Senior Thesis

Simulation of the two-dimensional square-lattice Lenz-Ising model in Python

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Abstract

A program to simulate the the two-dimensional square-lattice Lenz-Ising model with periodic boundary conditions and no external field was implemented in Python. The program uses the Metropolis-Hastings algorithm to quickly sample the distribution being investigated. The output of the program is a comma-separated list of values representing some parameters of interest at different lattice temperatures. These values can be examined to demonstrate several well-known properties of this version of the Lenz-Ising model.

Introduction to the Lenz-Ising Model

In 1920, Wilhelm Lenz proposed a new model of ferromagnetism which his student, Ernst Ising, later published a solution for in his 1924 dissertation. The Lenz-Ising model can be used to describe how the temperature of a ferromagnetic material affects its magnetic properties. This model treats the material as a lattice of elementary dipole magnets, such as electrons, each with their own spin magnetic moment. Ferromagnetic materials differ from other materials in that it is slightly energetically favorable for their constituent dipole moments to align with each other[i]. At high temperatures, the random movement of the molecules dominates and the spins become unaligned. However, at low temperatures the lack of thermal disturbance allows the spins to align.

The key difference between the Lenz-Ising model and one proposed earlier by Pierre Weiss in 1907 was the treatment of spin orientations. In the Lenz-Ising model, the spins of the dipoles in the lattice are allowed occupy one of two possible orientations, either up or down. Additionally, the Lenz-Ising model considers only adjacent sites on the lattice to have any effect on one another, disregarding long-distance interactions.[?] In 1924, Ising published a solution for the one-dimensional case of the Lenz-Ising model, which displayed no phase transition,[ii] but he incorrectly extrapolated from this result that a three-dimensional lattice would display the same lack of a phase transition.[?,?] Later, in 1942, Lars Onsager published an exact solution to the two-dimensional Lenz-Ising model (with no external field) which *did* display a phase change, and later authors expanded on his work to find solutions to other versions of the model.[?]

[i] This is due to the exchange interaction, an explanation of which can be found on pages 207 - 210 of Griffiths' *Introduction to Quantum Mechanics*, second edition.[?]

[ii] A *phase transition* is a change in a system's physical properties, such as the transition between a ferromagnetic state and a paramagnetic state.

Introduction to a Solution

Ideally, parameters of interest such as specific heat capacity, magnetic susceptibility, average energy, and average magnetization could be calculated from the partition function of the system. Unfortunately, a method for calculating the partition function of such a system exactly is not currently possible for anything above the two dimensional case; however, there are techniques that allow study of lattices easily on consumer hardware with only a beginner's understanding of programming.

For a given temperature, all that is required to make predictions about the future state of this spin lattice system is its current state, which means that the process by which the lattice changes configurations can be modeled as a Markov chain.[?] Let A and B represent two possible states of the system (configurations of the lattice). Let E represent the total energy of a configuration, which is the sum of all spin-spin interaction energies plus any external field component. Let Z represent the partition function, which is the sum over every possible lattice state of every state's associated Boltzmann factor.[iii] From this, $p(A)$ and $p(B)$ are the probabilities of finding the system in their respective states,

$$p(A) = \frac{e^{-E(A)/\tau}}{Z} \qquad \text{and} \qquad p(B) = \frac{e^{-E(B)/\tau}}{Z}. \tag{1}$$

Let $w(A, B)$ be the probability of transitioning from A to B. If the system is examined at equilibrium, then by the principle of detailed balance it is equally likely for the system to be in state A and then transition to B as for the system to be in state B and then transition to A.

$$p(A)w(A, B) = p(B)w(B, A) \tag{2}$$

Using (**??**) and (**??**), the ratio of transition probabilities can be calculated as the ratio of Boltzman factors of the two states:

$$\frac{w(A, B)}{w(B, A)} = e^{-(E(B)-E(A))/\tau} \tag{3}$$

$$= e^{-\Delta E/\tau} \tag{4}$$

This extremely convenient result is at the heart of the Monte Carlo Markov chain technique known as the Metropolis algorithm. The Metropolis algorithm is an importance sampling technique where instead of calculating values for a distribution itself, samples are calculated from a function proportional to it.[?] The Metropolis algorithm is implimented as follows:

[iii] The Boltzmann factor of a state, s, is given by $e^{E(s)/\tau}$. Further explanation of Boltzmann factors and partition functions can be found on pages 58-62 of Kittel and Kroemer's *Thermal Physics*, second edition.[?]

