Simulation of the Ising model
Michael Sova
December 18th, 2014

Abstract

The metropolis algorithm was used to simulate the 2D Ising model. Code for the simulation was written in Python using an object orientated programming approach. Behaviour of Ferromagnetic materials was studied using the results of the simulation. The average magnetization and energy per atom were calculated for different temperatures [figures 11, 12]. A critical temperature for the phase transition of a 2d lattice of atomic spins was found by plotting the magnetic susceptibility and specific heat capacity against temperature [figures 13, 14]. The temperature at the peaks of the magnetic susceptibility and specific heat capacity plots was calculated to be $T = 2.3\frac{J}{k_b} \pm 0.1$. The theoretical value for the critical temperature of the 2D Ising model is $T = 2.27\ \frac{J}{k_b}$ [4]. Therefore, the experimental value at which the lattice underwent a phase change corresponds well to theory. The system was also studied under the influence of an external magnetic field.

Background

Magnetic domains
Ferromagnetism [2] is found in many naturally occurring metals such as Iron or Nickel. These metals are ferromagnetic due to quantum mechanical interactions that cause quantum spins to be aligned [3]. Neighbouring atoms are likely to be ordered despite the randomizing effects of thermal excitations. This long range ordering effect results in areas of intense magnetic fields called domains [2]. In these domains electrons are lined up in the same direction. Magnetic domains can be clearly seen in figure 3. On average a ferromagnetic metal is not magnetized because the domains are randomly distributed and are not aligned with each other. The random distribution of domains is illustrated by figure 2. The Ising model can be used to study ferromagnetic materials as a two dimensional lattice. If the lattice experiences an external magnetic field, there will be a stronger preference for domains with a magnetic field pointing in the same direction as the external field. The preference for different domains under opposite magnetic fields is demonstrated in figures 9 and 10. If the entire lattice of atoms are aligned the net effect would be a highly magnetized system.

Hysteresis Loop
Ferro-magnets continue having macroscopic magnetization even after the external magnetic field is removed. Once magnetic domains are formed it takes energy to break them. Therefore an opposing magnetic field has to be used to drive the Ferro-magnet back to zero net magnetization. In essence ferromagnetic materials have memory of their previous orientation. This dependence on past states is called hysteresis [3]. As a result, the magnetization of a ferromagnetic material experiencing alternating magnetic fields will form a hysteresis loop (fig 19, 20). It can be seen in figures 19 and 20 that a decreasing temperature will make the hysteresis loop wider.

Critical temperature
An analytical solution for the two dimensional Ising model was derived by Lars Onsanger [4].
At this temperature the lattice ceases to be ordered. The formula for the Onsanger equation was

derived for an infinite lattice. Since a finite sized lattice had to be used in the computer simulation, some deviation from the analytical result should be expected. The precise value for the critical temperature is given by [4]:

$$T_{crit} = \frac{2J}{k_b \ln(1+\sqrt{2})}$$

Plotting the results revealed this critical temperature. Since all the plots are in natural units of $\frac{J}{k_b}$ the critical temperature should be $T = 2.27\ \frac{J}{k_b}$.

Methods

Ising Model

The 2d Ising model consists of a lattice of atomic spins. The spins can either be +1 or -1. Atoms interact with four neighbours (excluding diagonal neighbours). The model allowed the study of phase transition in ferromagnetic material using statistical mechanics. The metropolis algorithm is used to determine if a spin flips. The energy change is calculated from the spin interaction of neighbouring atomic spins. The energy change for flipping one atomic spin is therefore given by:

Formula 1: $$dE = 2\sigma_{i,j}(\sigma_{i+1,j} + \sigma_{i,j+1} + \sigma_{i-1,j} + \sigma_{i,j-1})$$

Where i and j are the positions of the atomic spin to be flipped in the lattice. Interaction energy is assumed to be constant and is not considered since all the calculations are in natural units. Therefore the maximum energy change for each flip $\pm 8J$.

