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THE ISING MODEL - AN EMPIRICAL STUDY OF MONTE CARLO SIMULATIONS AND THE METROPOLIS ALGORITHM

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ABSTRACT

In this project we will study the thermodynamic properties of the 2-D Ising model using Monte Carlo methods with the Metropolis Algorithm as a selection rule for proposed spin configuration changes. Of particular interest is the behavior of the mean energy, mean magnetization, heat capacity, and magnetic susceptibility near the Curie Temperature. Using our results for finite lattices, we extrapolated the Curie Temperature for an infinite lattice to be 2.275 k_BT/J which yields a relative error of 2.562×10^{-3} when compared to the analytical value of 2.269 found by Lars Onsager (5). We also found that a significant speed up can be achieved by parallelization, roughly by a factor of 3.

Subject headings: Monte Carlo methods — Metropolis Algorithm — Thermodynamics

1. INTRODUCTION

The Ising model is a simple but informative model when studying phase transitions in magnetic systems. For a given critical temperature, also known as the Curie temperature, this model undergoes a second degree phase transition from having a finite magnetic moment to having zero magnetic moment. The model can be built out of either a 1D, 2D, or 3D collection of spins taking on binary values. It is convenient to take these spin values to be +1 and -1 to represent spin up and spin down. For a finite number of spins, both the 1D and 2D case have analytical values for several important expectation values.

The systems of interest for this project are 2D Ising models of various sizes. These systems are microcanonical in nature and therefore follow Boltzmann Statistics. We will begin our study by deriving the analytical results for heat capacity, magnetic susceptibility, mean magnetization, and mean energy for a simple 2×2 model. Thereafter we will study the same quantities for larger systems using Monte Carlo simulations along with the Metropolis algorithm to validate energy transitions. Finally, we will attempt and estimate the Curie temperature for in the limit of infinite lattice size using our results from finite lattices.

The paper consists of 5 main following sections. In the theory section, we provide the fundamental theory for setting up the problem, as well as the theory behind the algorithms used to study the model. In the methods section, we present details on the implementation of the algorithms. In the results section, we provide the main results, focusing on expectation values, energy probabilities, and Curie temperatures. We discuss the results in the discussion section, and provide closing thoughts in the conclusions section.

2. THEORY

2.1. *The Ising Model*

The 2D Ising model we will study is made up of a microcanonical ensemble of spins. This means that the system is thermally isolated and does not exchange particles with its environment. Each point in our $L \times L$ model represents a particle with a magnetic dipole that assume binary values. We will define these dipole, or spin values, s as

$$s = -1, +1 \tag{1}$$

where -1 represents spin down and +1 represents spin up. Without the presence of an external magnetic field the energy or this system is given by

$$E = -J \sum_{<k,l>}^{N} s_k s_l \tag{2}$$

where J is a coupling constant. The $< k, l >$ notation represents a sum over the nearest neighbors of the spin in question. Thus the energy of the system is a sum of magnetic dipole interactions between each spin and its nearest neighbors. The magnetization of the system can then be give as

$$M = \sum_{i}^{N} s_i \tag{3}$$

Note: J will be set to 1 in this study.

2.2. *Boltzmann Statistics*

For a given system of an unchanging number of particles at a fixed temperature T the probability of finding the system in a state with energy E_i is given by

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z} \tag{4}$$

where $\beta = \frac{1}{k_B T}$ with k_B representing the Boltzmann constant, E_i is the energy of the i^{th} microstate, and Z is the partition function given by

$$Z = \sum_{i=1}^{M} e^{-\beta E_i} \tag{5}$$

which is a sum over all microstates M. We can now conveniently calculate the expectation values for the physical

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quantities of the system using the expression

$$\langle X^n \rangle = \frac{1}{Z} \sum_{i=1}^{M} X^n e^{-\beta E_i} \tag{6}$$

where X^n is a quantity such as energy or magnetization.

