PHSX815 Project 4: Using Monte Carlo to Estimate the Curie Temperature of a Two-Dimensional Ferromagnetic Crystal

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May 2023

1 Introduction

Magnetic materials are normally characterized by their magnetic susceptibility (χ) and magnetization (M) in an external magnetic field. The magnetic susceptibility is a dimensionless proportionality constant that indicates the degree to which a material becomes magnetized in response to an external magnetic field, B_{ext}. The magnetization is a vector that is the measure of the magnetic moment of a material. Effectively the magnetization is the sum total of all the spins in the material and the susceptibility is defined by how much the magnetization changes when placed in a magnetic field.

$$M = \langle \sum_{i=1}^{N} s_i \rangle \quad \text{and} \quad \chi = \frac{\partial M}{\partial B_{ext}} \tag{1}$$

From these two properties magnetic materials are commonly divided into three groups of materials: paramagnetic, diamagnetic, and ferromagnetic materials. Both paramagnetic and diamagnetic materials do not exhibit remanence [1], i.e. $M = 0$ if the external magnetic field is removed, but paramagnetic materials have $\chi > 0$ while diamagnetic materials have $\chi < 0$. Ferromagnetic though do exhibit remanence ($M > 0$ at $B_{ext} = 0$) and have $\chi > 0$. These properties are based on a few key assumptions. The first assumption is that the temperature is well below the Curie temperature, T_c. This temperature is so named because Pierre Curie showed that for $T > T_c$ the spins in the system become no longer align and become randomized with only a weak form of paramagnetism existing above this temperature [2]. The second assumption is that the material exist in greater than one dimension. The Ising model for magnetism assumes nearest-neighbor spin interaction. In one dimension, Ernst Ising showed that there is no phase transition [3]. However, in two dimensions and up phase transitions have been shown to exist.

The temperature this phase transition occurs at in a two dimensional lattice has is shown to be 2.268 K in Onsager [4]. Based on this we will be calculating the magnetization, energy, and specific heat of the two dimensional lattice by simulating it.

2 Code

The calculation required to simulate this system in principle requires us to construct all possible permutations of the spin-grid. This however, is impractical given that there are 2^{L^2} possible states to consider (over-counting slightly due to symmetry in some of the systems). To circumvent this issue the code exhibited here uses the Metropolis-Hastings Monte Carlo method, a Markov chain. The reason for this is to minimize the energy of the free energy of the lattice under study.

In order to do this, the code prepares a $L \times L$ grid of spins. The code then passes over the grid and flips spins randomly throughout the grid. The change in energy resulting from the spin flips is calculated and if the resulting energy is lower than the previous energy the new state is accepted. However, if the energy change is positive, the new state is accepted with a new probability of $P = e^{-dE/T}$. This process is repeated to minimize the energy of the system. Once this is done the specific heat, energy, and magnetization is calculated.

3 Analysis

The code that we are using assumes a two dimensional system. For these systems it calculates the magnetization, energy and specific heat. These calculations also allow us to see how accurately we can calculate T_c. Plotting T_c vs. temperature will result at a discontinuity at the T_c [5]. This allows us to calculate the T_cs for the different simulations. Since the size of the lattice and number of MC sweeps are variables we control, we will investigate the calculated values as we vary these controls. The lattice sizes that were used were all $L \times L$ where L is 10, 20, and 30 for 1,000,000 Monte Carlo sweeps. We also did simulations for the different numbers of Monte Carlo sweeps for the 20×20 lattice. Those simulations were done for 100, 10,000 and 1,000,000 sweeps.

3.1 Energy

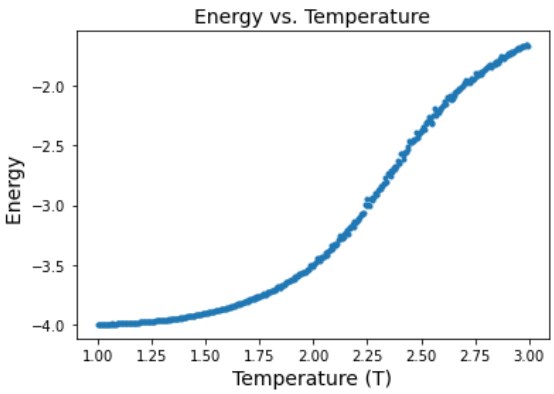
The energy vs temperature plots are mostly consistent for the different lattice sizes at 1,000,000 sweeps. The only difference is a slight steepening of the slope as the lattice size increases. There is not much difference due to the number of MC sweeps in the 20×20 lattice, perhaps some additional variation as the number of Monte Carlo sweeps decreases.

