Term Project Proposal: Applying the Metropolis Algorithm to the Ising Model of 2-D and 3-D Ferromagnetic Materials

Mason Hargrave

May 2, 2018

1 Introduction

A common problem in the field of solid state physics is determining the net magnetization of a ferromagnetic material when subjected to an external magnetic field. The net magnetization of such a material is the result of the "spin-states" of its lattice sites. A crystalline ferromagnet with net zero magnetization has an even number of spin-up lattice sites and spin-down lattice sites. It is seen experimentally with ferromagnets, that below some critical temperature T_c, even in the absence of an applied field, a ferromagnet either gains a next positive magnetization of net negative magnetization. This gain of a net magnetization is called "spontaneousness breaking of symmetry".

By far the most popular model of a two-state ferromagnet is called the Ising Model in which each lattice site is assigned a spin position (up or down) and there is some energy associated with that position due to spin-spin interactions (between lattice sites) and due to magnetic interactions (with an external magnetic field).

2 Background

The 2-D Ising model was solved by Lars Osanger in his 1944 paper "Crystal Statistics. i. a two-dimensional model with an order-disorder transition". The Ising model **has never been solved** analytically in more than two dimensions. As such, mean field theory was developed in part by Pierre Weiss in order to approximate solutions for the 3-D case. The man field theory relies on only considering the mean effect of the nearest neighbors of a given lattice site.

Determining the net-magnetization of a ferromagnet boils down to determining the proportion of spin up lattice sites to spin down lattice sites. Such a determination can in theory be made by finding the lowest (and thus most thermodynamically favorable) set of lattice site spin states. Such a calculation however becomes computationally ridiculously very quickly even when using the simplifications of mean-field theory. For instance, to find the lowest combination of spin states in a 10x10 lattice would require you to calculate the energy associated 10^{21} different combinations of spin states.

To make these problems more computationally reasonable, one might adopt a naive Monte Carlo approach in which spin states are randomly generated for a lattice and the energy of the spin states individually evaluated. This method however only serves to inefficiently survey a small subset of sample space and does not favor the generation of lower energy spin states.

A much better idea is to use the Boltzman factors to help us determine which elements of sample space are worth simulating in order to more effectively find energetically favorable spin states.

This method is known as the Metropolis algorithm and has been implemented in our class to solve the "1-D ferromagnetic chain" in which each lattice site only had two neighbors. The Metropolis algorithm is useful not only in solving the 1-D "ferromagnetic chain" but can in fact be generalized to solve much more complicated lattices (such as the 2-D square lattice or the 3-D cubic lattice).

3 Project Summary

I would like to carry out some the problems listed in section 8.2 of the textbook *Thermal Physics* by Daniel V. Schroeder.

The project goals are:

1. Implement the Metropolis algorithm in python for the 2-D square lattice.
2. Run the metropolis algorithm with a 20x20 lattice at $T = 10$, 5, 4, 3, and 2.5 (above the critical temperature) for at least 100 iterations per dipole per run. At each temperature make a rough estimate of the size of the largest clusters.
3. Repeat part 2 with a 40x40 lattice and check to see if the cluster sizer are any different.
4. Run the program with a 20x20 lattice at T - 2, 1.5, and 1 (below the critical temperature). Estimate the average magnetization at each of these temperatures.
5. Run the program with a 10x10 lattice at T=2.5. Watch it run for 100,000 iterations.
6. Use successively larger lattices to estimate the typical cluster size at temperatures from 2.5 down to 2.27 (the critical temperature). Watch to see how large the cluster size gets.
7. Modify the ising program to simulate the 3-D Ising model with a a simple cubic lattice. Show that they stem has a critical point at around T=4.5.
8. Create a visualization of the spin states generated by the Metropolis algorithm.

These problems are paraphrased or taken directly out of the textbook. As such, I will be able to compare my results to the results that the textbook suggests I should get in order to confirm my results.

4 Project Details

There is a pseudo code implementation of the metropolis algorithm on page 249 of *Thermal Physics* by Daniel V. Schroeder. The challenge will be converting this pseudo code to python, and then modifying it to solve the problems laid out in the book.

The Metropolis Algorithm is the definitive method for solving these problems so the challenge will be in the correct implementation of the algorithm, not in developing a new method do solve the Ising model.

Most challenging I think will be development of an aesthetically pleasing visualization of the Ising Model spin states.

If time permits, I would like to also take on the challenge of developing an animation that will show the changes in the spin sates of a 2-D lattice over the many iterations of the Metropolis algorithm. It would be fun to see the development of spin domains in the lattice.

References

[1] N. W. Ashcroft and N. D. Mermin, *Solid state physics.* Saunders College, 1988.

[2] T. H. Cormen, C. E. Leiserson, R. L. Rivest, and C. Stein, *Introduction to algorithms.* MIT Press, 2014.

[3] J. Kleinberg and E. Tardos, *Algorithm design.* Addison-Wesley, 2011.

[4] R. H. Landau, M. J. Paez, and C. C. Bordeianu, *Computational physics: problem solving with Python.* Wiley-VCH, 2015.

[5] D. V. Schroeder, *An Introduction to Thermal Physics.* Addison Wesley Longman, 2000.

[6] S. H. Simon, *The Oxford solid state basics.* Oxford Univ. Press, 2017.

[7] L. Onsager, “Crystal statistics. i. a two-dimensional model with an order-disorder transition,” *Phys. Rev.*, vol. 65, pp. 117–149, Feb 1944.

[8] P. Weiss, “L’hypothèse du champ moléculaire et la propriété ferromagnétique,” *J. Phys. Theor. Appl.*, vol. 6, no. 1, pp. 661–690, 1907.