2.3. *Thermodynamic Quantities and Phase Transitions*

Using 6, the expectation value for the energy of a given arrangement is

$$\langle E \rangle = \sum_{i=1}^{M} E_i P_i(\beta) = \frac{1}{Z} \sum_{i=1}^{M} E_i e^{-\beta E_i} \tag{7}$$

The variance of the energy is then defined as

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 \tag{8}$$

Finally, the specific heat at constant volume C_V can be given by

$$C_V = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2} \tag{9}$$

We can similarly define the magnetic susceptibility of the arrangement χ as

$$\chi = \frac{\langle M^2 \rangle - \langle M \rangle^2}{k_B T} \tag{10}$$

where the expectation values for M and M^2 are derived from 6.

Near the Curie temperature T_C and subsequent phase change, the heat capacity and magnetic susceptibility both diverge. The thermodynamic quantities follow power law behavior near this point

$$\langle M(T) \rangle \sim (T - T_C)^{\beta} \tag{11}$$

$$C_V(T) \sim |T_C - T|^{\alpha} \tag{12}$$

$$\chi(T) \sim |T_C - T|^{\gamma} \tag{13}$$

with $\beta = \frac{1}{8}$, $\alpha = 0$, and $\gamma = \frac{7}{4}$. Another quantity of interest is the correlation length ξ. For $T >> T_C$ the correlation length is on the order of the lattice point separations. As T approaches T_C, the spins become more correlated and ξ begins to exhibit divergent behavior given by

$$\xi(T) \sim |T_C - T|^{-\nu} \tag{14}$$

Due to computational limitations, we are always restricted to a finite lattice and thus ξ is proportional to our lattice size. Despite this, we are able to scale our results using finite scaling relations

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu} \tag{15}$$

where a is a constant and ν is defined in 14. a can then be calculated by comparing 15 for grids of two sizes L_1 and L_2 giving the following

$$a = \frac{T_C(L_1) - T_C(L_2)}{L_1^{-1/\nu} - L_2^{-1/\nu}} \tag{16}$$

15 can now be rearranged to solve for $T_C(L = \infty)$ using a given finite lattice size. The analytical Curie temperature for an infinite lattice is given by (5)

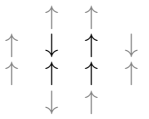
$$T_C(L = \infty) = \frac{2}{ln(1 + \sqrt{2})} \approx 2.269 \tag{17}$$

2.4. *Periodic Boundary Conditions*

To avoid discontinuous behavior at the edges of our lattice, we study our model using periodic boundary conditions. If we picture our lattice points as an $L \times L$ matrix, all points along the edge of the matrix are missing one of their nearest neighbors. To remedy this we say that if a point is on the edge, say somewhere in the top row, its missing top 'neighbor' is replaced by the particle at the bottom of its column. This is done similarly for points on the left, right and bottom edges.

2.5. *2 × 2 Analytical Solution*

For any lattice of size L, we have L^2 lattice points and thus 2^{L^2} possible spin configurations. The 16 configurations for a 2×2 lattice consist of permutations of the following grid



here, the light arrows present a visual for the periodic boundary conditions. Using 2 and 3 we calculate the Energies and Magnetizations for the various configurations

# of Spin Up	Multiplicity	Energy	Magnetization
4	1	-8J	4
3	4	0	2
3	2	8J	0
2	4	0	0
1	4	0	-2
0	1	-8J	-4

We now use 5 to calculate Z

$$Z = \sum_{i=1}^{16} e^{-\beta E_i} = 2e^{-8J\beta} + 2e^{8J\beta} + 12 = 4cosh(8J\beta) + 12 \tag{18}$$

With Z in hand, 4 becomes

$$P_i(\beta) = \frac{e^{-\beta E_i}}{4cosh(8J\beta) + 12} \tag{19}$$

We are now interested in finding $\langle E \rangle$, $\langle E^2 \rangle$, $\langle M^2 \rangle$, $\langle M \rangle$, C_V, χ.

