Investigations of the Ising Model in 2D and 3D

Sean Ghaeli's Submission

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1 Ising Into Things

In this paper, we will introduce the Ising Model (pronounced easing) of a Ferromagnet, and use its theory to implement a working 2D and 3D simulation to investigate the phenomena of phase transitions, magnetization, and specific heat capacity. In particular, we will look at critical exponents and how the fundamental mechanism of heat capacity in 2D exhibits behavior that is completely distinct from the 3D case. We have attached our code to the end of this document.

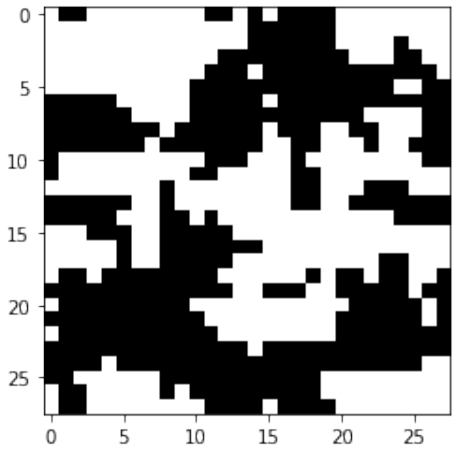

Figure 1: Random arrangement of a 2D lattice of dipoles

2 Background

In a magnet, neighboring dipoles have a measurable tendency to align in parallel. Whether this tendency arises from regular classical magnetic forces, or

through more complicated quantum-mechanical interactions such as those involving the Pauli exclusion principle, there is always a contribution to the energy of the system depending on the alignment of neighboring dipoles. Some materials require the application of external magnetic fields in order to overcome the required energy to become magnetized, these materials are known as paramagnets. Other materials align their dipoles without any additional field applied, and these materials are known as ferromagnets. A ferromagnet has a property known as Curie temperature, which is the temperature at which the material no longer magnetizes on it's own without an external field. Such a cutoff exists because the magnitude of random fluctuations (which decreases magnetization) is proportional to temperature.

With these properties of a ferromagnet in mind, the Ising Model is an attempt to model ferromagnetism. The model comprises of an assortment of two-state variables (either +1 or -1) which are arranged in some manner, in our case a 2D and 3D lattice. Each two-state variable represents the magnetic dipole moment, and each dipole can interact with its neighbors, where neighboring dipoles in parallel yield a lower overall energy to the system. The model does not take longer range effects into account. The model is such that lower energy microstates of the lattice are favored, but as temperature increases, thermal effects take over this tendency. The specific point at which this transition between the competing drivers occurs is the Curie temperature, or critical temperature.

While our model doesn't consider the principles of quantum mechanics, and is thus not particularly useful for accurately analyzing the specific behavior of ferromagnets, the Ising Model is still widely investigated for its ability to demonstrate phase transitions. This aspect of the Ising Model coupled with its relative simplicity (consider that we have made very few assumptions so far) makes it useful in analyzing the underlying physics of phase transitions in general. Since we have not made any assumptions about magnets, the Ising Model could be used as a simplistic model for any physical system which can be treated as a lattice of two-state variables, such as fluids like liquid helium(6), systems of neurons, and more. However, we will proceed in this paper with the context for ferromagnets in mind.

We will be using an algorithm to implement the Ising Model which we will demonstrate to be consistent with Boltzmann statistics when the algorithm has run through many iterations. Real world magnets are also consistent with Boltzmann statistics (if we are to operate under the assumption that Boltzmann statistics is correct), and this is how we will convince ourselves that our model is useful.

