2D Ising Model Simulation with Varying Adjacent Site Configurations

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June 8, 2019

I. Introduction

The Ising model is a model which displays the termodynamic 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.

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 - 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 $kT = 1$

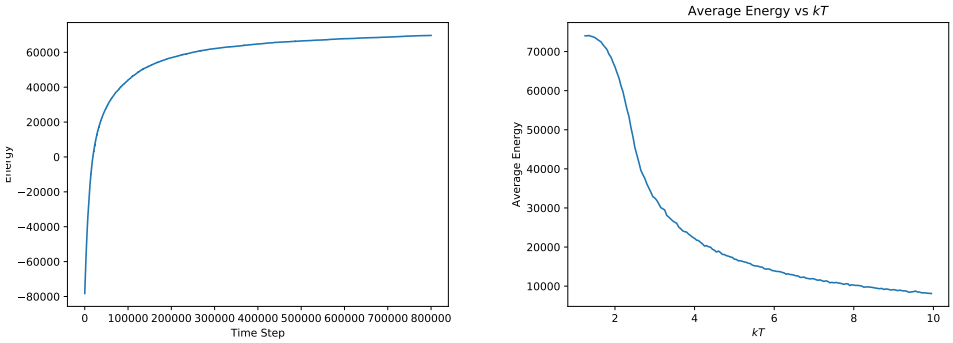

Figure 2: *(right)* plot of average energy vs kt. note an inflection at $\approx kt = 2.5$, which is evidence of a phase transition.

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

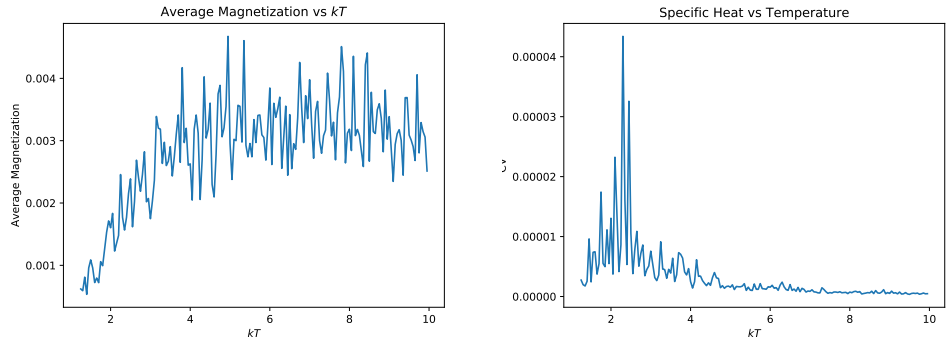

Figure 4: *(right)* Plot for specific heat vs temperature. Note a peak at $kT \approx 2.5$, also indicating a phase transition.

All-adjacent

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

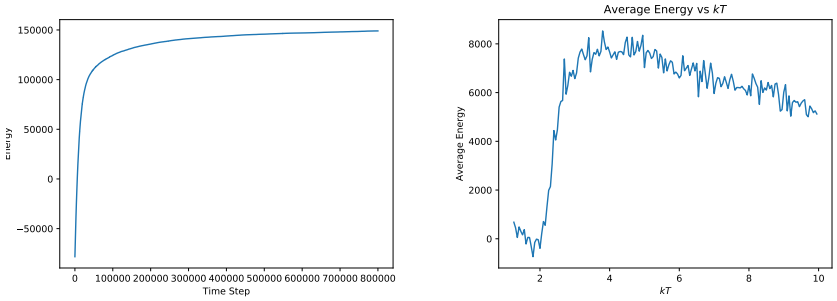

Figure 6: *(right)* plot of average energy vs kt. note an inflection at $\approx kt = 2.2$, which is evidence of a phase transition.

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

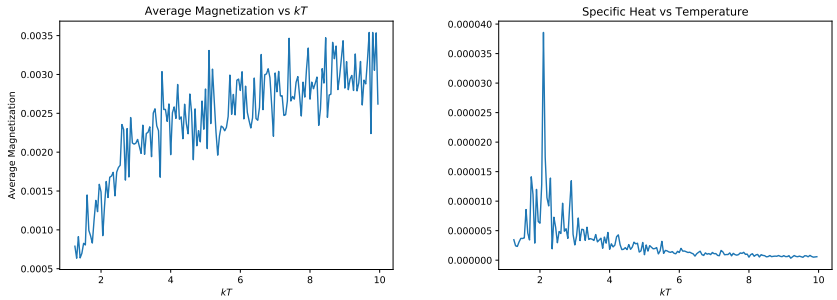

Figure 8: *(right)* Plot for specific heat vs temperature. Note a peak at $kT \approx 2.2$, also indicating a phase transition.

Diag-adjacent

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

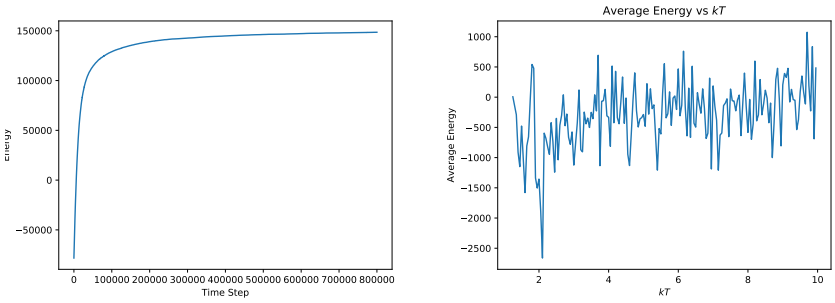

Figure 10: *(right)* plot of average energy vs kt. This graph is very noisy and no inflection point seems immediately discernable.

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

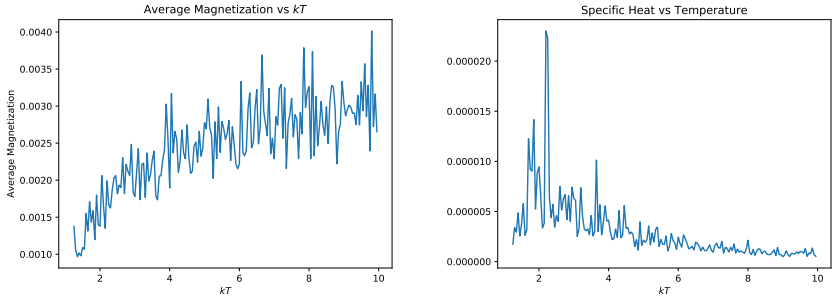

Figure 12: *(right)* Plot for specific heat vs temperature. Note peaks at $kT \approx 1.8$ and $kt \approx 2.1$

V. Analysis

VI. Conclusion