$$\langle E \rangle = \sum_{i=1}^{16} E_i P_i(\beta) = -\frac{8Jsinh(8J\beta)}{cosh(8J\beta) + 3} \tag{20}$$

$$\langle E^2 \rangle = \sum_{i=1}^{16} E_i^2 P_i(\beta) = \frac{64J^2 cosh(8J\beta)}{cosh(8J\beta) + 3} \tag{21}$$

$$C_V = \frac{1}{k_B T} \left(\frac{64J^2 cosh(8J\beta)}{cosh(8J\beta) + 3} - \left(\frac{8Jsinh(8J\beta)}{cosh(8J\beta) + 3} \right)^2 \right) \tag{22}$$

$$\langle M \rangle = \sum_{i=1}^{16} M_i P_i(\beta) = 0 \tag{23}$$

$$\langle M^2 \rangle = \sum_{i=1}^{16} M_i^2 P_i(\beta) = \frac{8e^{8J\beta} + 8}{cosh(8J\beta) + 3} \tag{24}$$

$$\chi = \frac{1}{k_B T} \frac{8e^{8J\beta} + 8}{cosh(8J\beta) + 3} \tag{25}$$

Since $\langle M \rangle = 0$ for this configuration, we also consider $\langle |M| \rangle$ given by

$$\langle |M| \rangle = \sum_{i=1}^{16} |M_i| P_i(\beta) = \frac{2e^{8J\beta} + 4}{cosh(8J\beta) + 3} \tag{26}$$

These expressions can now but used to validate our algorithm by solving for computationally solving the 2×2 case.

2.6. *Monte Carlo and Metropolis Algorithm*

Our problem will be initialized by a grid of either random or ordered spins that will evolve with time to an equilibrium energy configuration for a given temperature. Advancing forward in time in our problem will be represented by progressing through a given number of Monte Carlo cycles. Here, a general explanation of the algorithm will be given, with more details given in Section 3.

We first use 2 and 3 to calculate the initial energy and magnetization of the $L \times L$ system. We then loop over a given number of Monte Carlo cycles. During each cycle, we loop over the grid L^2 times, each time picking a random spin and flipping it. We calculate the energy and magnetization change of the system for the flip of each spin s_l by

$$\Delta E = 2 s_l \sum_{<k>} s_k \tag{27}$$

$$\Delta M = 2 s_l \tag{28}$$

In our problem, each spin only sees its four nearest neighbors resulting in five possible ΔE values

$$\Delta E = [-8j, -4J, 0, 4J, 8J] \tag{29}$$

We now employ the Metropolis algorithm as an acceptance rule for each spin flip. A thorough treatment of the topic is given in Chapter 13 of (4). We do not know the explicit transition or acceptance probability for this system. We can bypass this problem by taking a ratio of the probabilities of the two states in question and applying an acceptance rule to it. Our probability ratio for the transition from E_i to E_j is

$$A(i \to j) = \frac{P(E_j)}{P(E_i)} = e^{-\beta \Delta E} \tag{30}$$

where $\Delta E = E_j - E_i$. We now impose the condition to only accept this transition if

$$\zeta \leq e^{-\beta \Delta E} \tag{31}$$

where ζ is a random number between 0 and 1 drawn from the uniform distribution. This acceptance rule allows us to always accept transitions to lower energy states while sometimes accepting the less likely transitions to higher energy states, thus preserving the possibility to reach all possible states from any given starting configuration. If the transition is accepted, the spin flip and and new total grid energy are calculated. The E, E^2, $|M|$, and M^2 are then updated and the next Monte Carlo cycle begins.

3. METHODS

In this section we will describe the methods we utilized to acquire our results.

3.1. *Code*

The main simulations are run in the file *mainPara.cpp*. There is also an unparallelized version used to acquire results for the equilibrium time and the different thermal quantities as a function of Monte Carlo cycles, called *main.cpp*. The results are then saved to text files, and imported and plotted in python, in the files *plot2.py* for the thermal quantities and critical temperature, and *plot.py* for the equilibrium time estimation. The estimation of the Curie temperature is also done in the program *plot2.py*.

3.2. *Algorithm*

The overarching algorithm structure in the program is outlined in the following pseudo-code.

```
for temp_iterations
    for mc_iterations
            for flip_iterations
                >Pick a random r
                >Pick random lattice point to flip

                if r<= precalculated e^(-beta(E_j-E_i))
                    >accept flip
                    >calculate E and M
                end if
            end for
    end for
    >save relevant expectation values
end for
```

The algorithm is run for $1E6$ Monte Carlo cycles, and an equilibrium time of $1E5$, I.E. we don't start collecting statistics before $1E5$ MC cycles. This is more than our previously calculated equilibrium time of $1E4$, but we found that the statistics will be even more stable, as long as you have the computational power for it.