Metropolis algorithm

The metropolis algorithm is used to minimize free energy of the system. In order not to get stuck in a local minima the energy has to have some probability of increasing. Local energy minima in Ferro-magnets are created by relatively stable orientations of magnetic domains. Some positive thermal fluctuations (increase in free energy) are needed to break the magnetic domains to reorder the system into a lower energy state (shown by hysteresis loop in figure 19). Once the system enters a global minima the probability of the system escaping is sufficiently small. Since the number of possible states of the system is 2^N, the simulation would be far too complex to fully generate. Instead, the problem was solved probabilistically from a statistical mechanics perspective. Numbers based on averages of the physical attributes of the system were used. All the microstates of the system are assumed to be accessible and probabilistically proportional to their energy. As a result, the probability of the states is determined by the Boltzmann distribution is $P = e^{-dE\beta}$. Where β is $\frac{1}{T}$ and dE is the change in energy given by formula 1.

The steps in the algorithm are:

- Initialize a N by N lattice of spins (a cold start or a hot start)
- A state is selected at random in the lattice
- Compute the energy change of flipping the spin (formula 1).
- If the energy change for flipping is negative, the energy change is favourable since free energy is minimized. Therefore the change is accepted.
- If the energy change for flipping the spin is greater than zero the probability of the spin is given by the Boltzmann distribution. A random function is used to select a number

between zero and one. If the number is smaller than $P = e^{-dE\beta}$ then the change is accepted.

- To measure the variables over a range of temperatures, the metropolis algorithm is run until the system equilibrates. Only then is data collected.

Thermodynamic variables

The net magnetization of a system is given by the following formula [1]:

$$\mathbf{M} = N^{-2} \sum_k \mathbf{S}_k$$

Where N is the number of atomic spins in the lattice and the sum is over all spins. The system has maximum magnetization when all the spins are aligned. The magnetization has two possible global minima (+1 and -1) between which it can oscillate given enough time. An external magnetic fields can force the magnetization of the system in either direction (figures 15 and 16). Increasing an external magnetic field can also shorten the stabilization period of the system (figures 15 and 16).

The total energy is given by [1]:

$$E = -\frac{1}{2} \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - \mu \sum_k \mathbf{S}_k \cdot \mathbf{B}$$

The interaction energy J_{ij} is assumed to be constant for all neighbours. The system is in a minimal energy state when all the spins are parallel. The interaction energy is greater than zero for Ferro-magnets [1]. In case of no external magnetic field the right side of the formula goes to zero. The ½ constant prevents counting the energy twice. The energy has one possible global minima. An external magnetic field can shift the system to a lower global minima and therefore lower energy state, which can be seen in figure 18.

The specific heat capacity C and the magnetic susceptibility X are given by [1]:

$$C = N^{-2} \frac{1}{k_B T^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right)$$

$$\chi = N^{-2} \frac{J}{k_B T} \left(\langle S^2 \rangle - \langle S \rangle^2 \right)$$

Where N is the number of atomic spins in the lattice and the averages are computed for Energy and Spin. The magnetic susceptibility and specific heat capacity peak at the critical temperature (fig 13, fig 14). However, the analytical derivation assumes an infinite lattice. But limitations in computational power prevent the simulation of an infinite lattice. As a result, some deviation from the expected result should be expected.

Programming

Boundary conditions were solved by connecting the lattice along its borders (top to bottom, left to right). The lattice therefore assumes the shape of a torus. An object oriented approach was taken with relevant methods and attributes held in the appropriate classes. A class called Lattice holds all the attributes and methods relevant the simulation of the 2d Ising model. The attributes include size of lattice, strength of external magnetic field, temperature, total magnetization and total energy. The methods allow for initializing the system with random spins (hot start) or aligned spins

(cold start) and running the metropolis algorithm for a specified number of steps. A plotting class was also written to simplify the generation of plots for the project. The plotting class also holds methods for normalizing and averaging data. Graphs were plotted using the matplotlib library. The numpy library was used to simulate the 2d lattice as an N-dimensional array object and its random number methods were used for the metropolis algorithm.

Discussion of Results

The system was left to equilibrate for 50 000 steps. The results were averaged over several sweeps. The averages were calculated for the relevant thermodynamic variable (magnetization and energy). All the plots of thermodynamic variables were simulated using a 10x10 array. The lattice plots were simulated with a 150x150 array. The peaks of the plots of magnetic susceptibility and specific heat capacity revealed that Ferro-magnets underwent a phase transition at a critical temperature of $T = 2.3\frac{J}{k_b} \pm 0.1$ (units of $\frac{J}{k_b}$). The error came from the approximate width of the peak.

