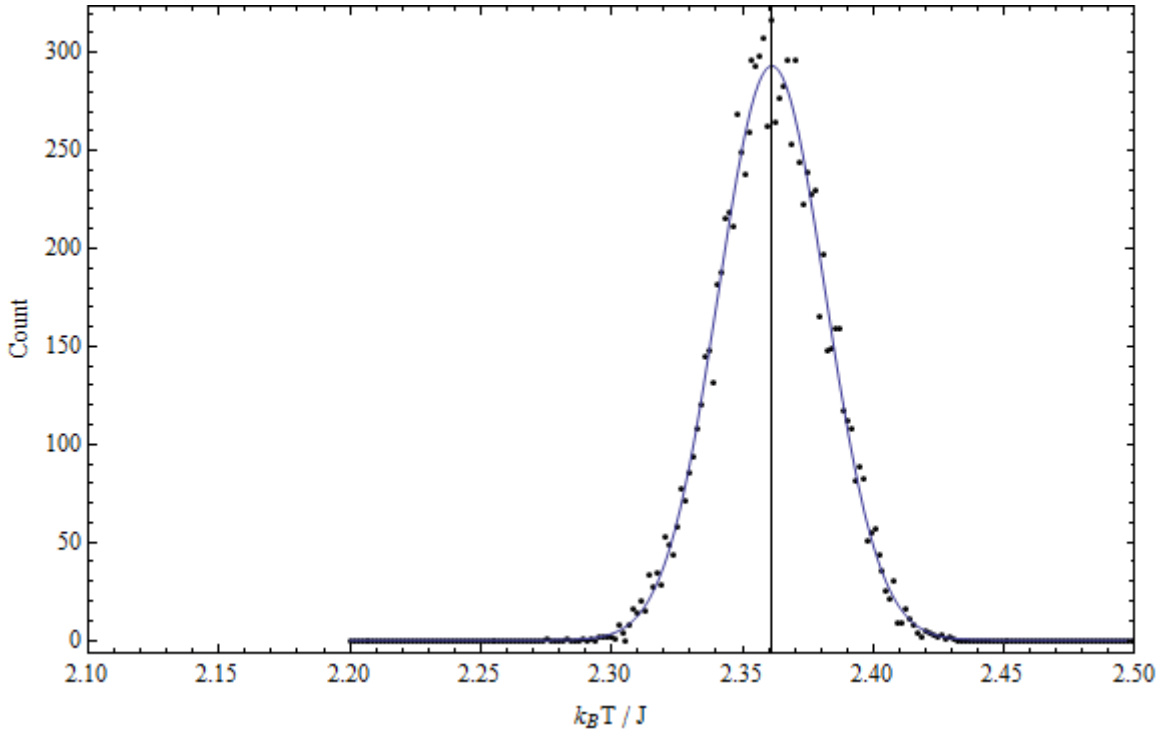


Figure 9: Histogram of 10,000 critical temperature measurements for an 8 x 8 lattice calculated by the Wang Landau algorithm and the fitted Gaussian distribution. The mean is at $k_BT/J = 2.361$ and the coefficient of variation is 0.864%.