3.2 Magnetization

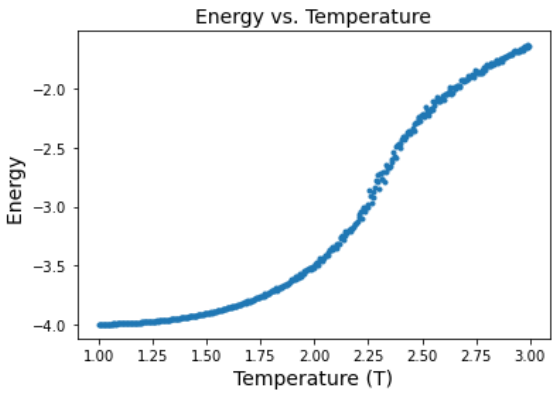
There was some increased instability as the lattice size decreased, with a bifurcation of the plot at the 10×10. As for the number of Monte Carlo sweeps, the plot had the largest variance at 10,000 steps.

3.3 Specific Heat

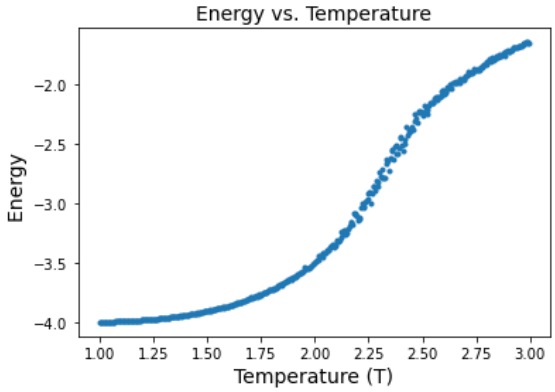
The specific heat shows that as the lattice size is increased, the peak of the of the specific heat curve is more obviously discontinuous. This discontinuity corresponds to the critical temperature of our system. The number of Monte Carlo sweeps in the 20×20 seems to become more discontinuous with more Monte Carlo sweeps.