3.3. *Smoothing and polynomial fitting for the Curie temperature*

For smoothing the values of C_v and χ, we use a Savitzky-Golay filter, from the *scipy.signal* library. We use a windows size of 5, and a polynomial degree of 3. For acquiring the critical temperature, we use the *np.polyfit* from the numpy library, with polynomial degree of 1.

3.4. *Parallelization*

We used MPI to make our program parallel. The temperature loop is divided with equal work between the different cores. We ran the program on 4 cores. The parallelization is initialized through this code snippet

```
    MPI_Init (&argc, &argv);
    int numprocs;
    MPI_Comm_size (MPI_COMM_WORLD, &numprocs);
    int my_rank;
    MPI_Comm_rank (MPI_COMM_WORLD, &my_rank);
    ...
    int N_temp = 32;
    int N_temp_local = (N_temp) / numprocs;
    double T_start_local=T_start + my_rank*delta_T*N_temp_local;
    double T_end_local=T_start + (my_rank+1)*delta_T*N_temp_local -
        delta_T;
    arma::vec
        T_vec=arma::linspace(T_start_local,T_end_local,N_temp_local);
```

such that every core gets their own unique vector of temperature values to loop over. The number of temperature points, N_{temp} should be divisible by the number of cores to avoid complications. The parallel regions are finally gathered in the root process via the *MPI_ Gather* function.

4. RESULTS

4.1. $L = 2$ *Study*

We will first analyze a system of $[2 \times 2]$ spins at a fixed temperature unit-less temperature $T = 1.0 k_B T/J$. In the following plots, Each Monte Carlo cycle can be interpreted as a unit of time.

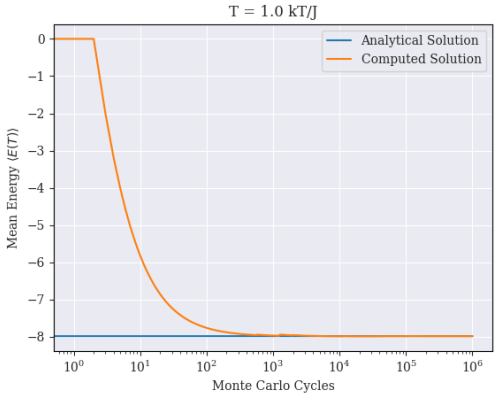


FIG. 1.— The evolution of $\langle E(T) \rangle$ as a function of time for a fixed temperature $T = 1.0$. The blue line represents the analytical solution calculated in Subsection 2.5.

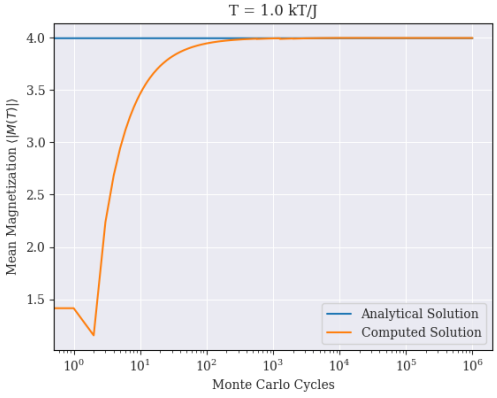


FIG. 2.— The evolution of $\langle |M(T)| \rangle$ as a function of time for a fixed temperature $T = 1.0$. The blue line represents the analytical solution calculated in Subsection 2.5.

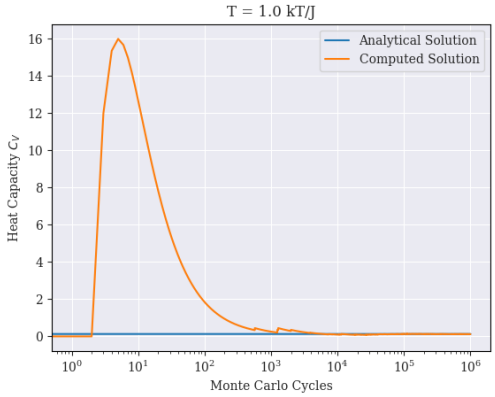


FIG. 3.— The evolution of C_V as a function of time for a fixed temperature $T = 1.0$. The blue line represents the analytical solution calculated in Subsection 2.5.