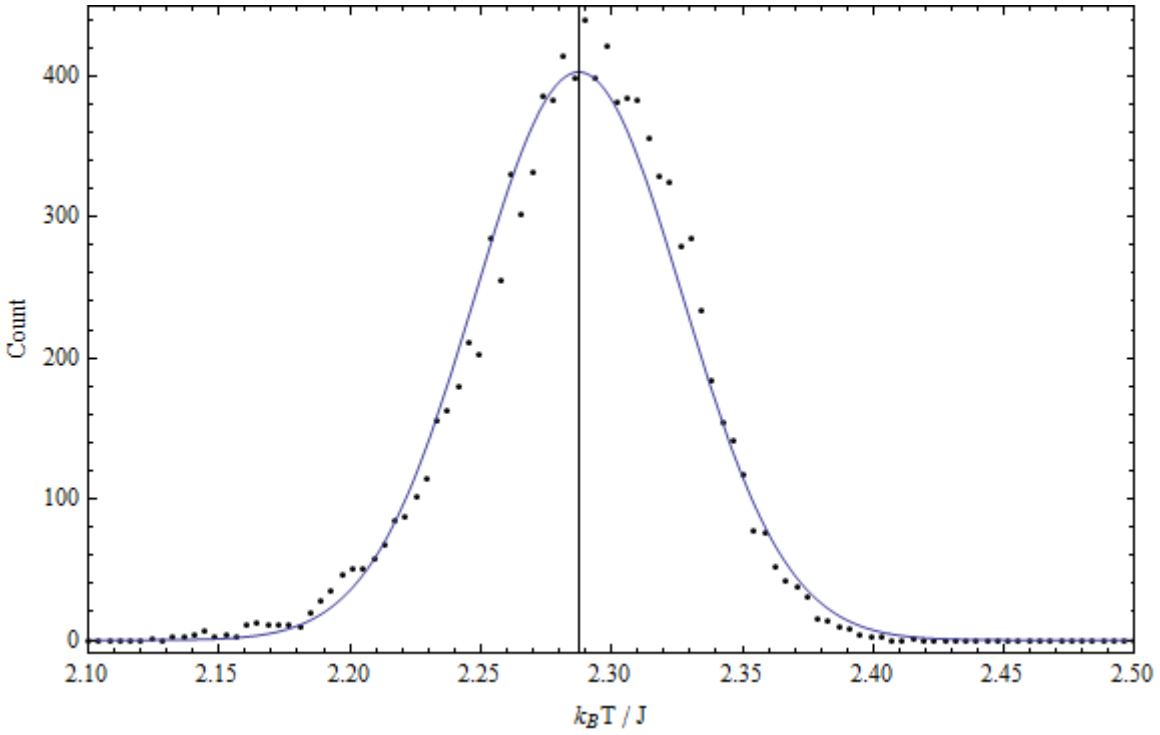


Figure 10: Histogram of 10,000 critical temperature measurements for a 16 x 16 lattice calculated by the Metropolis algorithm and the fitted Gaussian distribution. The mean is at $k_BT/J = 2.287$ and the coefficient of variation is 1.73%.

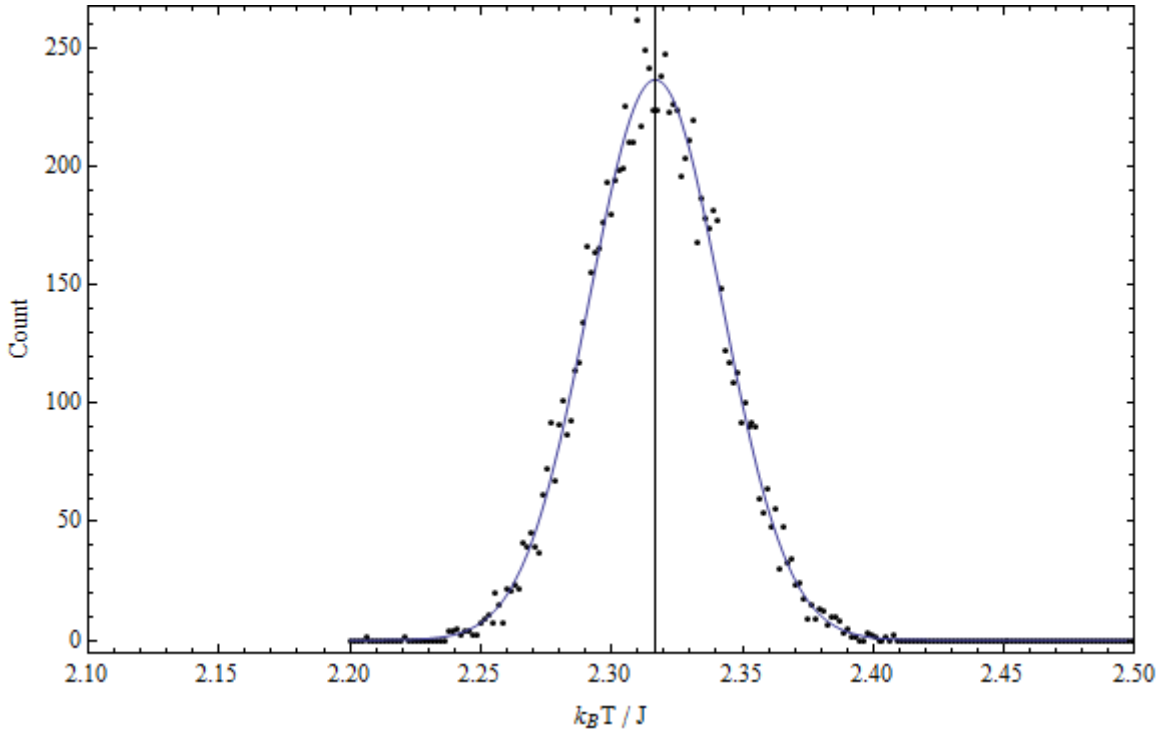


Figure 11: Histogram of 10,000 critical temperature measurements for a 16 x 16 lattice calculated by the Wang Landau algorithm and the fitted Gaussian distribution. The mean is at $k_BT/J = 2.317$ and the coefficient of variation is 1.09%