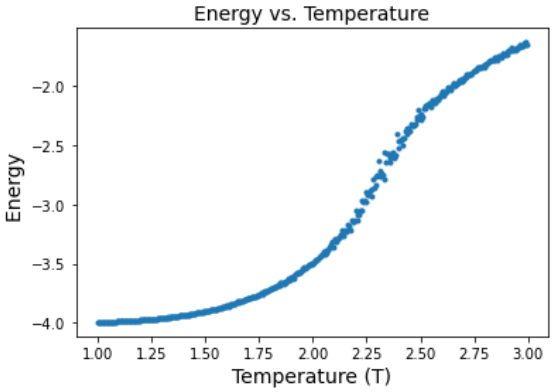
(a) 10×10 lattice with 1,000,000 sweeps



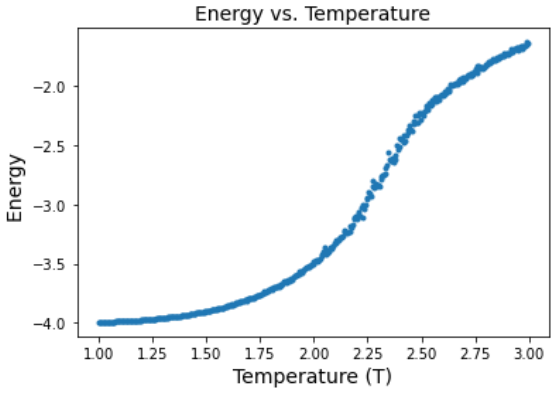
(b) 20×20 lattice with 1,000,000 sweeps



(c) 30×30 lattice with 1,000,000 sweeps

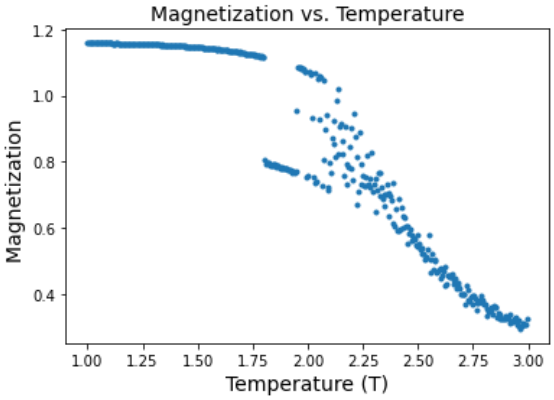


(d) 20×20 lattice with 10,000 sweeps

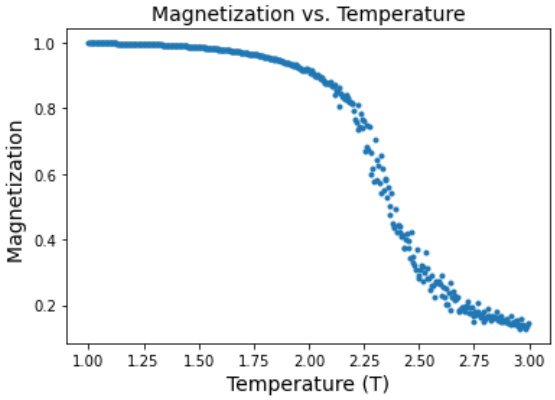


(e) 20×20 lattice with 100 sweeps

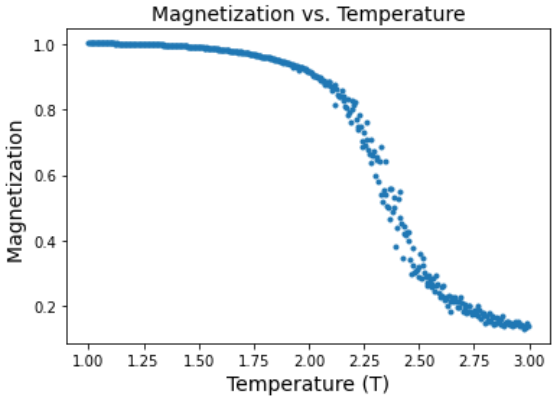
Figure 1: Energy vs. Temperature. (a) 10x10 lattice grid with 1,000,000 Monte Carlo Sweeps. (b) 20x20 lattice grid with 1,000,000 Monte Carlo Sweeps. (c) 30x30 lattice grid with 1,000,000 Monte Carlo Sweeps. (d) 20x20 lattice grid with 10,000 Monte Carlo Sweeps. (e) 20x20 lattice grid with 100 Monte Carlo Sweeps.