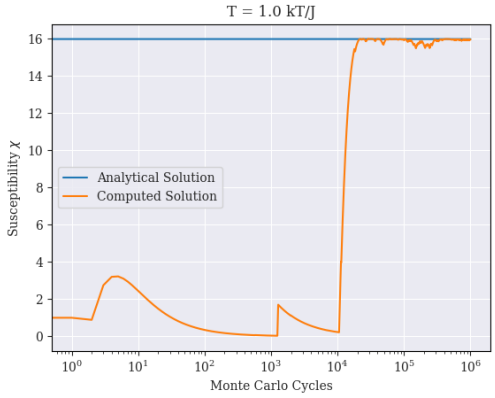


FIG. 4.— The evolution of χ as a function of time for a fixed temperature $T = 1.0$. The blue line represents the analytical solution calculated in Subsection 2.5.

4.2. $L = 20$ *study*

Next we will study a $[20 \times 20]$ lattice. This lattice will be initialized with both ordered and random starting spin configurations. The property of interest is how quickly the system converges to the expectation values for both E and $|M|$. We will also study the number of spin flips as a function of Monte Carlo cycles and the probability of being in given energy configurations.

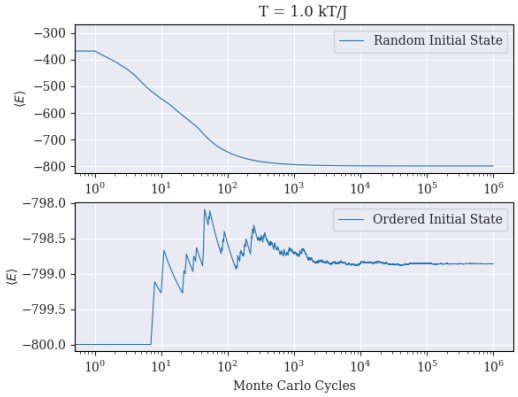


FIG. 5.— The evolution towards $\langle E \rangle$ is shown above for $T = 1.0$ Note the y-scale difference between the ordered and random starting configurations.

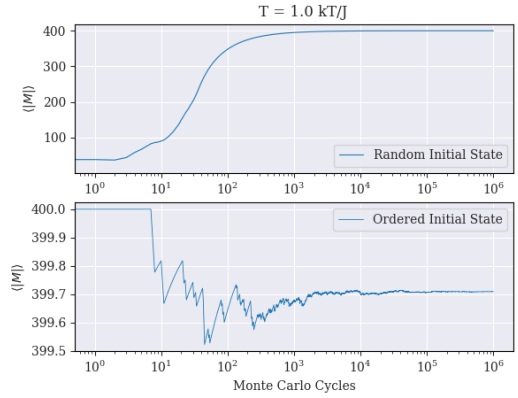


FIG. 6.— The evolution towards $\langle |M| \rangle$ is shown above for $T = 1.0$ Again, note the y-scale difference between the ordered and random starting configurations.

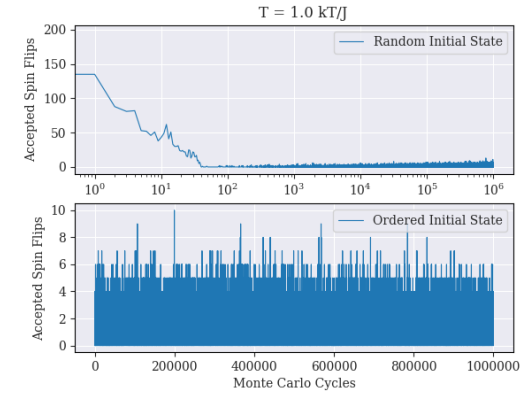


FIG. 7.— Here we see the accepted spin flips versus Monte Carlo cycles for $T = 1.0$. Note the low occurrence of flips for the ordered state vs the random state.

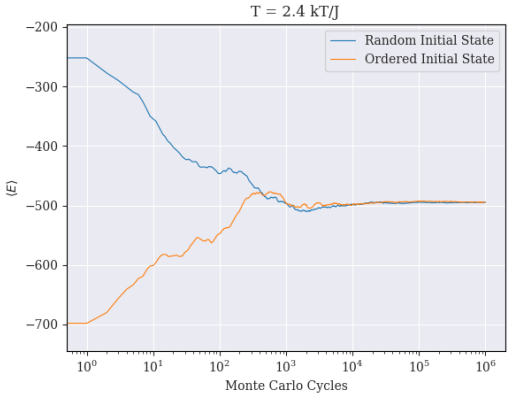


FIG. 8.— The evolution towards $\langle E \rangle$ is shown above for $T = 2.4$. We observe noticeably different convergence behavior than for the lower temperature system.