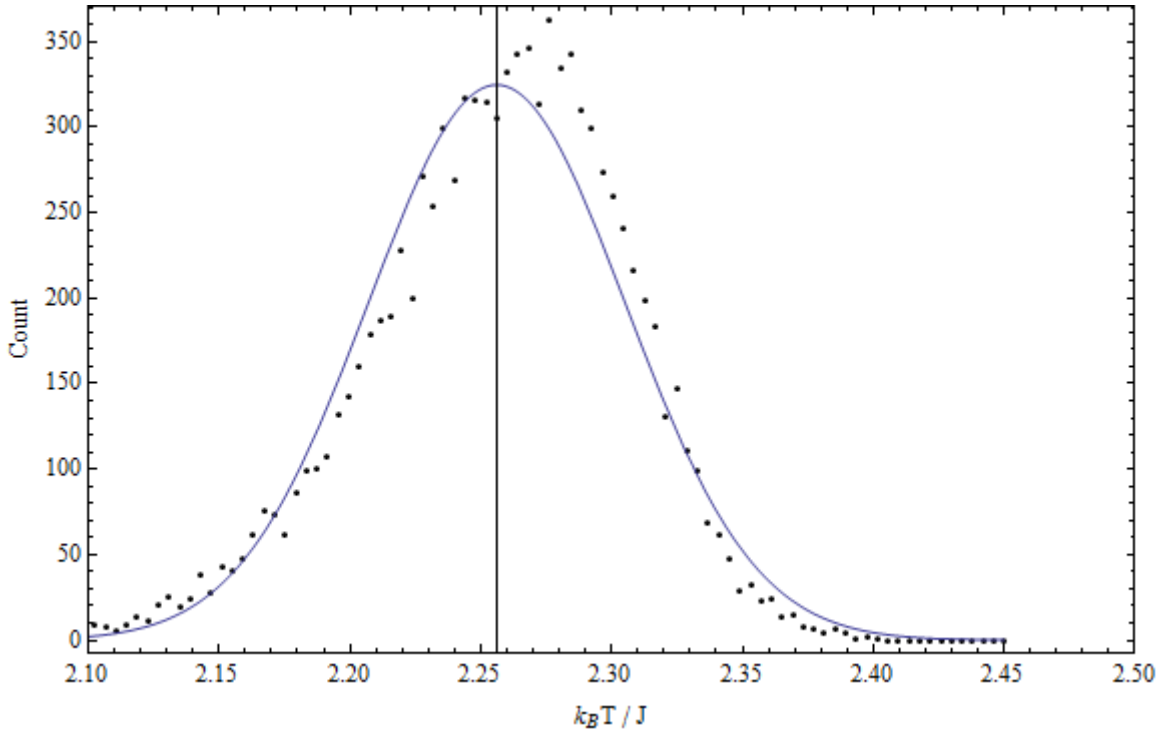


Figure 12: Histogram of 10,000 critical temperature measurements for a 24 x 24 lattice calculated by the Metropolis algorithm and the fitted Gaussian distribution. The mean is at $k_BT/J = 2.256$ and the coefficient of variation is 2.18%

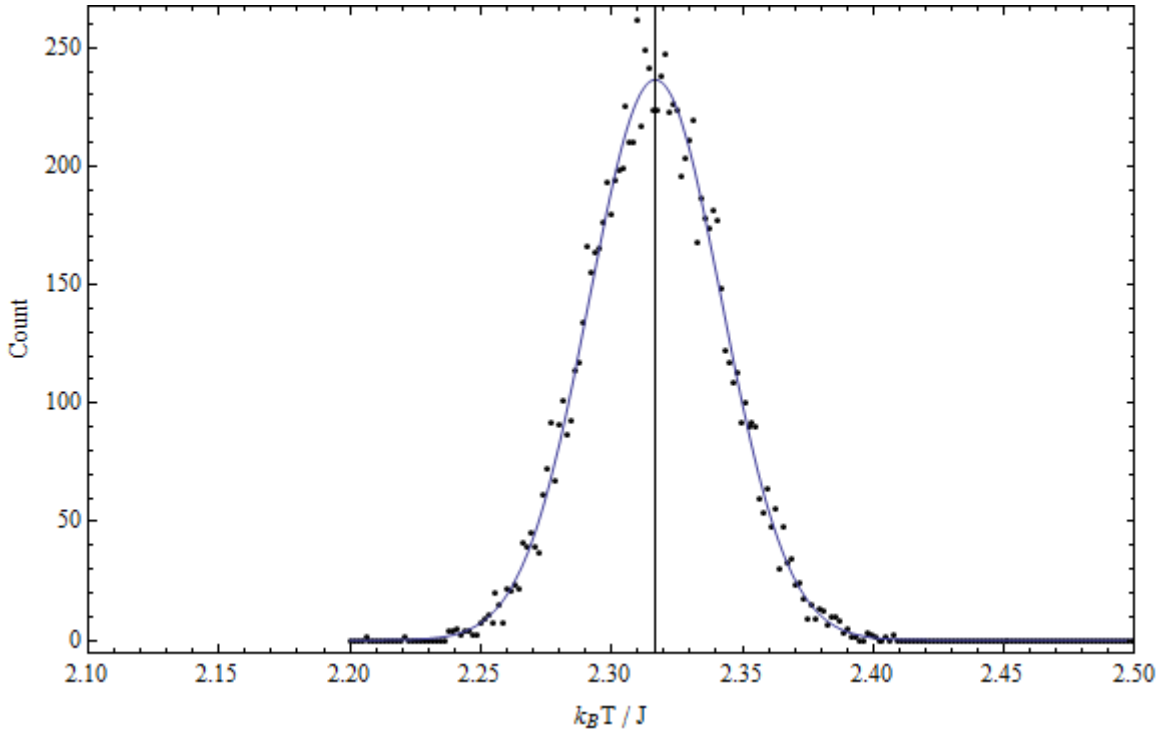


Figure 13: Histogram of 10,000 critical temperature measurements for a 24 x 24 lattice calculated by the Wang Landau algorithm and the fitted Gaussian distribution. The mean is at $k_BT/J = 2.299$ and the coefficient of variation is 1.31%