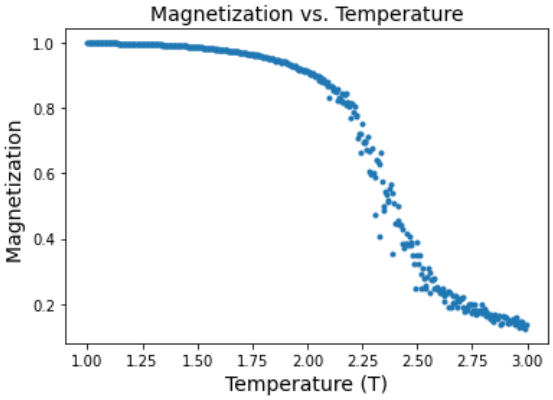
(a) 10×10 lattice with 1,000,000 sweeps



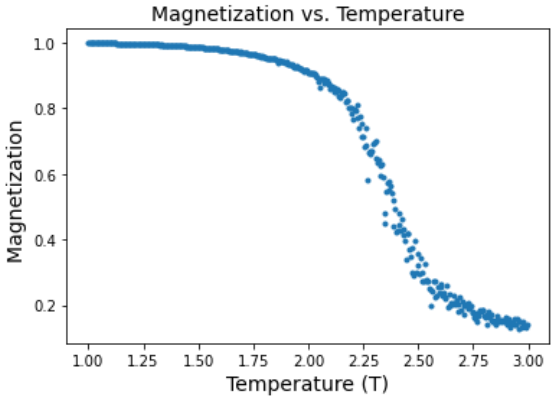
(b) 20×20 lattice with 1,000,000 sweeps



(c) 30×30 lattice with 1,000,000 sweeps

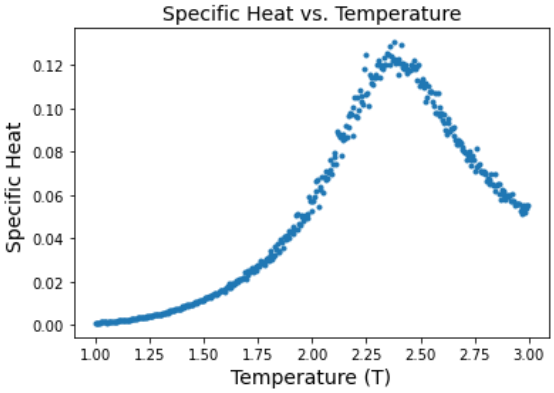


(d) 20×20 lattice with 10,000 sweeps

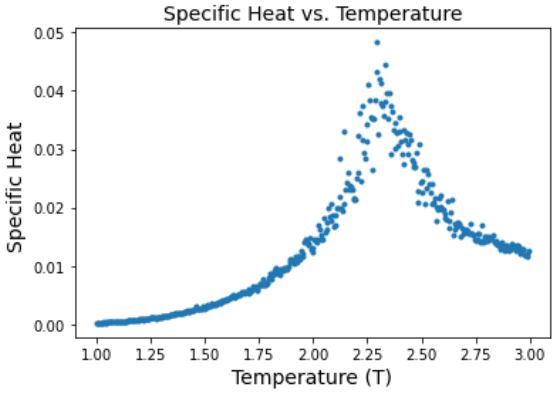


(e) 20×20 lattice with 100 sweeps

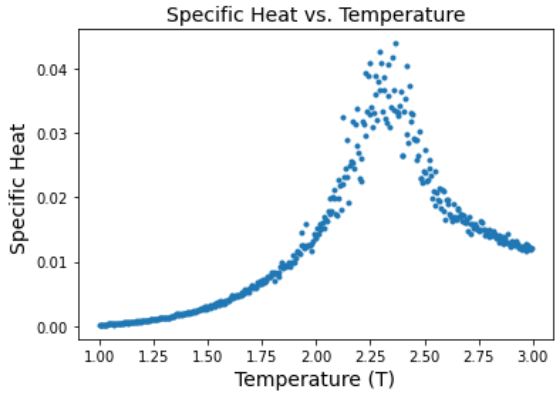
Figure 2: Magnetization vs. Temperature. (a) 10x10 lattice grid with 1,000,000 Monte Carlo Sweeps. (b) 20x20 lattice grid with 1,000,000 Monte Carlo Sweeps. (c) 30x30 lattice grid with 1,000,000 Monte Carlo Sweeps. (d) 20x20 lattice grid with 10,000 Monte Carlo Sweeps. (e) 20x20 lattice grid with 100 Monte Carlo Sweeps.