Figure 1 describes a possible state of a 10x10 grid 2D lattice of dipoles, where white cells correspond to one dipole direction and black cells correspond to the other. Remember that the Ising model assumes that there are only two possible dipole directions. Let's go ahead and introduce some mathematics so we can implement the Ising Model. Each pair of neighboring dipoles has some interaction energy, let's call it's magnitude to be ϵ. Our convention will be that the interaction energy between two neighboring dipoles is $-\epsilon$ when parallel and $+\epsilon$ when anti-parallel. Let σ_i be the state of the ith dipole, and that $s_i = 1$

when dipole is pointing up and $s_i = -1$ when pointing down. We can use the expression $-\epsilon s_i s_j$ to describe the interaction energy of two neighboring dipoles i, j. Now, our system's energy will be:

$$U = -\epsilon \sum_{neighbor\ pairs\ i,j} s_i s_j \tag{1}$$

This is also the *Hamiltonian* of our system. Notice that this energy is dependent on the number of neighbors a dipole has. We've considered lattices where a 2D dipole has 4 neighbors and a 3D dipole has 6 neighbors. As is standard with any thermal system: to talk about its behavior we will compute the partition function:

$$Z = \sum_{\{s_i\}} e^{-\beta U} \tag{2}$$

Where U is the energy of the system calculated in equation 1. As it turns out, calculating an exact solution for the average energy of the system has been done in 1D and 2D, but not yet in 3D. For this reason, we cannot rely on analytical mathematics alone to investigate the Ising model.

Additionally, we also cannot expect to compute the probability of all possible microstates, because even a small system –such as a 100 dipole system shown in Figure 1– would be too computationally intensive for the fastest supercomputer to evaluate in a reasonable amount of time; a ferromagnet such as a bar magnet could easily contain trillions and trillions of dipoles. Although, it could be possible that a random sampling of microstates, perhaps on the order of a few million, would be enough to capture the macroscopic behavior of our system. This is the idea of a *Monte Carlo Simulation*. Even this, however, is not enough to capture the macroscopic behavior of our system. This is because, as it turns out, there is a very small subset of states that are considered "important" in the representation of a ferromagnet, and our random sampling of a few million microstates could very easily not traverse enough of these "important" states. What we will do then is use an algorithm known as the *Metropolis Algorithm*, which uses Boltzmann factors to determine which microstates are likely to be worth sampling. Our algorithm is outlined as follows:

1. Start with some random initial state, for example the state shown in Figure 1

2. Choose a random dipole, and decide whether or not to flip it based on the following principles:

   - Compute ΔU of the system that would occur if the dipole is flipped. If $\Delta U \leq 0$ (decrease in system's energy or unchanged), flip the dipole.
   - If $\Delta U > 0$ the Boltzmann factor $e^{\Delta U/kT}$ is the probability of flipping the dipole.

3. Repeat process enough times so that it is statistically likely for each dipole to have changed states several times.

The procedure we've just outlined is called *Importance Sampling*, which is a technique that can be applied to the Monte Carlo method. To see where the term "importance sampling" comes from, let us consider the following from page 347 of Schroeder (1). Consider two microstates state 1 and state 2: state 1 being some random microstate such as the one shown Figure 1, and state 2 being the same as state 1 but with one dipole at random having been flipped. So the only difference between these two states is the flipping of one dipole. These two states both have an energy U, which we will call U_1 and U_2 respectively. Let's have it such that $U_1 \leq U_2$. If our system starts out in state 2, then the probability of recovering state 1 is simply $\frac{1}{N}$, N being the number of dipoles in our system. This is because there is a $\frac{1}{N}$ chance that we randomly land on the one dipole that is not polarized in the same direction as state 1, and since flipping this dipole reduces our overall energy, with $\Delta U \leq 0$, step 2 of our algorithm tells us that there is a 100% probability of flipping this dipole if it is chosen. Now for the reverse: if we start in state 1, there is still a $\frac{1}{N}$ chance of picking the one dipole that is in the opposite direction of state 2, but since flipping this dipole would add energy to our system, $\Delta U > 0$, step 2 of our algorithm tells us that there is a $\frac{1}{N}e^{-\Delta U/kT}$ probability for the dipole to flip, where $\Delta U = U_2 - U_1$. So in our setup, the probability of going from state 1 to 2 is:

$$\mathcal{P}(1 \to 2) = \frac{1}{N}e^{-\Delta U/kT} \tag{3}$$

And the probability from going from state 2 to 1 is:

$$\mathcal{P}(2 \to 1) = \frac{1}{N} \tag{4}$$

The ratio of these probabilities gives us:

$$\frac{\mathcal{P}(1 \to 2)}{\mathcal{P}(2 \to 1)} = \frac{\frac{1}{N}e^{-\Delta U/kT}}{\frac{1}{N}} = e^{-\Delta U/kT} = \frac{e^{-U_2/kT}}{e^{-U_1/kT}} \tag{5}$$