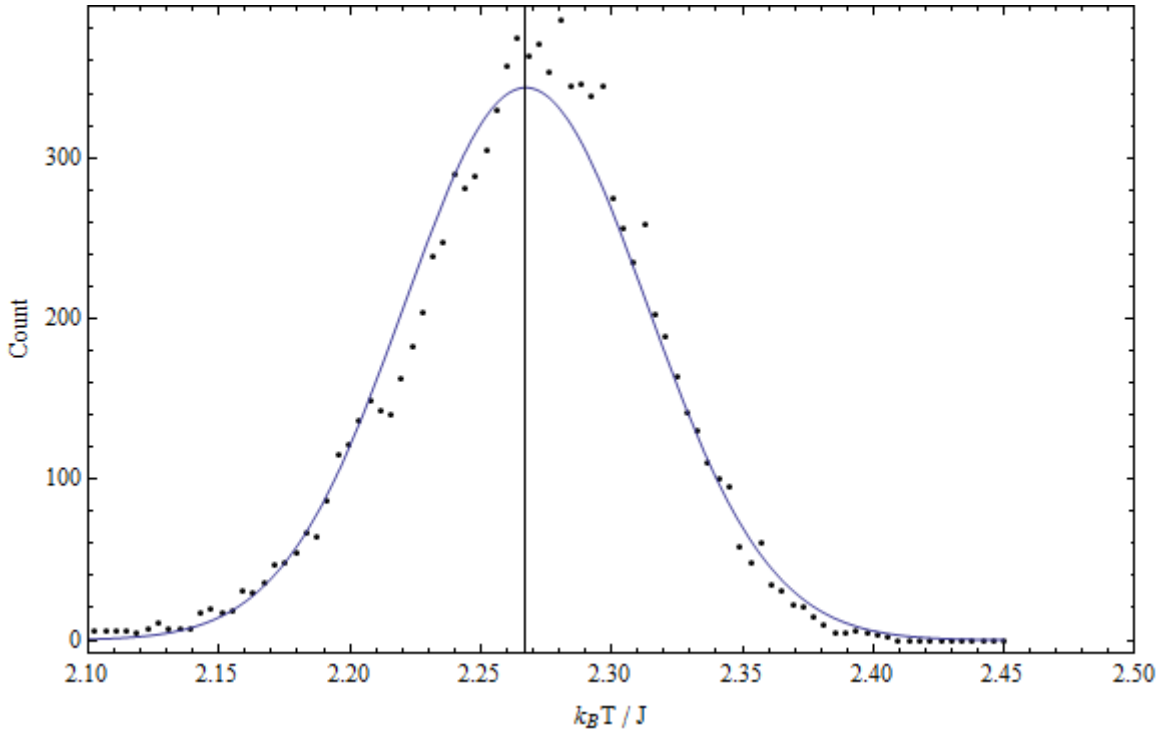


Figure 14: Histogram of 10,000 critical temperature measurements for a 32 x 32 lattice calculated by the Metropolis algorithm and the fitted Gaussian distribution. The mean is at $k_BT/J = 2.267$ and the coefficient of variation is 2.05%