1. A random spin site is chosen in the lattice.

2. A trial flip of the spin is made and the energy difference, ΔE, is calculated. If $\Delta E < 0$ (flipping the spin leads to a lower energy state), the flip is made and the lattice is updated to the new configuration.

3. If $\Delta E \geq 0$, a random number $0 \leq x \leq 1$ is generated. Using (**??**) and comparing the randomly generated variable to this transition probability, the spin flip is only accepted if $x \leq e^{-\Delta E/\tau}$.

Implementation

At each temperature the program must determine which spins should get flipped and which should not. At sufficiently low temperatures, all the spins should be aligned, but as the temperature rises, the probability that sites might have sufficient energy to flip orientations increases.

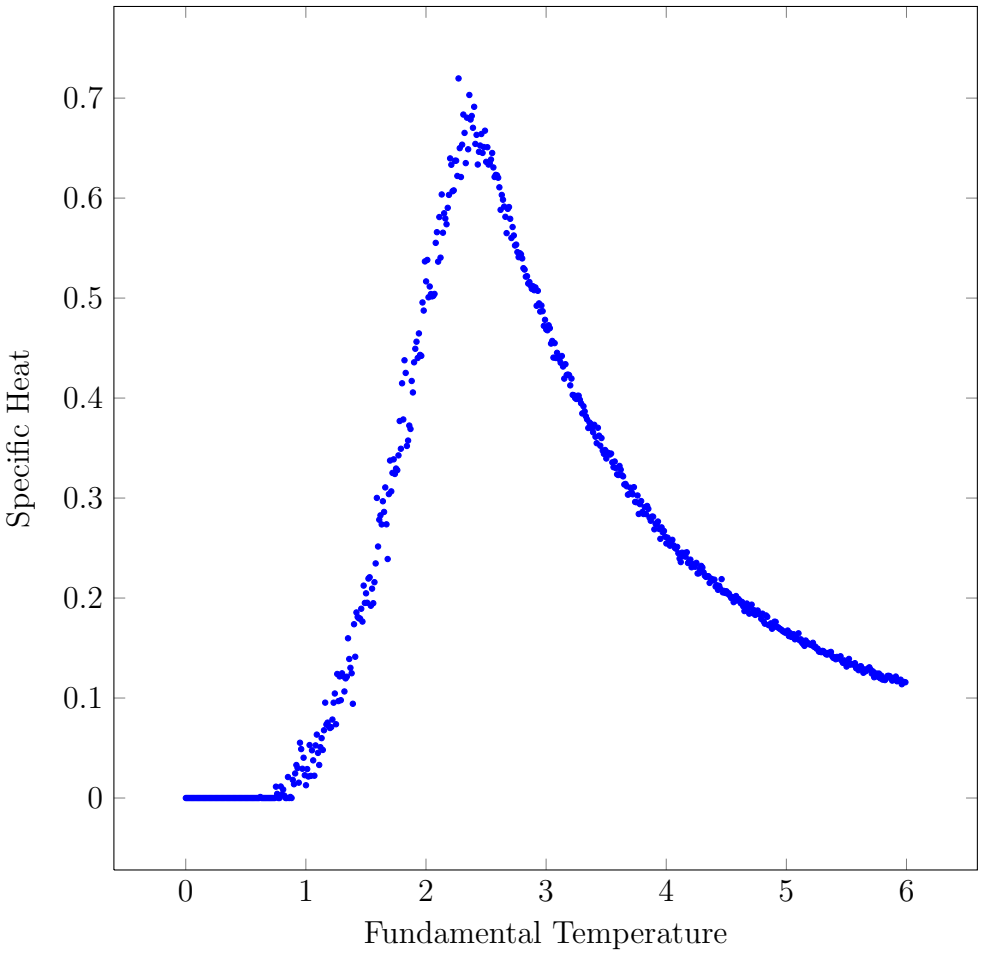
In this program, the lattice is represented by a two dimensional nested list of lists. Each element in the list is an integer (either -1 or 1) representing a spin down or spin up site. The lattice starts out very close to absolute zero with every spin site pointing in the same direction. In addition, several lists are initialized to store values of interest.