Which is just the ratio of the two Boltzmann factors. Boltzmann statistics demands that if these were the only two possible microstates the system could explore, then the ratio of the probability of their occurrence is the above ratio, given by their Boltzmann factors. So far, our algorithm agrees with Boltzmann statistics, but these are obviously not the only two microstates that can be explored by any system worth modelling. Luckily, this exact logic can be extrapolated for any number of states, not only just two like we have done, which tells us that our conclusion is generally valid. So we've seen that our algorithm is such that the system evolves with low-energy states being more favored than high-energy states, but it only couples with Boltzmann statistics after it has ran infinite iterations. Our goal, however, is to minimize the amount of time the algorithm runs while still being confident the simulation is showing

us the accurate macroscopic behavior of the system. The word "accurate" in this context is loosely used to refer to the accuracy of the expected energy and magnetization of the system. What we mean by "accuracy" of these quantities themselves is also hard to pin definitions onto, as there are many states a ferromagnet can possibly find itself in. For example, Boltzmann statistics tells us that it is quite likely to find a state where nearly all dipoles are aligned in the "up" direction as well as a state where nearly all dipoles are aligned in the "down" direction. However, for our Metropolis algorithm to traverse to both states could take an exceedingly long amount of time since the two states are so different. However, our limitation of not being able to compute all states is not purely a vice, considering real world systems also does not have time to explore all microstates.

3 Calculation of Observable Quantities

We will define magnetization, M, as follows:

$$M = \sum s_{up} - \sum s_{down} \tag{6}$$

Where $\sum s_{up}$ is the number of dipoles polarized in the "up" direction, and the corollary applies to $\sum s_{down}$. So it is quite simply a measure of the imbalance of dipoles in the lattice. An unmagnetized lattice would have an equal number of up dipoles as it would down dipoles.

From Equation 1, we will use our Hamiltonian of the system to find the average energy (2):

$$\langle U \rangle = \frac{1}{2}\langle \sum_{i}^{N} U_i \rangle = \frac{1}{2}\langle -\epsilon \sum_{i}^{N} \sum_{dipoles\ i,j} s_i s_j \rangle \tag{7}$$

Knowing that we can write variance as: $(\Delta X)^2 = \langle X^2 \rangle - \langle X \rangle^2$, we can define Specific Heat Capacity, C, as the following (2):

$$C = \frac{\delta U}{\delta T} = \frac{(\Delta U)^2}{k_b T} = \frac{\langle U^2 \rangle - \langle U \rangle^2}{k_b T^2} \tag{8}$$

4 Implementation and Results

Now that we have a grasp of the Metropolis Algorithm and how it implements the Ising Model, let's go ahead and simulate it and extract results. Our code can be found in the Appendix of this paper. Let's start off by running our algorithm and seeing what our lattices look like in 2D and 3D at a certain value for temperature:

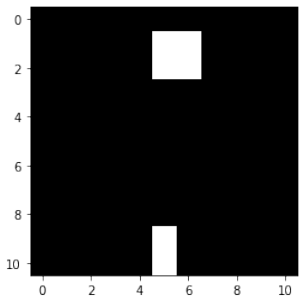

Figure 2: Steady state of a 10x10 2D grid at T=2.1K after many Monte Carlo steps

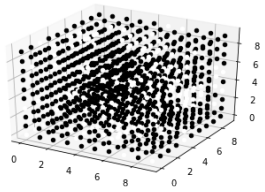

Figure 3: Steady state of a 10x10x10 3D grid at T=4.5K after many Monte Carlo steps

Qualitatively speaking for the 2D case, most of the dipoles are aligned (black dipoles), with a few exceptions (white dipoles). For the 3D case, the lattice is mostly magnetized (black dipoles), with a few clusters of dipoles (white dipoles) that go against the net magnetization of the lattice. Notice that these clusters come in various sizes.