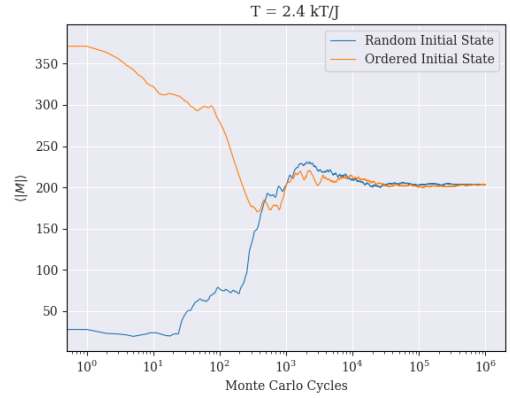


FIG. 9.— The evolution towards $\langle |M| \rangle$ is shown above for $T = 2.4$. As with $\langle E \rangle$, we observe noticeably different convergence behavior than for the lower temperature system.

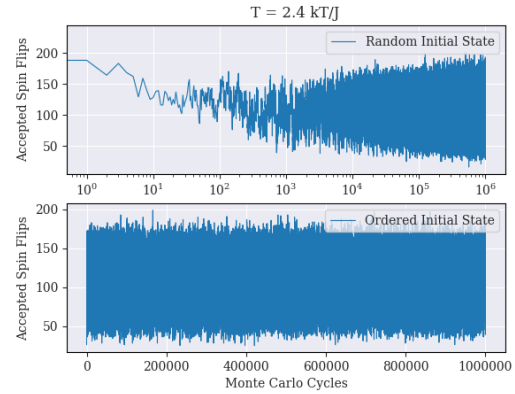


FIG. 10.— Here we see the accepted spin flips versus Monte Carlo cycles for $T = 2.4$. Note the high occurrence of flips for both the ordered and random states.

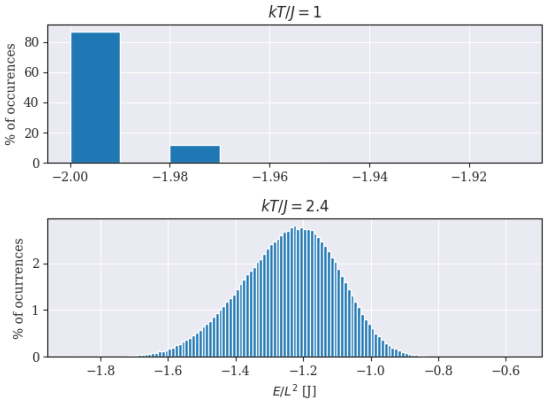


FIG. 11.— Above are the probabilities of being found in an energy configuration that gives a specific energy per spin. Note the distribution difference between $T = 1.0$ and $T = 2.4$.

The variances for the distributions in Figure 11 were calculated to be

k_BT/J	$\sigma_E^2[J^2]$
1.0	6.5175×10^{-5}
2.4	2.0181×10^{-2}

4.3. *Curie Temperature*

Now we have studied the system for fixed temperature, we will observe the quantities $\langle E\rangle$, $\langle|M|\rangle$, C_V, and χ as functions of both temperature and lattice size. We are interested in studying the effect of lattice size on the Curie Temperature which is where the system undergoes a second degree phase change. For an ideal infinite $2-D$ lattice $T_c = 2.269$.

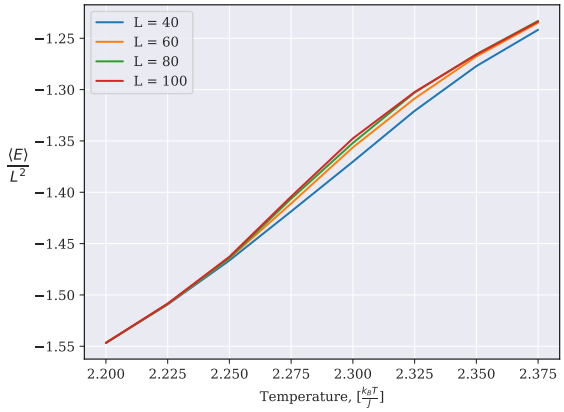


FIG. 12.— $\langle E\rangle$ as a function of temperature and lattice size. Here, the energies have been normalized by the number of spins in the grid.