At this point, the program enters a loop where the temperature will be increased by a set amount each cycle. For every increment of the temperature, the lattice is first brought to thermal equilibrium and then a random site is chosen to be investigated. With the lattice at thermal equilibrium, individual sites are chosen at random and flipped or not flipped according to the Metropolis algorithm.

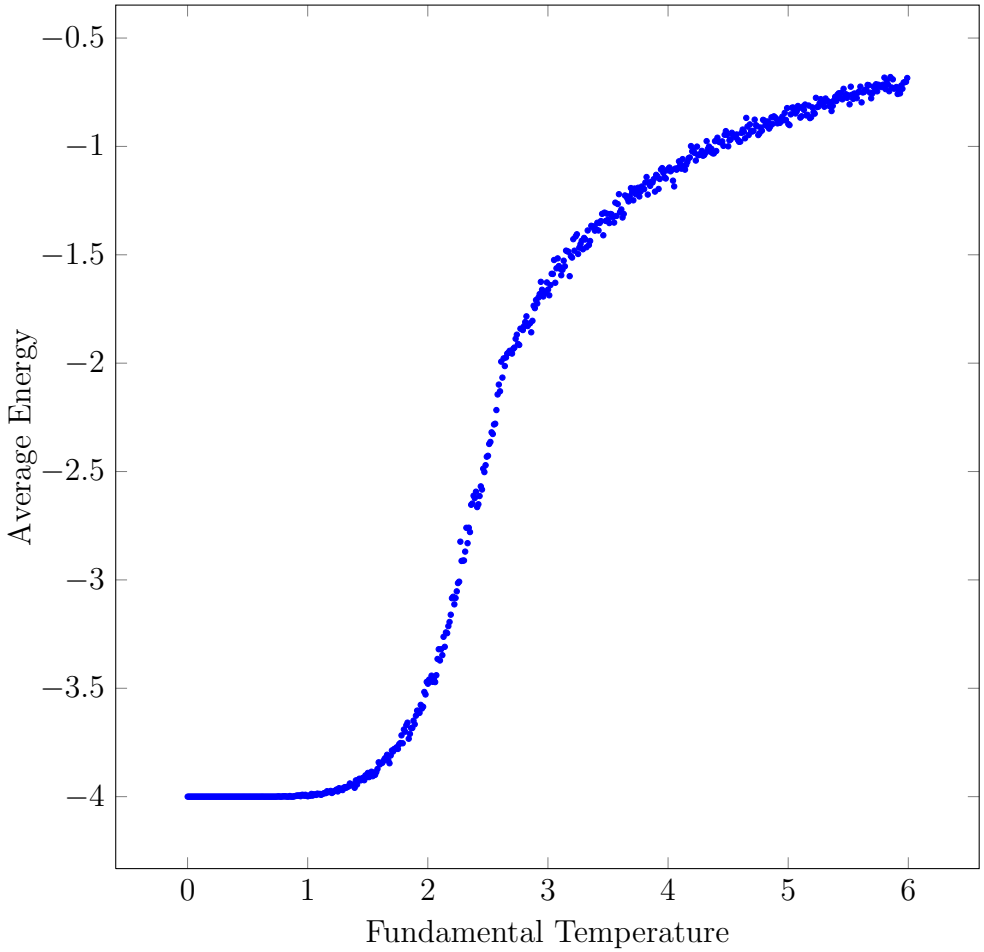
After the flip has been attempted, the difference in energy between the pre-step lattice and the current lattice is recorded, as well as the magnetization at that site. Each of these attempts constitutes one step. The number of steps carried out is proportional to the size of the lattice. After the appropriate number of steps are carried out, the average energy, average magnetization, and energy variance are calculated for this temperature from the data gathered at the end of each step for this temperature. Then, the temperature is increased by a set amount and the whole process is started over again. This is repeated up until some maximum specified temperature is reached.

