2D Ising Model Simulation with Varying Adjacent Site Configurations

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I. Introduction

The Ising model is a model which displays the thermodynamic properties of a ferromagnet by simulating the interactions of N^2 atoms (or spin-sites) on an $N \times N$ grid. The simulation flips a random spin-site by a factor of -1 and if the change in spin causes the energy change in the system to follow the Boltzmann Distribution, then the model saves that change.

The change in energy is proportional to the sum of the spin-states adjacent to the test spin-site, typically the 2D ising model considers the spin sites $S_{i+1,j}$, $S_{i,j+1}$, $S_{i-1,j}$, and $S_{i,j-1}$ to be adjacent to a spin site $S_{i,j}$. In this experiment, different definitions for adjacent spin-sites are implemented to observe how the physical properties and structure of the lattice change over time and over temperature.

II. Background and Theory

The $2D$ Ising model contains some characteristics not present in the $1D$ Ising model, such as phase transitions. These transitions can be observed qualitatevly by watching how the structure of the model gradually decomposes, and quantitavely via notable inflection points in the energy E, magnitization M, and specific heat C_v vs k_bT graphs.

The initial energy of the state is determined by implementing a checkerboard algorithm over the state, and is vectorized to improve effiency. In the following function, $Roll(\vec{V}, n)$ is defined to rotate all elements in a vector $\vec{V}$ by n indices, with end elements rotating to the front. Therefore, the total energy of a state composed of R row vectors and C column vectors, with transfer energy J, magnetic moment μ, in a magnetic field B is given by

$$E = -J\sum_{0}^{R} Roll(\vec{V_R}, 1)\cdot\vec{V_R} + \sum_{0}^{R} -\mu B\vec{V_R}\cdot\vec{I} - J\sum_{0}^{C} Roll(\vec{V_C}, 1)\cdot\vec{V_C} + \sum_{0}^{C} -\mu B\vec{V_C}\cdot\vec{I} \tag{1}$$

Where $\vec{I}$ is the identity matrix. M is given simply by

$$\sum_{i,j} S_{i,j} \tag{2}$$

and C_v is given by

$$C_v = \frac{1}{N^2}\frac{\langle E\rangle^2 - \langle E^2\rangle}{k_B T^2} \tag{3}$$

The change in energy ΔE depends on how we define what is considered adjacent spin-sites, and is detailed in **Section III**. In matter, the shape of the electron orbitals influence what are adjacent spin-sites. For example, if two sheets of a material are parallel in the $x-z$ plane, and have electron orbitals that extend in the $x-z$ plane, then the two sheets do not interact and the interacting neighbors would only be along the $x-z$ plane, but if the electron orbitals span the $x-y$ plane, then the two sheets are able to interact. When the adjacent spin-sites of $S_{i,j}$ are defined to include all 8 adjacent neighbors (including the diagonal

elements) then we begin to see the structure of the material begin to resemble a maze like pattern, seemingly similar to bizmuth (although I am uncertain if bizmuth's electron configuration matches this definition of adjaceny).

III. Implementation

This simulation follows from the logic behind the Metropolis algorithm and Monte Carlo methods. For each temperature kt in the domain of all temperatures T, run the simulation for given values of J, μ, and B. Calculate the initial energy (as described above) and the initial magnetization. Generate a list of random spin-site locations, the length of which is the number of time steps to iterate for. In this simulation we chose 20 times the number of spin-sites. For each coordinate co in our list, multiply the value of the spin-site by -1. If the change in energy follows the Boltzmann's distribution, we keep the change, and update our values of energy. The change in magnitization is also calculated. After the simulation runs for that value of kt, the energy versus time is plotted, and other physical parameters are recorded. After the simulation is done running for all valus of kt, the average equilibrium energy vs kT, the average magnitzation vs kT and the specific heat versus kT are plotted. Finally, an animation is rendered showing how the simulation changes from our initial kT to our final, for all time steps.

ΔE depends on the definition of what is an adjacent spin-site. Our trials included three main definitions for adjacent sites: grid-adjacent, all-adjacent, and diag-adjacent. Grid-adjacent is defined above in the **Introduction** and is the standard used in the 2D Ising model. All-adjacent is defined to include the diagonal sites as well, and diag-adjacent is only the diagonal components.

IV. Results

Figures 1 through 12 are provided below, and contain for each different site adjacency type the energy vs time graphs at $kT = 1$, the average energy vs kT, the average magnitzation vs kT, and the specific heat vs kT. The source code for this project, as well as pdfs containing the energy vs time graphs for each kT, as well as animations displaying the change in our state configuration, are all available in the zipped filesystem this report is contained in.