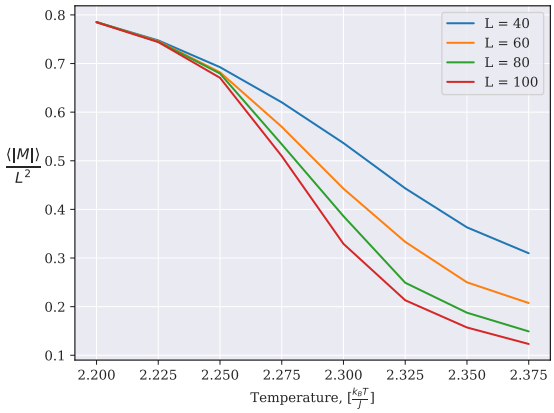


FIG. 13.— $\langle|M|\rangle$ as a function of temperature and lattice size. Here, the energies have been normalized by the number of spins in the grid.

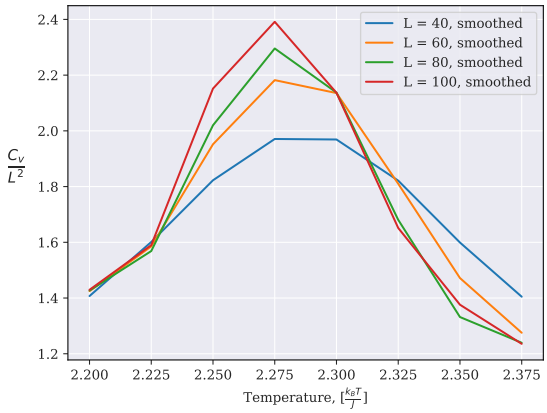


FIG. 14.— C_V as a function of temperature and lattice size. Here, the peaks of the lines are the Curie Temperature for the respective lattice size.

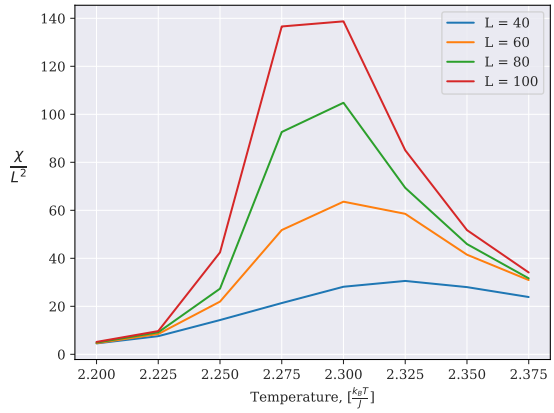


FIG. 15.— χ as a function of temperature and lattice size. Here, the peaks of the lines are the Curie Temperature for the respective lattice size.

TABLE 1
Calculation of $T_c\,(L = \infty)$ using the both the heat capacity and susceptibility, with and without a Savitzky-Golay filter.

Source	T_c	Total error	Relative error
C_v	2.254	$1.564 \cdot 10^{-2}$	$6.891 \cdot 10^{-3}$
Smoothed C_v	2.275	$5.815 \cdot 10^{-3}$	$2.562 \cdot 10^{-3}$
χ	2.279	$9.362 \cdot 10^{-3}$	$4.126 \cdot 10^{-3}$
Smoothed χ	2.279	$9.362 \cdot 10^{-3}$	$4.126 \cdot 10^{-3}$

4.4. *Optimization and speed up*

TABLE 2
Runtime of the temperature loop with and without optimization. All comparisons were run with 1E4 MC cycles just for comparing speed up, final results acquired with 1E6 MC cycles. The optimization flag used was -O3.