Above the critical temperature the system became paramagnetic [2]. Thermal effects cause random flips of spins. A higher temperature will increase the number of flips, which will disturb the creation of domains. If the temperature is high enough, the thermal excitations will dominate the system. Therefore, the size of the domains is inversely proportional to temperature (shown in figures 1 and 2). At temperatures close to $T_{critical}$, the system took longer to stabilize. It was therefore crucial to check if the lattice had reached an equilibrium. At higher temperatures of about *T*=10*JKB* the system was not allowed to reach equilibrium since the domain formation was precluded by the thermal fluctuation (figure 5).

At a higher than critical temperature (T>>2.3) the system was random with zero net magnetization and in its highest energy state (fig 11, fig 12). At low temperatures (T<<2.3) when thermal excitations were minimal all the atomic spins were parallel and the system was in the lowest energy state and highest magnetization state (fig 11, fig 12).

Below the critical temperature the thermal excitation had a lower frequency and the system became more aligned (fig 3, fig 4). Lattices initialized at high temperatures and equilibrated at temperatures below $T_{critical}$ are shown in figures 3 and 4. Below the critical temperature the system is allowed to drop to the minimum energy state (given enough time). However, even above the critical temperature an external magnetic field can be used to align the lattice (shown in figures 6 and 8). Increasing an external magnetic field can also shorten the stabilization period of the system (figures 15,16,17,18). An external magnetic field can shift the system to a lower global minima and therefore lower energy state, which can be seen in figures 18 and 21.

As shown in the average magnetization plot, the lattice becomes a paramagnet at the critical temperature given by Onsanger. The value of magnetization plummets rapidly from 1 to 0 at this point (figure 12). Based on the plot for net magnetization, it was expected that energy would oscillate around zero after the critical energy was reached. But energy is dependent only on closely neighbouring spins (Formula 1). Even after the critical temperature is reached some local relatively stable domains persist lowering the free energy. At a temperature high enough to break all local domains a zero value for energy would be expected.

The phase transition of the system was further illustrated by plotting the specific heat capacity and magnetic susceptibility of the system [fig 13, fig 14]. Initially the magnetic susceptibility is low because there is not enough energy for the electrons to flip. Once sufficient energy is reached many spins are flipped to change the net magnetization. This change increases susceptibility. Susceptibility is increased until the phase transition occurs at the critical temperature. Then thermal fluctuations dominate and net magnetization tends to zero. Therefore

the magnetic susceptibility decreases and there is a peak for magnetic susceptibility at the critical temperature. The specific heat capacity peaks for a similar reason. It makes sense that specific heat capacity peaks at the phase change, since the temperature of a system undergoing a phase change should not change no matter how much energy is put into the system.

