Modeling long-range interactions in a 2D Ising ferromagnet

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ABSTRACT

Various physical characteristics of a two-dimensional Ising ferromagnet are investigated using a Monte Carlo simulation in MATLAB. Nearest- and next-nearest-neighbor spin interactions are considered. The ensemble's sample configurations are generated using the Metropolis algorithm, which is a specific Monte Carlo method used to produce the simulation. Several order parameters are computed for the system, which are used in indicating the occurrence of phase transitions such as spontaneous magnetization below the critical temperature (Curie point). The results are compared to those predicted by the analytic solution for nearest-neighbors case given by Onsager, as well as results predicted by Zandvliet which also include next-nearest-neighbor interactions.

BACKGROUND INFORMATION

The Ising model is mathematical model of ferromagnetism. It is primarily used to study the mechanics of phase transitions, which occur when a single parameter of a given physical system is changed, resulting in a qualitatively different behavior in the overall state of the system [1]. For this work, we are concerned with phase transitions that occur in magnetic materials.

Each electron in the lattice structure of a given magnetic material has its own intrinsic spin angular momentum (which we will refer to simply as *spin*) which is the vector quantity that contributes to the electron's magnetic dipole moment. The magnetic properties of the overall material is due to the collective influence of each electron's magnetic moment [2].

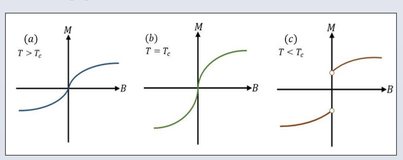

Figure 1. Idealized graphs representing total magnetization M as a function of the external magnetic field B: (a) above, (b) at, and (c) below the Curie point.

When these materials are subjected to an applied external magnetic field $\vec{B}$, it exerts a torque on the electrons, which rotates them until their dipole moments align parallel with the field. If the dipole moments remain aligned after the field is turned off, the material is said to be *ferromagnetic*. If the dipole moments revert to random directions, the material is said to be *paramagnetic* [1]. There exists a temperature T_c called the *Curie point*, at which materials undergo a phase transition from being paramagnetic to ferromagnetic, where thermal effects no longer inhibit a global alignment of the dipole moments. This effect is called *spontaneous magnetization*. This is demonstrated in Figure 1, which displays the net magnetization of the material as a function of the external field strength. It is the subject of this research to determine the Curie point for a specific model of a magnetic material.

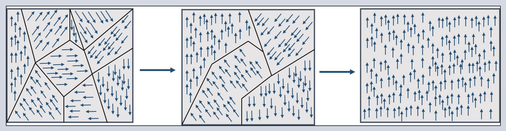

Figure 2. Independent magnetic domains becoming aligned under the influence of an applied external magnetic field.

In ferromagnetic materials, it is energetically favorable for each dipole moment in the material to point in the same direction [2]. This causes the formation of *magnetic domains*, which are regions in the material where large numbers of dipoles are pointing in the same direction. The application of an external magnetic field causes these domains to merge until all are parallel with the applied field, as depicted in Figure 2.

SYSTEM MODELING

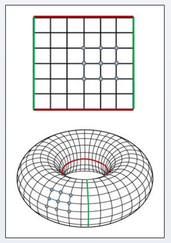

Figure 3. The square lattice adapted onto a torus.

As mentioned earlier, the Ising model is a mathematical model of a simplified system of interacting electron spins that exhibits phase transitions. In two dimensions, the electrons are arranged equidistant from each other in a square lattice. However, to avoid unnecessary complications, the edges of the lattice are wrapped around each other to make the actual shape of the system toroidal (Figure 3). Each site is assigned a state variable $\sigma_i = \pm 1$, which indicates whether the electron is *spin up* or *spin down* in the i^{th} lattice site. An assignment of particular values to each site indicates a *configuration* of the system [1]. We then assume something critically important: that each site only interacts with its nearest- and next-nearest-neighbors' spins, as well as an external magnetic field. The aforementioned neighbors are depicted in Figure 4.

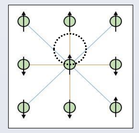

Figure 4. A representation of an arbitrary lattice point and its nearest (orange) and next-nearest (blue) neighbors.

The energy of any arbitrary configuration of spins is given by the Hamiltonian $H(\sigma)$ of the configuration,

$$H(\sigma) = J_1 \sum_{[i,j]} \sigma_i \sigma_j + J_2 \sum_{]i,j[} \sigma_i \sigma_j + B \sum_i \sigma_i$$

where $[i,j]$ and $]i,j[$ indicate the sum is over nearest- and next-nearest neighbor pairs, respectively. J_1 and J_2 are parameters that describe the two interaction "strengths," and B is the strength of the external magnetic field.

The probability of a system being in any configuration is proportional to its Boltzmann factor $e^{-\beta H}$ with $\beta = 1/k_b T$, where k_b is Boltzmann's constant and T is the temperature of the system measured in Kelvin. We then form the partition function Z by summing over all the Boltzmann factors corresponding to every possible configuration of the system.

$$Z(J_1, J_2, B, \beta) = \sum_{\sigma_i = \pm 1} e^{-\beta H(\sigma_i)}$$

For a system of N particles, the number of terms in this sum is 2^N, which makes explicit numerical computation a daunting, if not impossible task. It is for this reason that Monte Carlo simulations were chosen to carry out this numerical experiment. Additionally, all relevant thermodynamic quantities such as magnetization, specific heat, and magnetic susceptibility. The Gibbs free energy F of the system is stated (without proof) as follows.

$$F(T, Z) = -k_b T \cdot \ln\big(Z(J_i, B, \beta)\big)$$

EXACT SOLUTION/ZANDVLIET'S PREDICTIONS

Onsager analytically solved the problem of nearest-neighbor interactions ($J_2 = 0$) in a 2D square lattice by showing that the phase transition manifested as a discontinuity in the free energy, resulting in the following expression for the Curie point [3],

$$T_c = \frac{2J_1}{k_b \ln\big(1 + \sqrt{2}\big)} \approx 2.269$$

provided that the interactions are *isotropic*, meaning that all nearest-neighbor interactions were of equivalent strength. This is represented in Figure 5.