Spin	1 core	Parallel	Parallel&flag	Parallel(1E6)
40	51.47s	20.60s	13.51s	20.9m
60	240.6s	84.59s	69.75s	1.95h
80	732.6 s	224.7s	193.3s	5.5h
100	1574 s	484.0s	450.1 s	13.1 h

5. DISCUSSION

Beginning with a simple $[2 \times 2]$ lattice at a fixed temperature of $T = 1.0$, figures 1 and 2 show the mean magnetization and energy to approach there respective analytical values at around 10^3 Monte Carlo Cycles. The heat capacity C_V seen in 3, and especially the susceptibility χ seen in 4, exhibit less desirable behavior. While χ eventually approaches its analytical value just after 10^4 Monte Carlo cycles, it does not behave as smoothly as the other three once it nears its analytical value. This is a good sanity check to ensure that our algorithm approaches the proper value as time progresses.

We then increase the lattice size to $[20 \times 20]$ and consider systems for $T = 1.0$ and $T = 2.4$. From figures 5 and 6 we see that by starting in an ordered configuration (in this case all spin up) the system is already very close to its lowest energy state for $T = 1.0$. Interestingly, while the random initial state begins much farther away from the lowest energy state, it takes roughly the same 10^4 Monte Carlo cycles to reach the favorable state that it takes the ordered state. Figure 7 shows the large disparity between number of accepted spin flips between the ordered and random systems. When starting in an ordered system, the maximum amount of spin flips for one Monte Carlo cycle is 10. The maximum for the disordered system is roughly 140.

We notice slightly different behavior for the system when increasing the temperature from $T = 1.0$ to $T = 2.4$. Figures 8 and 9 show that both the ordered and disordered states must change significantly to reach the lowest energy state. One point to note is that for $\langle E \rangle$ and $\langle |M| \rangle$ to stabilize, it still takes roughly 10^4 Monte Carlo cycles. This is the same as it took for $T = 1.0$. For $T = 2.4$, we also see from Figure 10 that the number of accepted spin flips for the entire calculation remains somewhere between 50 and 160. This is significantly higher than the results for $T = 1.0$. Because of this, the system has higher likelihood to be found in different spin configurations with different energy expectation values. This is property is illustrated by Figure 11 which shows the probabilities of finding the system in a certain energy per spin state. For $T = 1.0$ we only get non negligible probabilities for two energies and a small variance of 6.5175×10^{-5}, while the results for $T = 2.4$ show more of a Gaussian behavior with a variance of 2.0181×10^{-2}.

Next the behavior of the Ising model around the Curie temperature is explored. We run our code to calculate the expectation value of the energy $\langle E \rangle$, the expectation value of the absolute value of the magnetization $\langle |M| \rangle$, the heat capacity C_V, and the susceptibility χ per particle in the lattice. This is done using 10^6 Monte Carlo cycles and only considering data points after the lattice had reach its energy expectation value. We loop over a range of 8 temperatures in the range $[2.2, 2.4)$ for lattices of size 100, 80, 60, and 40. Figures 12, 13, 14, and 15 show the resulting behavior. Notice that for each lattice size, the C_V and χ peak at slightly different temperatures. We then take these points and perform a polynomial fit described in 3.3 to find the Curie temperature for an infinite lattice. These results displayed in Table 1 are in good agreement with the theoretical value shown in equation 17 in section 2.3. When applying the Savitzky-Golay filter to smooth our C_V function, we obtained a total error of $5.815 \cdot 10^{-3}$, and a relative error of 2.562×10^{-3}.

The parallelization of the program showed a significant speedup, with an average speed up of a factor of 2.96. This speed up is very significant for run times as long as these, as the longest simulation would take around 39 hours compared to 13 hours. Adding compiler flag -O3 also showed an average speed up of factor 1.24. Not as significant, but still helpful in large calculations.

6. CONCLUSIONS

In this project we have simulated a lattice of particles with different spins, using Monte Carlo simulation and the Ising model. We found that the numerical results match very well with the analytically derived value by Lars Onsager. We also found that the system consistently reached the most likely state at 1E4 Monte Carlo cycles, regardless of lattice size and temperature. Moving forward, one could acquire more statistically significant results by increasing the amount of Monte Carlo steps. One could also test for more temperatures, to get a higher resolution result for the thermal quantities as a function of temperature.

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7. APPENDIX

All source code, data and figures can be found at the github repository: https://github.com/marbjo/FYS4150/tree/master/Project4