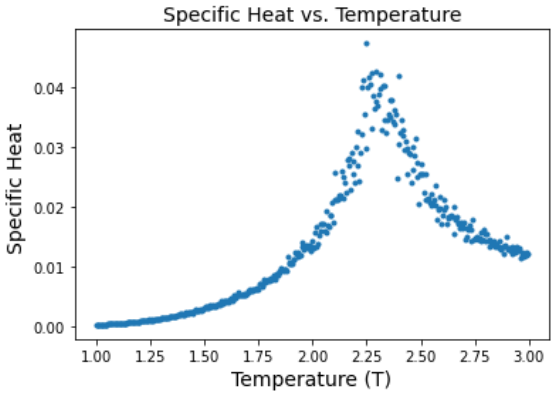
(a) 10×10 lattice with 1,000,000 sweeps



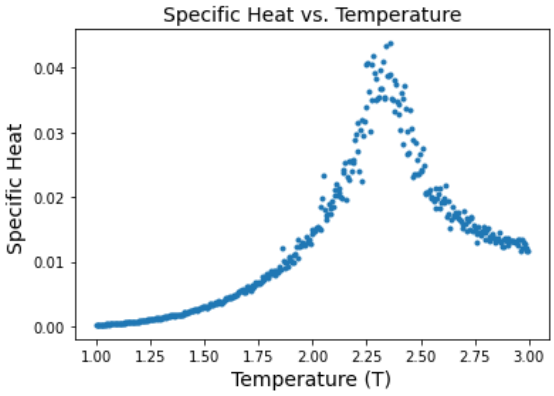
(b) 20×20 lattice with 1,000,000 sweeps



(c) 30×30 lattice with 1,000,000 sweeps



(d) 20×20 lattice with 10,000 sweeps



(e) 20×20 lattice with 100 sweeps

Figure 3: Specific heat vs. Temperature. (a) 10x10 lattice grid with 1,000,000 Monte Carlo Sweeps. (b) 20x20 lattice grid with 1,000,000 Monte Carlo Sweeps. (c) 30x30 lattice grid with 1,000,000 Monte Carlo Sweeps. (d) 20x20 lattice grid with 10,000 Monte Carlo Sweeps. (e) 20x20 lattice grid with 100 Monte Carlo Sweeps.

4 Error Analysis

Error in our simulation arises from the size of the lattice. There are also other sources of variation such as defects (Frenkel defects, Schotky defect, etc.) in the crystals. For this project, only the error due to randomness will be analyzed.

A natural way of determining the error of our estimation would be to run multiple iteration of the same experiment and interpret the average as the estimated parameter and standard deviation as uncertainty. Also, we expect the distribution of the approximations of the T_c to be Gaussian. This can be done using the scipy library. The fit then would give us the expected value of T_c which is also the value that maximizes the likelihood. Finally, we perform a two tailed t-test and calculate the p-value for the hypotheses: $H_0 : T_c = 2.268K, H_1 : T_c \neq 2.268K$.