Grid-adjacent

Figure 1: *(left)* Plot of Energy vs Time for $kT = 1$

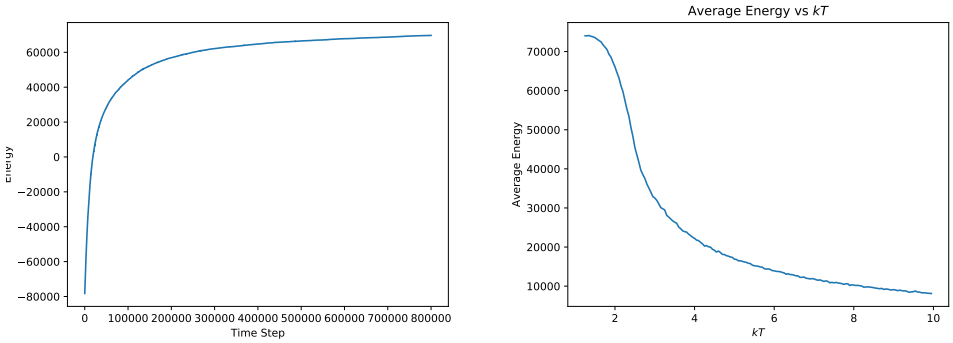

Figure 2: *(right)* plot of average energy vs kt. note an inflection at $kt \approx 2.5$, which is evidence of a phase transition.

Figure 3: *(left)* Plot for average equilibrium magnitzation vs temperature. Note after a value of $kT \approx 2.5$ it begins to equilbriate.

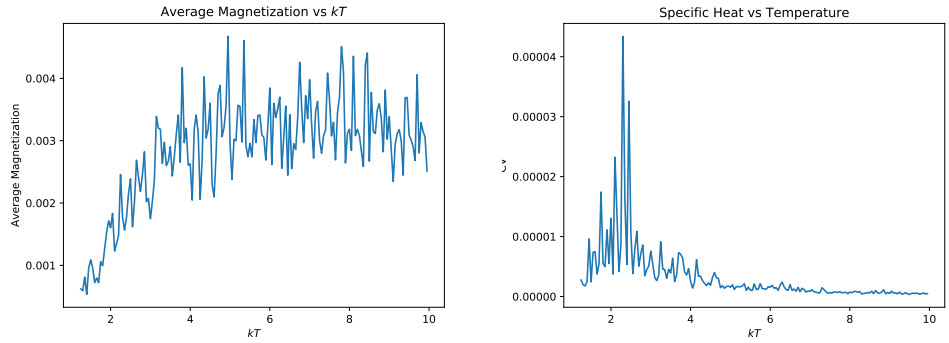

Figure 4: *(right)* Plot for specific heat vs temperature. Note a peak at $kT \approx 2.5$, also indicating a phase transition.

All-adjacent

Figure 5: *(left)* Plot of Energy vs Time for $kT = 1$

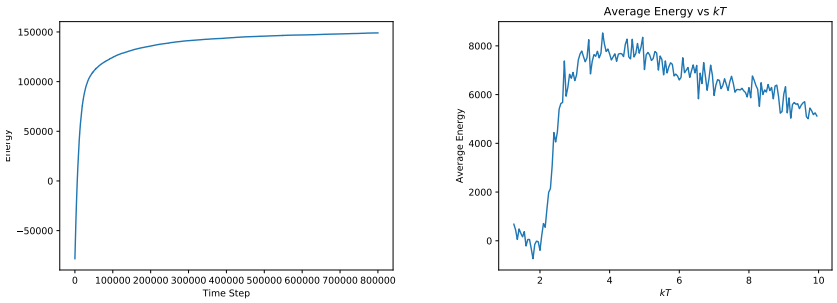

Figure 6: *(right)* plot of average energy vs kt. note an inflection at $kt \approx 2.2$, which is evidence of a phase transition.

Figure 7: *(left)* Plot for average equilibrium magnitzation vs temperature. Note after a value of $kT \approx 2.2$ it begins to equilbriate.

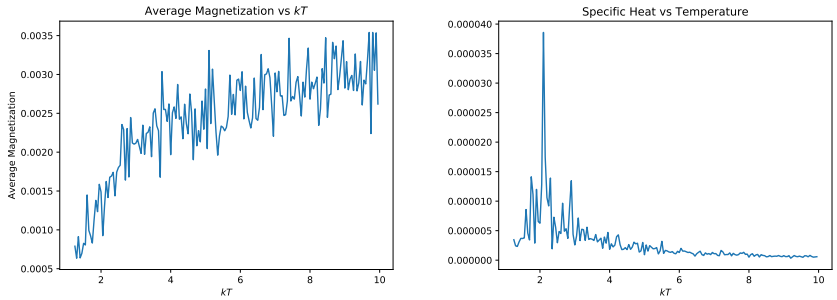

Figure 8: *(right)* Plot for specific heat vs temperature. Note a peak at $kT \approx 2.2$, also indicating a phase transition.