Results

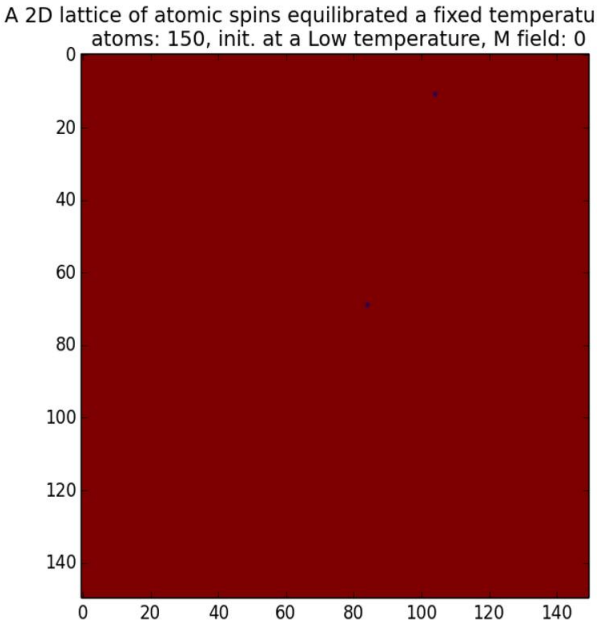

Figure 1

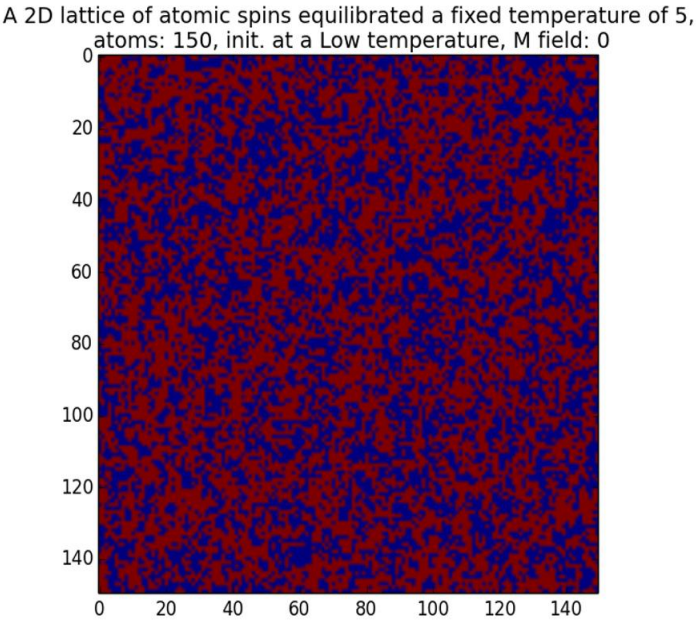

Figure 2

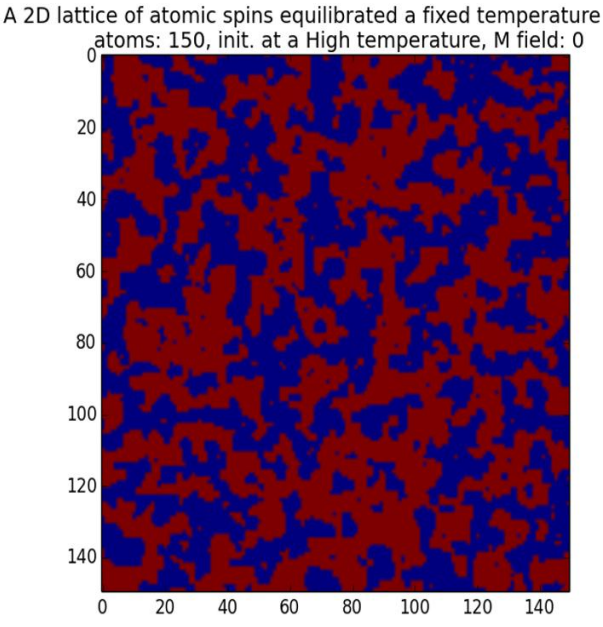