Results

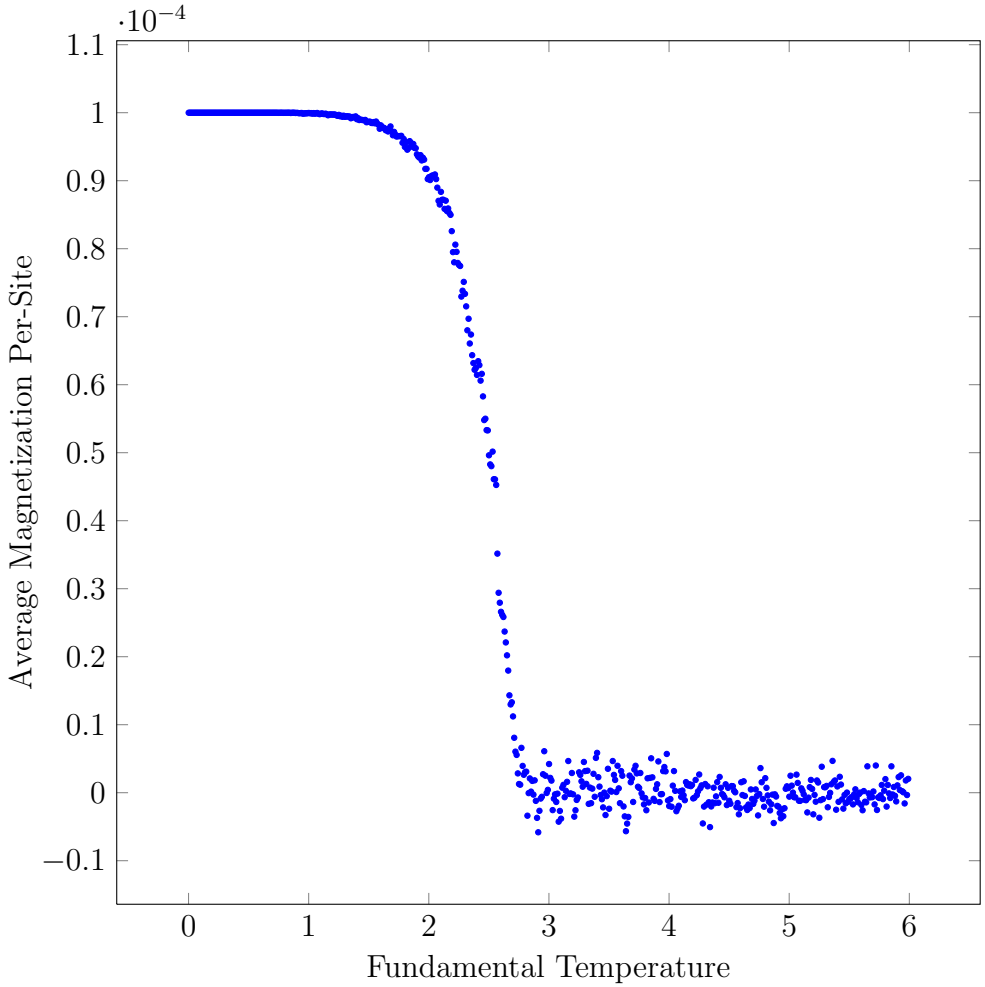
The following data were obtained by running the Python simulation with the following parameters: columns = 100, rows = 100, maximum temperature = 6.0, temperature step size = 0.01, number of equlibrium steps = 3, number of sweeps = 1. I have used fundamental temperature, $\tau = Tk_B$, in the simulation.



The phase transition causes a spike in the specific heat around $\tau = 2.3$, which is close to the critical temperature of 2.269 obtained in the literature.



The lowest energy state is associated with uniform spin alignment. As the lattice becomes disordered as the temperature increases, the average energy decreases.



At low temperatures, the lattice exhibits near-uniform magnetization until the critical temperature is approached, at which point the magnetization drops sharply and the system turns to a disordered state.

Additional Remarks

This program could be optimized for speed, but it has been left in its current state so that it can be more easily followed by a student who is new to programming or to this subject.