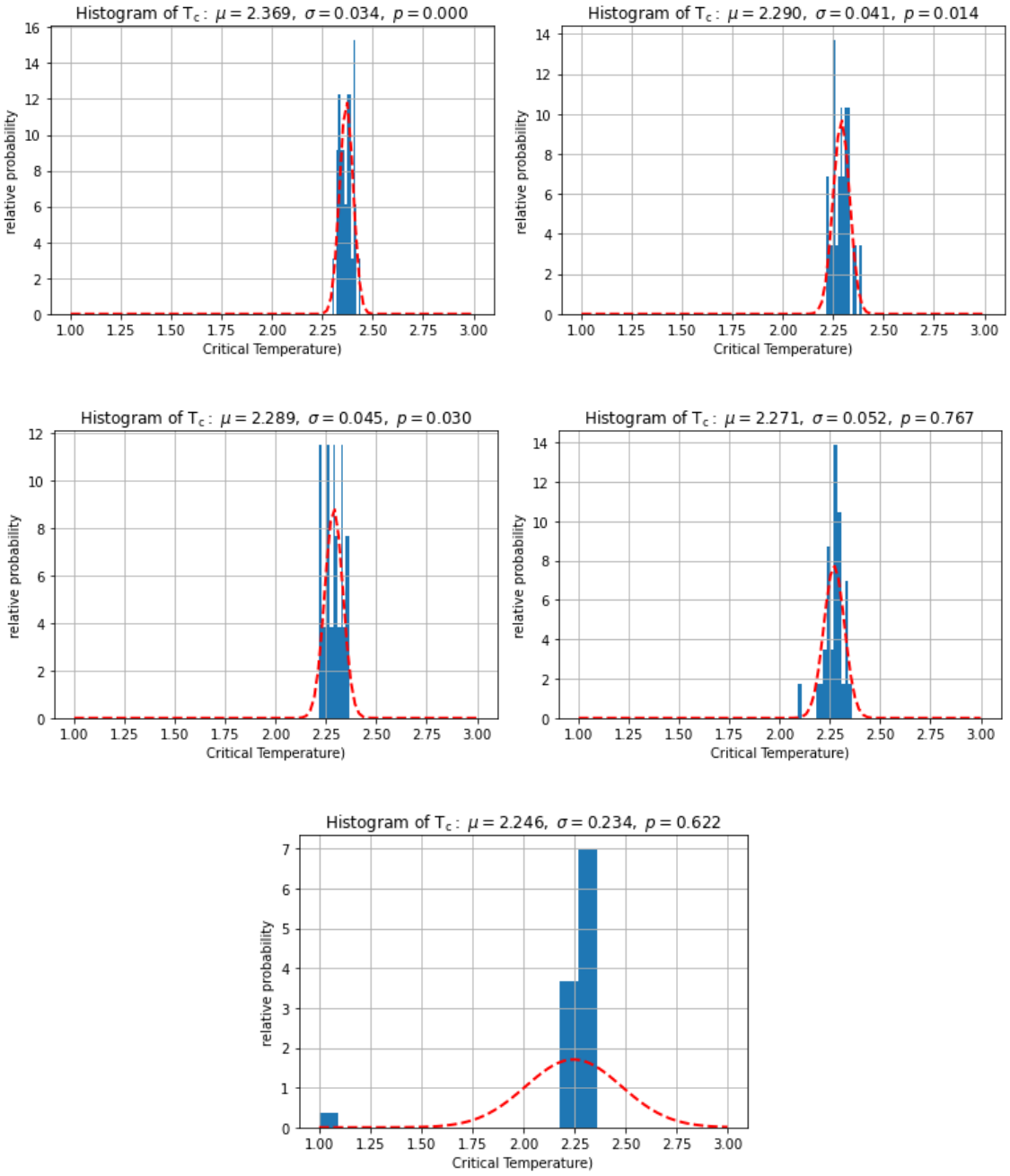


Figure 4: Gaussian fit of the distribution of T_c. (a) 10x10 lattice grid with 1,000,000 Monte Carlo Sweeps. (b) 20x20 lattice grid with 1,000,000 Monte Carlo Sweeps. (c) 30x30 lattice grid with 1,000,000 Monte Carlo Sweeps. (d) 20x20 lattice grid with 10,000 Monte Carlo Sweeps. (e) 20x20 lattice grid with 100 Monte Carlo Sweeps.

From the Figure 4, we can see that our standard deviation is not bad considering we are using small number of iterations only, due to computational limitations. Also, the fit shows that our expected T C is very close to the theoretical value of 2.268 K. Similarly, the p-values are also quite high and we can comfortably reject the alternative hypothesis at 95 percent confidence level. Of course, this does not let us accept the null hypothesis but it does gives us some confidence in our simulation. The error was not calculated, but could have been done with a bootstrap method. This would be done by taking N independent measurement of the same quantity several times. q is then calculated through q = Q/N with it's own uncertainty as its standard deviation.

5 Conclusion

The simulations and analysis reveals that 2D Ising model could explain the magnetic phase transition occurring in materials. The simulation used various lattice sizes, different numbers of MC sweeps and different number of iterations of the MC simulation to demonstrate the phase transition. We saw that in general lattice size does affect the T_c as well as the number of MC sweeps.

6 Acknowledgements

Feedback on this project came from Kenny Couberly who provided peer feedback on this project. Kushal Rijal was consulted for this project and his advice was helpful in finding the inspiration for this project. The work done in The hobbyhorse of magnetic systems: the Ising model [6] and Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition [4] was the foundation of the code for the project.

Here are the references

[1] K. Chesnel, A. S. Westover, C. Richards, B. Newbold, M. Healey, L. Hindman, B. Dodson, K. Cardon, D. Montealegre, J. Metzner, T. Schneider, B. Böhm, F. Samad, L. Fallarino, and O. Hellwig, *Morphological stripe-bubble transition in remanent magnetic domain patterns of Co/Pt multilayer films and its dependence on Co thickness*, *Phys. Rev. B* **98** (Dec, 2018) 224404.

[2] P. Curie, , *Propriétés magnétiques des corps à diverses températures*. thesis, University of Paris, 1895.

[3] E. Ising, , *Beitrag zur Theorie des Ferro-und Paramagnestismus*. thesis, Universität Hamburg, 1924.

[4] L. Onsager, *Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition*, *Phys. Rev.* **65** (Feb, 1944) 224404.

[5] J. Shi, *Chapter 7. Canonical and Grand Canonical Ensemble*, April, 2023.

[6] C. G. M.-F. Eduardo Ibarra-García-Padilla and F. J. Poveda-Cuevas, *The hobbyhorse of magnetic systems: the Ising model*, *Eur. J. Phys.* **37** (Sept, 2016) 065103.