Let's also go ahead and plot magnetization as a function of temperature for both 2D and 3D:

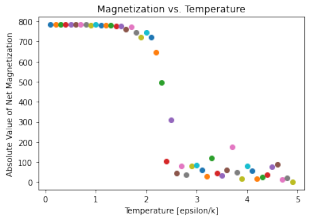

Figure 4: Magnetization vs temperature for 10x10 2D grid. The units of temperature are $\frac{\epsilon}{k_b}$

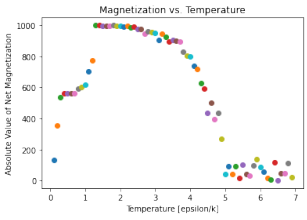

Figure 5: Magnetization vs temperature for 10x10x10 3D grid. The units of temperature are $\frac{\epsilon}{k_b}$

The sharp cutoff we see for both the 2D and 3D case is where the lattice stops being magnetized, or the phase transition of the system, which as we recall is the Curie Temperature of the system. This phase transition is a crucial result of the Ising Model, and it is one of the ways it exhibits *Universality*, making it applicable to modelling many systems in physics which are near the point of their phase transition (3). However, the Ising model stops being useful when far away from the critical point, and this can be visually seen in Figure 5 where we see a weirdly behaved portion of the graph on the low temperature side.

As a complete visual guess, it looks like the 2D critical point is somewhere around $2.2[\frac{\epsilon}{K_b}]$ and the 3D critical point is somewhere around $4.5[\frac{\epsilon}{K_b}]$. As a

general result, it turns out that the critical points are about T=2.27[$\frac{\epsilon}{K_b}$] in 2D (analytically solvable), and T=4.50[$\frac{\epsilon}{K_b}$] in 3D (numerical approximation) (1). Since our graphs match these known results, we can start to gain some confidence that we have correctly implemented the model.

Now, let's move onto heat capacity in 2D and 3D. Note, we use "heat capacity" and "specific heat capacity" interchangeably at times:

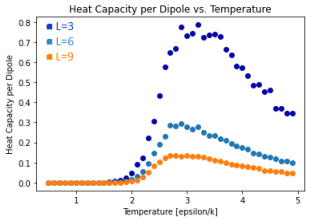

Figure 6: Specific heat capacity vs temperature for 10x10 2D grid. The various lines are for certain lattice sizes, as defined in the legend (L=3 corresponds to 3x3 lattice). The units of temperature are $\frac{\epsilon}{k_b}$

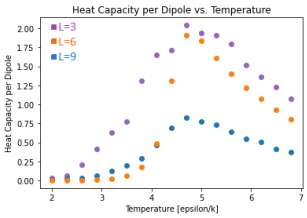

Figure 7: Specific heat capacity vs temperature for 10x10x10 3D grid. The various lines are for certain lattice sizes, as defined in the legend (L=3 corresponds to 3x3 lattice). The units of temperature are $\frac{\epsilon}{k_b}$

To investigate the specific heat capacities in 2D and 3D and to understand how its behavior differs depending on the dimension, we made an attempt to turn to the concept of *Critical Exponents*, although a much more thorough paper would be required to discuss this in greater depth than what we've considered in this paper. A critical exponent is used to describe how a system behaves near a critical point, or in our case a phase transition. They are useful in physics because they are thought to be a fundamental measurement of the characteristics of a system, and are often independent of certain parameters of the system, such as scale. As a loose explanation, let's consider the following: let $\tau = \frac{T-T_c}{T_c}$, where T is the temperature of the system and T_c is the Curie temperature, or critical temperature, of the system. We assert that heat capacity has behavior $C \approx \tau^{\alpha}$, where α is the critical exponent. In order to find said critical exponent, we have that:

$$\alpha = \lim_{\tau \to 0^+} \frac{\ln |C|}{\ln \tau} \tag{9}$$

Let's attempt to find α in 2D and 3D:

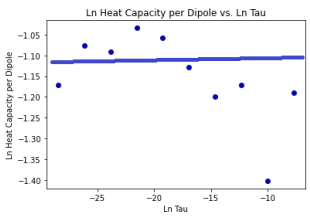

Figure 8: Ln C vs Ln τ near the critical temperature $T = 2.27\frac{\epsilon}{k_b}$ for 10x10 2D grid, with a weak trendline