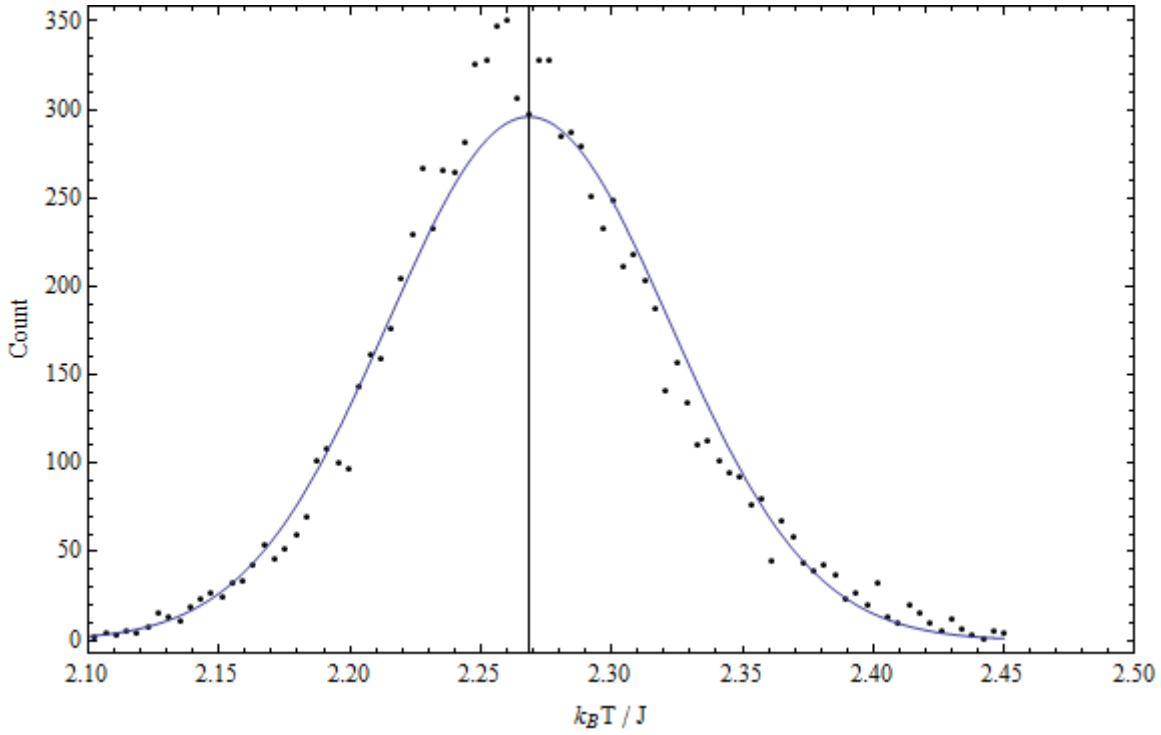


Figure 15: Histogram of 10,000 critical temperature measurements for a 64 x 64 lattice calculated by the Metropolis algorithm and the fitted Gaussian distribution. The mean is at $k_BT/J = 2.268$ and the coefficient of variation is 2.38%

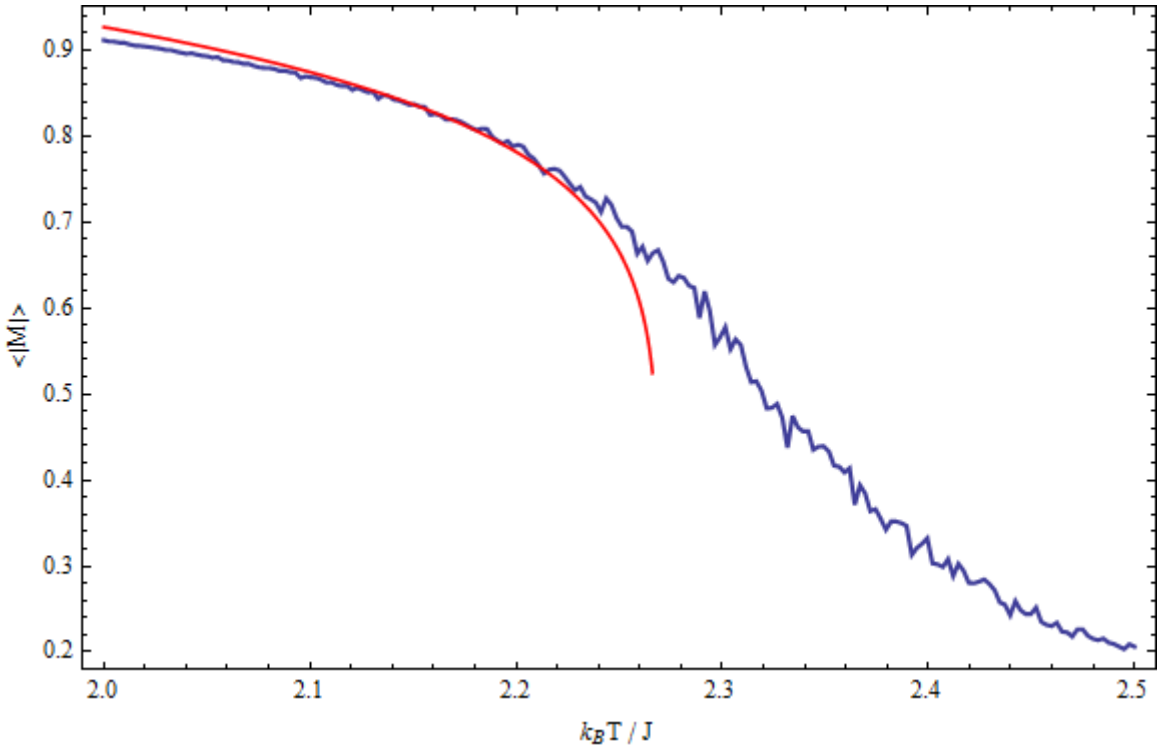


Figure 16: Fit of the average magnetization predicted using the critical theoretical power law and exponent, $\beta = \frac{1}{8}$ , (red line) to the calculated behaviour of a 32 x 32 lattice evaluated using the Metropolis algorithm (blue line).