Figure 3

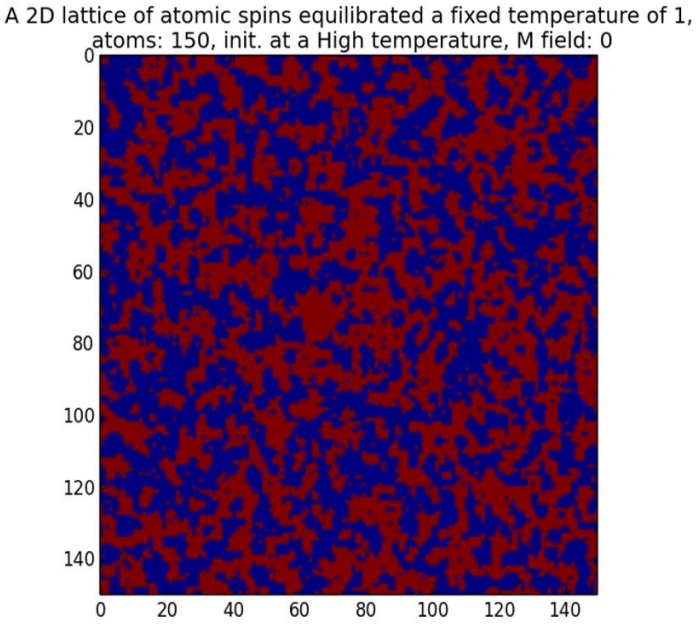

Figure 4

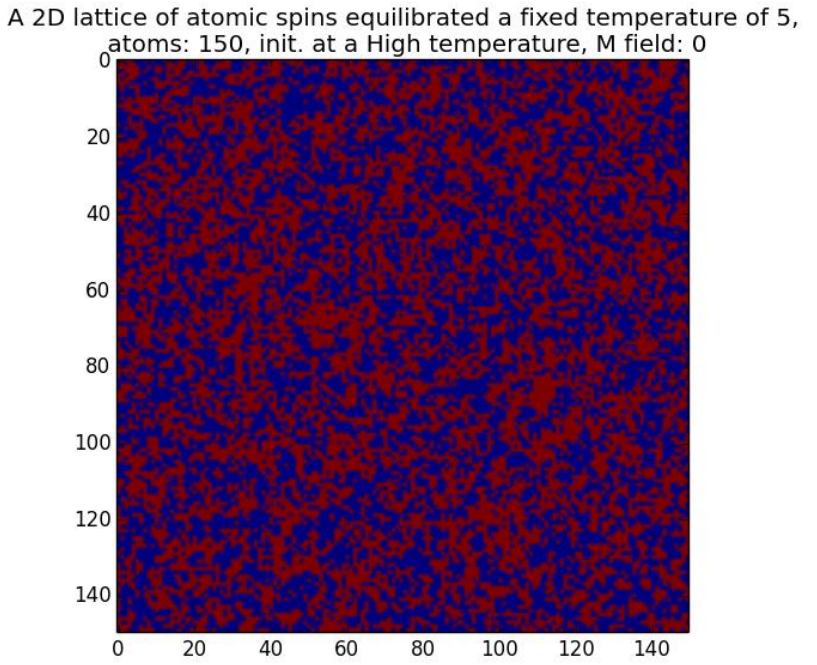

Figure 5

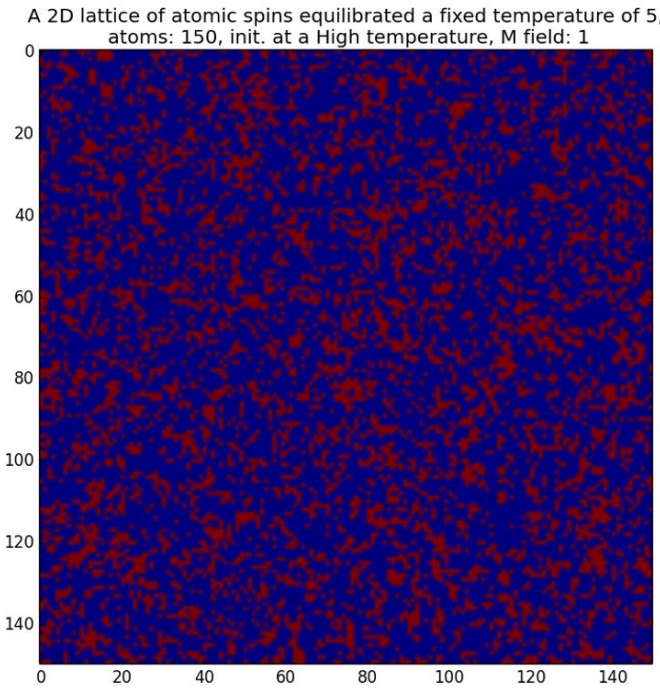