Diag-adjacent

Figure 9: *(left)* Plot of Energy vs Time for $kT = 1$

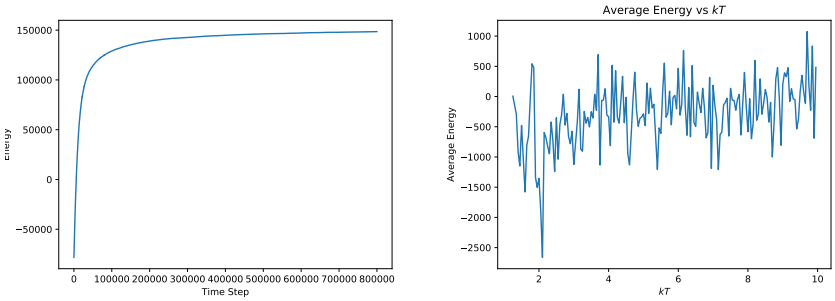

Figure 10: *(right)* plot of average energy vs kt. This graph is very noisy and no inflection point seems immediately discernable.

Figure 11: *(left)* Plot for average equilibrium magnitzation vs temperature. Due to the noise this graph is hard to determine a phase transition temperature

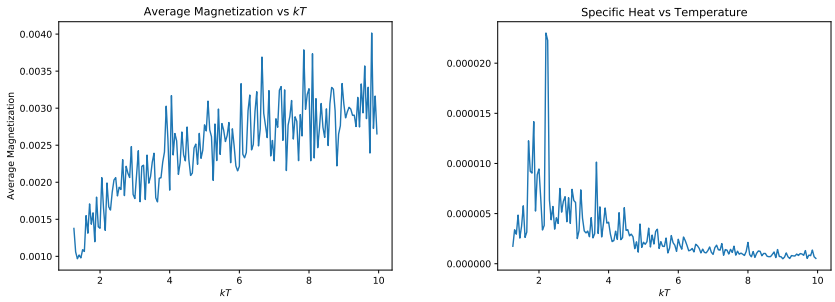

Figure 12: *(right)* Plot for specific heat vs temperature. Note peaks at $kT \approx 1.8$ and $kt \approx 2.1$

V. Analysis

Comparing the graphs to the analytical solutions provided in the textbook *Computational Physics: Problem Solving with Python* by Rubin H. Landau, Manuel J. Paez, and Cristian C. Bordeianu, my graphs for the grid-adj configuration appears flipped vertically for both the average energy and the average magnitization. The simulation was ran multiple times, with different methods for calculating E, ΔE, and M but yielded the same results. The inflection points occur at roughly the same value for kT however, which is a promising sign that the simulation shows some sign of success. The magnitization also appears flipped, as in my model the initial average magnitization is zero and jumps to its maximum after the phase transition, the book has it initially at a maximum and dropping to zero. The Specific heat graph looks promising for this configuration, as we have a peak right at $kT \approx 2.5$, in agreement with the text.

The all-adjacent configuration has similar defects as the grid-adjacent configuration - flipped values for average energy and average magnitization but the specific heat is nominal. It appears in this configuration the critical temperature is a little lower - closer to 2.2 - than in the previous configuration. We can see this critical change occur at a value of kT in **Figure 7** as the slope becomes less steep.

Lastly, the diag-adjacent configuration looks the least promising to deliver any interesting results, as it almost appears to have two critical temperatures on **Figure 12**. The average energy does not behave consistently with the other graphs, so it is unlikely to make any strong conclusions from this particular model.

VI. Conclusion

Although the diag-model appears to be a failure, there is still a possibility that it is accurate, implying atoms with electrons that are aligned 45° off from the material they constitute really do exhibit these properties. Additionally, the structure of the material appears to maintain some order, so there is still some uncertainty on what conclusions we can make from this particular configuration. For now, areas to expand this project in the future should focus on generalizing the model to even more (if not all) dimensions, implementing and observing the wavelike behaviour of spin pulses, and attempting to solve for the physical properties in the 2D ising model by starting from the 4D Ising model which has a closed form solution, then slowly decreasing the length of one of the axes to be on the scale of the coherence length, making the model and its physical properties behave like a 3D model. Lastly, shorten again the length of one of the other remaining dimensions to the scale of the coherence length, and determine the physical properties of the 2D Ising model.