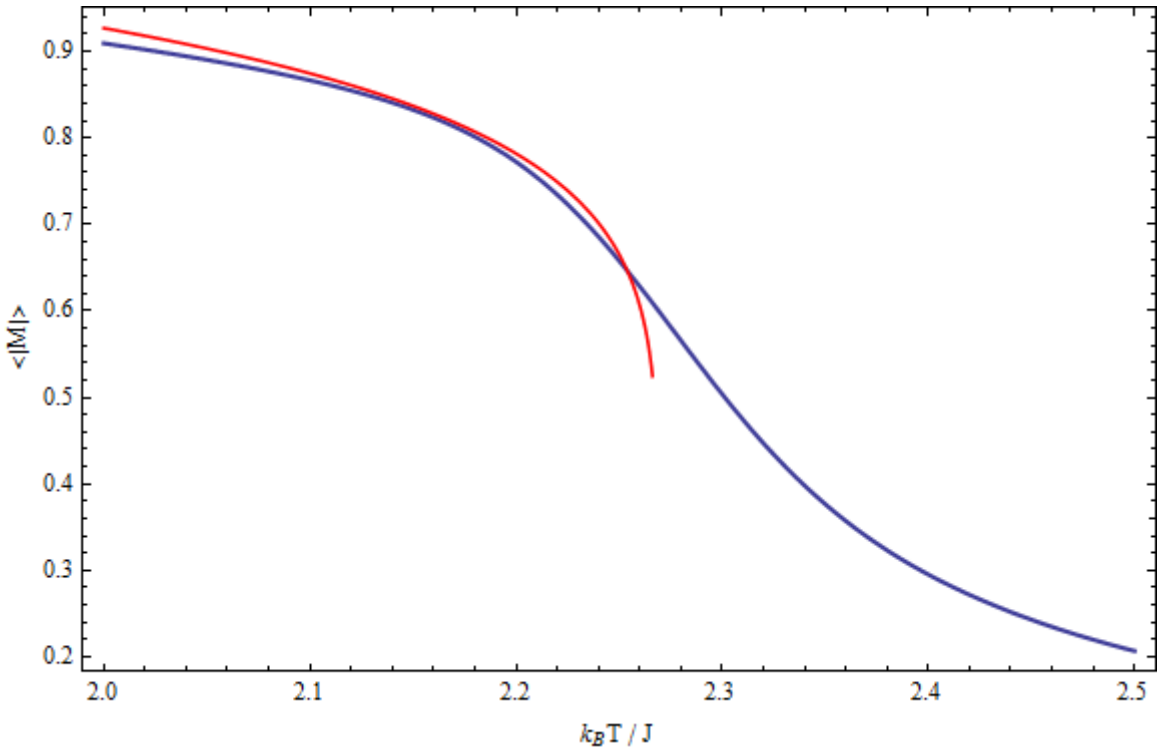


Figure 17: Fit of the average magnetization predicted using the critical theoretical power law and exponent, $\beta = \frac{1}{8}$ , (red line) to the calculated behaviour of a 32 x 32 lattice evaluated using the Wang Landau algorithm (blue line).