Figure 6

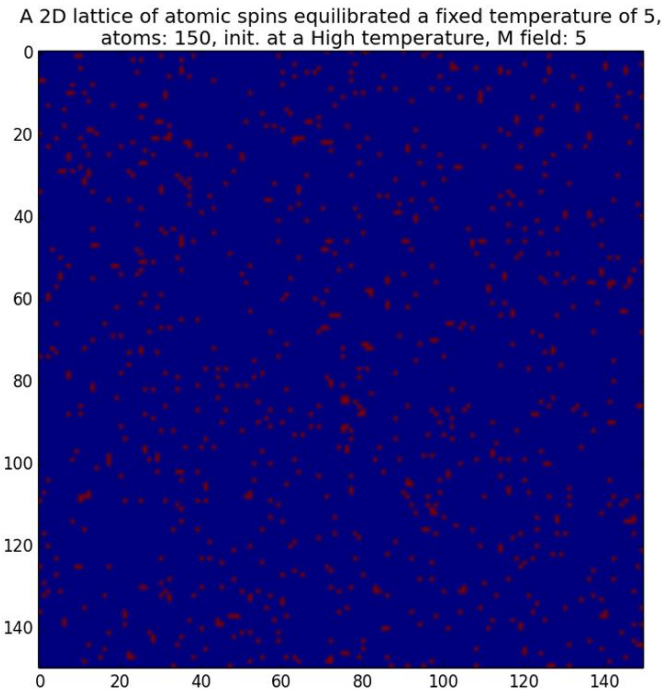

Figure 8

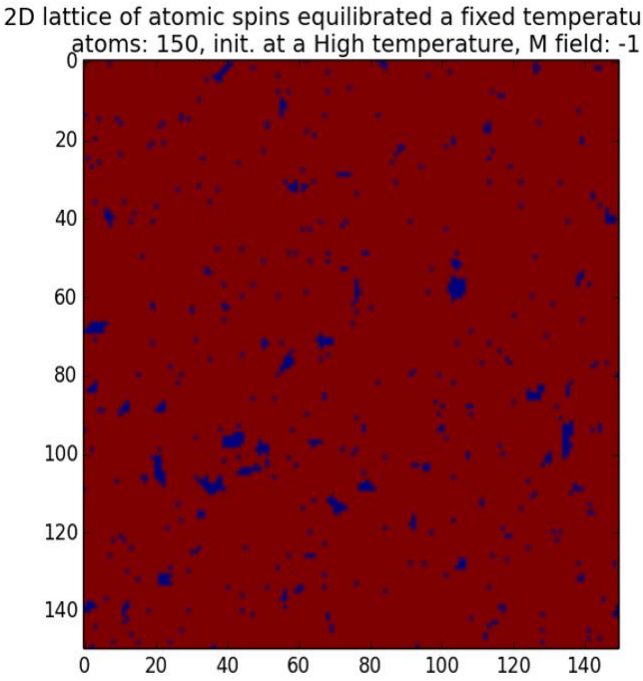

Figure 9