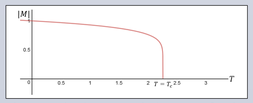

Figure 5. The Onsager solution curve for the magnetization as a function of temperature for systems with isotropic nearest-neighbor interactions.

The Ising model remains unsolved in the case that nearest- and next-nearest neighbor spin interactions are considered. However, Zandvliet demonstrated a possible partial solution based on similar methods to Onsager which gives the Curie point for this case as

$$T_c = \frac{4J}{k_b \ln(3)}$$

where J is a particular combination of J_1 and J_2 dependent on the modeling parameters used in a computer simulation [4]. It is important to note that Zandvliet's solution recaptures Onsager's original results in the case that the next-nearest-neighbor interaction strengths vanish.

MONTE CARLO AND METROPOLIS ALGORITHM

Monte Carlo simulations are a statistical computational technique used to predict outcomes of complex probabilistic systems with multiple interacting components [5]. These simulations come in the form of particular computer algorithms that randomize certain parameters in the system and evolve the system over a fixed number of steps and print out the results. There are several different established programs that have proven to be successful. For this experiment, we utilize the Metropolis algorithm, which chooses the randomized initial configurations in the lattice with a given probability proportional to each lattice site's Boltzmann factor, then weights them evenly [6]. A diagram describing the main functions of the program is displayed in Figure 6.

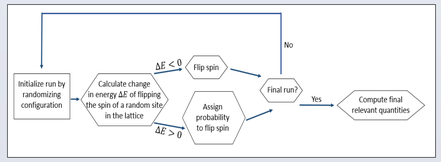

Figure 6. A basic program flowchart for the Monte Carlo simulation used.

The Metropolis algorithm functions through the weighting of probabilities, and a series of conditional statements, in a structured process as follows:

- An N X N square lattice of spins is randomly generated.
- The possible change in energy ΔE due to flipping a spin is calculated *for each spin*, based on its interactions with the spins of its nearest- and next-nearest-neighbor spins, as well as the external applied magnetic field.
- For each spin: If $\Delta E < 0$, the spin is flipped. This indicates that the interaction will cause the system to move towards a lower energy state and, subsequently, equilibrium.
- For each spin: If $\Delta E > 0$, a probability P is assigned to flipping the spin, which is determined by the site's Boltzmann factor $P(\Delta E) = \mathrm{e}^{-\frac{\Delta E}{k_b T}}$. This means the system's total energy is *increasing* due to the interaction, which is unfavorable.
- This process repeats for a fixed number of steps, which allows the system to move as close as possible to equilibrium.

RESULTS

For this work, units were chosen such that $J_1/k_b = 1$, and $J_2/k_b = 1/2$. This means that using the Zandvliet results, we predicted our system to have a Curie point of $T_c \approx 4.096$. First, the system was ran through randomized temperatures in order to determine whether the magnetization reflected the general trend of the Onsager solution shown in Figure 7.

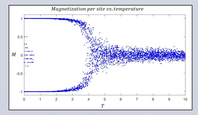

Figure 7. Graph of magnetization per site versus temperature, reflecting the general trend of the Onsager solution shown in Figure 5.

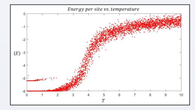

Figure 8. Graph of system energy at each lattice site versus temperature. The second curve near $T = 0$ indicates a second possible ground state energy.

Also, the total energy per lattice site was calculated (Figure 8) which will be discussed in the next section. Next, in order to determine the Curie point for the system, an additional loop was created in the program that increased temperature with each iteration, but the applied external magnetic field was randomized. The final result was that for this simulation, $T_c = 4.1 \pm 0.3$, which agrees with Zandvliet's prediction.

ANALYSIS AND CONCLUSION

Visuals of sample configurations at the end of the simulation are shown in Figure 9. Each lattice site is visualized as a square in the grid, where white and black squares represent that site as spin up or spin down, respectively. The magnetic domains are noticeable below the Curie point as large collections of white or black squares. At the critical temperature, the magnetic domains are visible, but are "struggling" to maintain themselves much like the configuration represented above the Curie point. Our results support Zandvliet's analytic solution, which indicates that this simulation is a good method to investigate possible solutions to the 2D Ising model where both nearest- and next-nearest-neighbor spin interactions are considered.

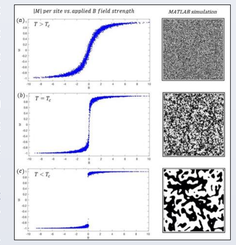

Figure 9. Here are results from the Monte Carlo simulation for magnetization as a function of external magnetic field (a) above, (b) at, and (c) below the Curie point. Compare these with the idealized graphs displayed in Figure 1.

One result worth noting is related to the total system energy, which is depicted in Figure 8. The bottom line indicates the ferromagnetic and antiferromagnetic ground state energies. The system sees total spin alignment with and against the external applied field as being energetically equivalent. However, the second line above that minimum energy indicates that this system may have more than one ground state energy. It is unknown if this result has physical implications or if it is an artifact of the program. It is our intent to run additional simulations varying the interaction strengths J_1 and J_2 in order to determine the root cause of this phenomenon.

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