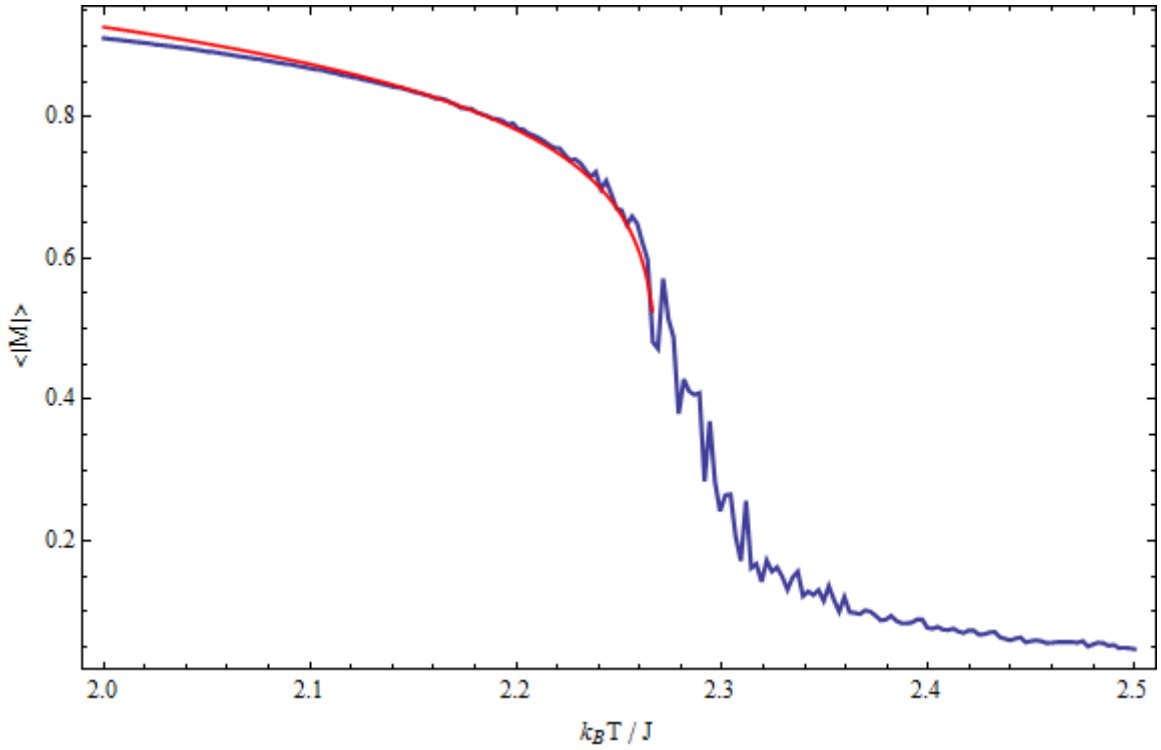


Figure 18: Fit of the average magnetization predicted using the theoretical critical power law and exponent, $\beta = \frac{1}{8}$ , (red line) to the calculated behaviour of a 128 x 128 lattice evaluated using the Metropolis algorithm (blue line).

# 5 Discussion

## 5.1 Success of the algorithms in computing the Ising model

The charts of the calculated Ising model state variables (magnetization, energy, and heat capacity) as a function of temperature are consistent between the two algorithms (Figs. 2 - 7) and also with other sources[7]. The expected Ising model phase transitions are visible in all of the 2, 3, and 4 dimensional cases (Figs. 2 and 3). In two dimensions, the critical temperature as indicated by charts appears close to the theoretically expected value (for an infinite lattice) of $k_B T/J = 2.27$ . This demonstrates that the implementations of both algorithms are, at least to a reasonable level of comfort, valid.

## 5.2 Ising model characteristics in three and four dimensions

In three and four dimensions the phase transitions seen in two dimensions are also visible but they occur at higher temperatures and are less sharply defined.

The higher temperatures of the phase transitions in three and four dimensions indicate that a greater quantity of thermal energy is required to disrupt the stable low temperature configuration. This may be because whilst in two dimensions each lattice site only forms bonds with four nearest neighbours, in three dimensions there are six nearest neighbour bonds and in four dimensions eight nearest neighbour bonds. With more bonds to be broken, more thermal energy is required to reach the disordered phase.

The decreased sharpness of the phase transitions in higher dimensions is probably just a consequence of the chosen lattice sizes rather than a genuine physical effect. It is known that in two dimensions that the phase transition becomes less pronounced as the span of the lattice decreases[7]. For reasons of computational efficiency (computing time was found to significantly increase with the higher dimensional cases), whilst a 32 x 32 lattice was used in two dimensions, in three and four dimensions the span of the lattices is only 8 atoms wide.

The measurement of heat capacity in four dimensions (Figs. 6 and 7) with both the Metropolis and Wang Landau algorithms resulted in a less smooth plot than for two or three dimensions. This is almost certainly

simply because the computation effort of both algorithms in four dimensions was not sufficiently increased to compensate for the larger lattice size.

### 5.3 Critical temperature dependence on lattice size

The estimation of the critical temperature for two dimensional lattices of different sizes (Figs. 8 - 15 and Table 3) demonstrates that the critical temperature for small lattices is notably different from the theoretical value for an infinite lattice. This can clearly be seen with, for example, Figs. 8 or 9, by comparing the theoretical value of $k_B T/J = 2.269$ with the results histograms and fitted Gaussians for the 8 x 8 lattice. For larger lattices (Figs. 14 and 15), the observed results come much closer to the theoretical value for an infinite lattice. This suggests that the difference between the observed critical temperature and the theoretical is a consequence of lattice size, rather than being an artefact of the algorithms and implementation.

However there does not appear to be an easily discernible trend in critical temperature with lattice size for smaller lattices. With the Metropolis algorithm, 8 x 8 and 16 x 16 lattices show a notably higher critical temperature than the theoretical value, while 16 x 16, 24 x 24, and 32 x 32 lattices show a slightly lower critical temperature than the theoretical value.

It is reasonable to expect that the critical temperature measured on small lattices would differ in detail from the theoretical result expected for an infinite lattice, since any assumptions in the theoretical derivation that rely on the lattice being infinite would not be valid with the small lattice. Perhaps it is more remarkable that lattices as small as 8 x 8 still show a phase transition that is broadly the same as that expected for an infinite lattice.

### 5.4 Critical temperature calculations compared between the Metropolis and Wang Landau algorithms

The critical temperature results differ somewhat between the Metropolis and Wang Landau algorithms. The 8 x 8 and 16 x 16 lattices evaluated with the Wang Landau algorithm also show a critical temperature higher than the theoretical value, but so does the 20 x 20 lattice.