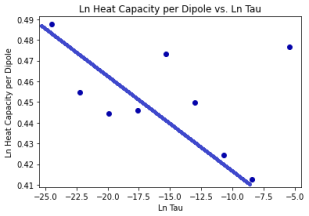

Figure 9: Ln C vs Ln τ near the critical temperature $T = 4.5\frac{\epsilon}{k_b}$ for 10x10x10 3D grid, with a weak trendline

From Equation 9, the slope of Figure 8 should be a very loose approximation for α in 2D, and similarly for Figure 9. Looking at the weak trend lines, it seems like the slope of Figure 8 is about zero, and the slope of Figure 9 is slightly nonzero, if we are to disregard the points which resemble outliers (namely the point where $\ln\tau = -10$ in Figure 8 and where $\ln\tau = -5$ in Figure 9). We do not attempt to extract an accurate value here, because for the sake of our discussion, the result that α is zero in 2D and non-zero in 3D hints at the existence of interesting underlying phenomena, which we will discuss in Section 5. As a general result, it is known from the analytical solution that α is actually zero in 2D, and known through numerical methods that it is nonzero in 3D, so our result agrees with the observations of others(4)(5).

5 Discussion of Results

With the minimal assumptions of the Ising Model, which we implemented by building upon the principles of statistical mechanics using the Metropolis algorithm, we were able to model a ferromagnet in 2D and 3D, determining the critical temperature in 2D and 3D, as well as the behavior of specific heat capacity in 2D and 3D. One thing that should be emphasized is that this model is in no way restricted to being a model of a ferromagnet, as our assumptions leading to the implementation of the Ising Model stated nothing about magnets, except that dipoles can only be polarized in one of two directions (which is not exclusive to magnets). Indeed, many physical systems which exhibit critical behavior such as phase transitions can potentially be analyzed near their critical point by the Ising model(6).

Our result that the critical exponent associated with specific heat capacity is zero in 2D and nonzero in 3D is a crucial result because it tells us that the heat capacity does not scale according to a power law in 2D and does scale according to a power law in 3D near the critical point. It is a much more profound result than finding that the critical exponents α are different but both nonzero, because in this case they would still scale according to the same functional form, which would be a much easier result to explain. A 2D system's heat capacity does scale

according to some function, and it happens to be logarithmic (4). Due to the two separate functional forms of the critical exponent for heat capacity in 2D and 3D, a 2D system described by the Ising Model has weakly scale-dependent specific heat capacity, whereas a 3D system has strongly scale-dependent specific heat capacity (near the critical point). By scale, we mean size of the system, or lattice. To reiterate simply, the heat capacity of a 2D system has a completely different dependence on scale than that of a 3D system. Knowing this, we can conclude that the underlying physics which drives the observable quantity of heat capacity near the critical point (in any physical system which can be modelled by the Ising Model) exhibits one behavior in 2D and a completely separate behavior in 3D.

References

[1] Daniel V. Schroeder *An Introduction to Thermal Physics*. Oxford University Press, 1999

[2] Jacques Kotze *Introduction to Monte Carlo methods for an Ising Model of a Ferromagnet*. https://arxiv.org/pdf/0803.0217.pdf

[3] Jeffrey Chang *The Ising Model*. https://stanford.edu/ jeffjar/statmech/intro4.html

[4] Tom Kennedy *The Ising Model*. https://www.math.arizona.edu/ tgk/541/chap1.pdf

[5] Andrea Pelissetto, Ettore Vicari *Critical Phenomena and Renormalization-Group Theory*. https://arxiv.org/pdf/cond-mat/0012164.pdf

[6] Hagen Kleinert *Critical exponents from seven-loop strong-coupling ϕ^4 theory in three dimensions*. http://users.physik.fu-berlin.de/ kleinert/279/279.pdf

6 Appendix

We've attached the code we used to achieve Figures 6 & 7, which required the most complex programming of all our plots. Every other plot is obtained using slightly simplified variations of the following code, which we have not included for the sake of keeping this paper at a reasonable length.