For reasons of computational efficiency the 32 x 32 and 64 x 64 lattices were not examined with the Wang Landau algorithm. It was found that whilst the Wang Landau algorithm is fast and efficient for smaller lattices, with larger lattices the random walk often gets "stuck" in patterns that do not allow the histogram to become flat. The solution to this is to divide the available energy levels into a series of smaller ranges and evaluate them separately[4], but that implementation option went beyond the scope of the current project.

A further observation that may be significant is whilst that the fit of the Gaussian distribution to the results histograms looks acceptable for both algorithms, for the Metropolis algorithm there does appear to be some asymmetry of results about the mean. This is most easily seen with the 16 x 16 lattice results (Fig. 10).

### 5.5 Fit of the phase transition with the theoretical power law and critical exponents

As noted in the discussion of results, the theoretical critical power law behaviour for the phase transition is best matched by computational results with larger lattices that allow the emergence of a sharper phase transition.

### 5.6 Computational efficiency

Figs. 8 - 15 illustrate a smaller coefficient of variation with the Wang Landau algorithm as to the Metropolis algorithm. However this is not a like-for-like comparison because no attempt was made to tune the running parameters of the two algorithms for similar accuracy or matched computation time. Broadly, the running parameters were set so that each run of 10,000 trials would complete within 24 - 36 hours on a desktop PC with Intel i7 processor.

It was beyond the scope of this project to attempt a direct quantitative comparison of the efficiency of the two algorithms, but anecdotally it was clearly observed that the Wang Landau algorithm produced accurate results more quickly for small lattices. However as noted above, a more sophisticated implementation of the Wang Landau algorithm would have been required to investigate larger lattices.

# 6 Conclusions

The Ising model is a important system exhibiting phase transitions that can be investigated computationally with Monte Carlo methods such as the Metropolis and Wang Landau algorithms.

The two algorithms differ in their approach. The Metropolis algorithm directly simulates the fluctuations in the system while the Wang Landau algorithm uses a random walk to compute the density of states of the system followed by a numerical summation of the partition function.

The two dimensional, infinite Ising model has been solved theoretically and both the Metropolis and Wang Landau algorithms give results that correspond well with the theoretically expected values, especially for larger experimental lattices. For smaller lattices, there are notable differences between the the theoretical results and the results of the two algorithms.

Computationally, both algorithms are relatively straightforward to implement. Whilst a direct quantitative comparison of computational efficiency was not made, anecdotally the Wang Landau algorithm produces faster and higher quality results for small lattices but a more sophisticated implementation would be required to deal adequately with larger lattices. The Metropolis algorithm, on the other hand, is somewhat slower and produces rougher results, but the basic implementation is good for both small or large lattices, with the latter only requiring a increase in the allotted computation time.

Further work could include the following:

- A more exhaustive survey of the effects of the lattice size on the observed critical temperature.
- A specific investigation of how increasing the lattice size impacts the performance of the Wang Landau algorithm in its basic implementation.
- An investigation of larger lattices using the more sophisticated implementation of the Wang Landau algorithm.
- Further experimental measurements of the Ising model, such as the additional critical exponents beyond those governing heat capacity and magnetization or the parameters of higher dimensional lattices.

# References


[1] Metropolis, N., Rosenbuth, A.W., Rosenbuth, M.N., Teller, A.H., Teller, E., J. Chem. Phys. 21, 1087 (1953)

[2] Wang, F., & Landau, D. P. (2001). An efficient, multiple range random walk algorithm to calculate the density of states, 30602, 1–4.

[3] Zhou, C., & Bhatt, R. N. (2003). Understanding and Improving the Wang-Landau Algorithm. Physical Review E - Statistical, Nonlinear and Soft Matter Physics, 72(2 Pt 2)

[4] Schulz, B. J., Binder, K., Müller, M., & Landau, D. P. (2003). Avoiding boundary effects in Wang-Landau sampling. Physical Review E - Statistical, Nonlinear and Soft Matter Physics, 67(6 Pt 2)

[5] Lee, H. K., Okabe, Y., & Landau, D. P. (2005). Convergence and Refinement of the Wang-Landau Algorithm. Computer Physics Communications, 175(1)

[6] Caparica, A., & Cunha-Netto, A. (2012). Wang-Landau sampling: Improving accuracy. Physical Review E, 85(4), 1–9.

[7] Blundell & Blundell (2006-2010). Concepts in Thermal Physics. Oxford University Press.

[8] Knuth, D. E. (1998-2012). The Art of Computer Programming, Vol 2, Seminumerical Algorithms, section 3.6.

[9] The author, 2013. https://github.com/Anding/Project2013A

[10] Landau, R. H., Paez, M.J., & Bordeianu C. A Survey of Computational Physics. Princeton University Press

[11] Binney, J. J., Dowrick, N. J., Fisher, A. J., and Newman, M. E. J (1992) The Theory of Critical Phenomena, Oxford University Press

[12] Mark Tuckerman, http://www.nyu.edu/classes/tuckerman/stat.mech/lectures/lecture_26/node2.html

[13] Stephen Brush, Reviews of Modern Physics, volume 39, number 4, (1967)