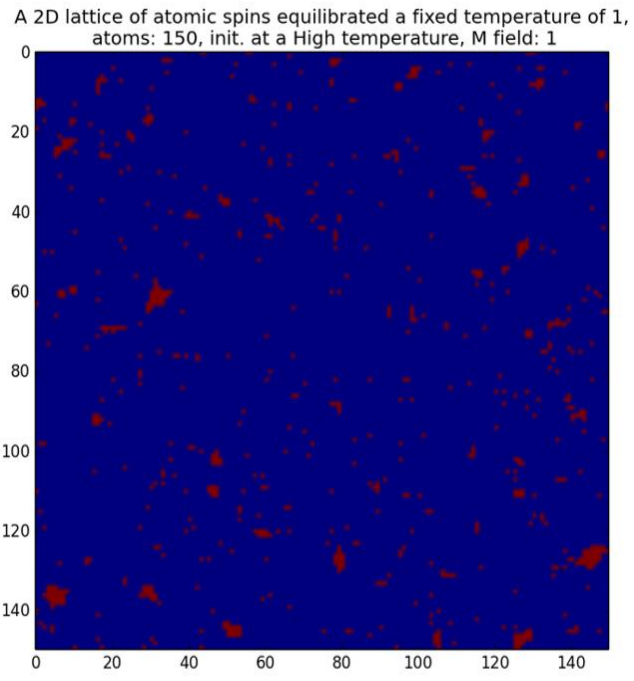

Figure 10

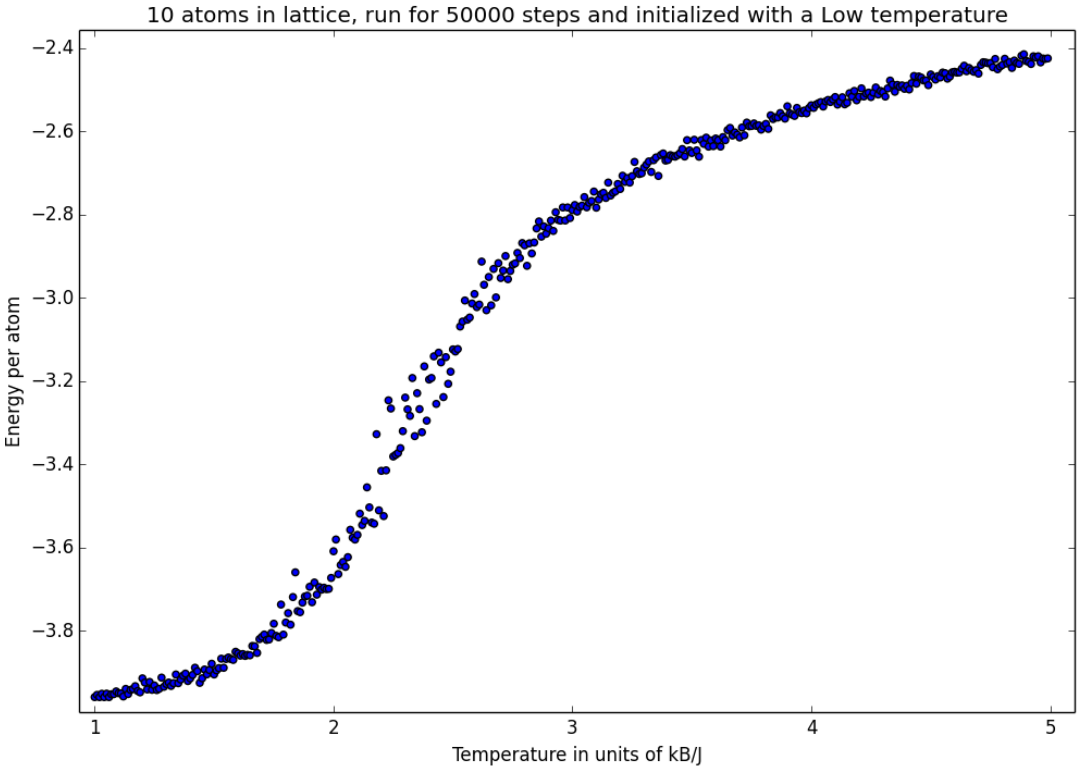

Figure 11

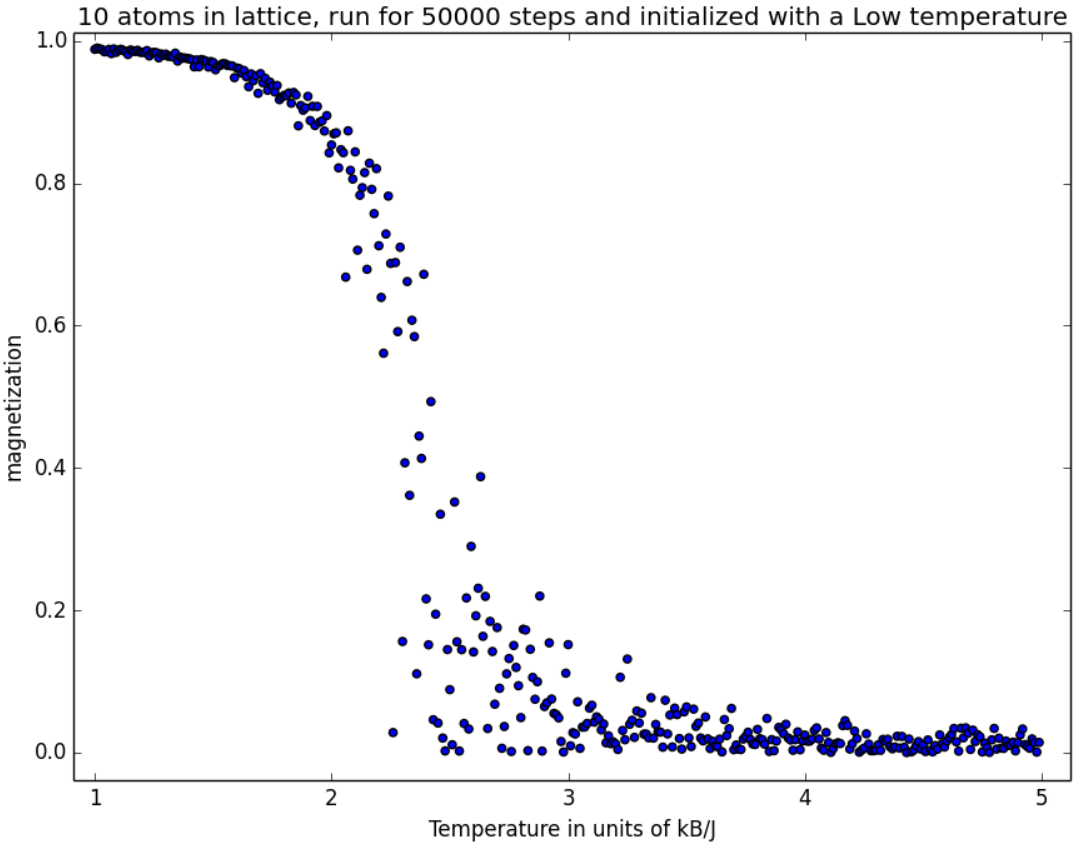

Figure 12

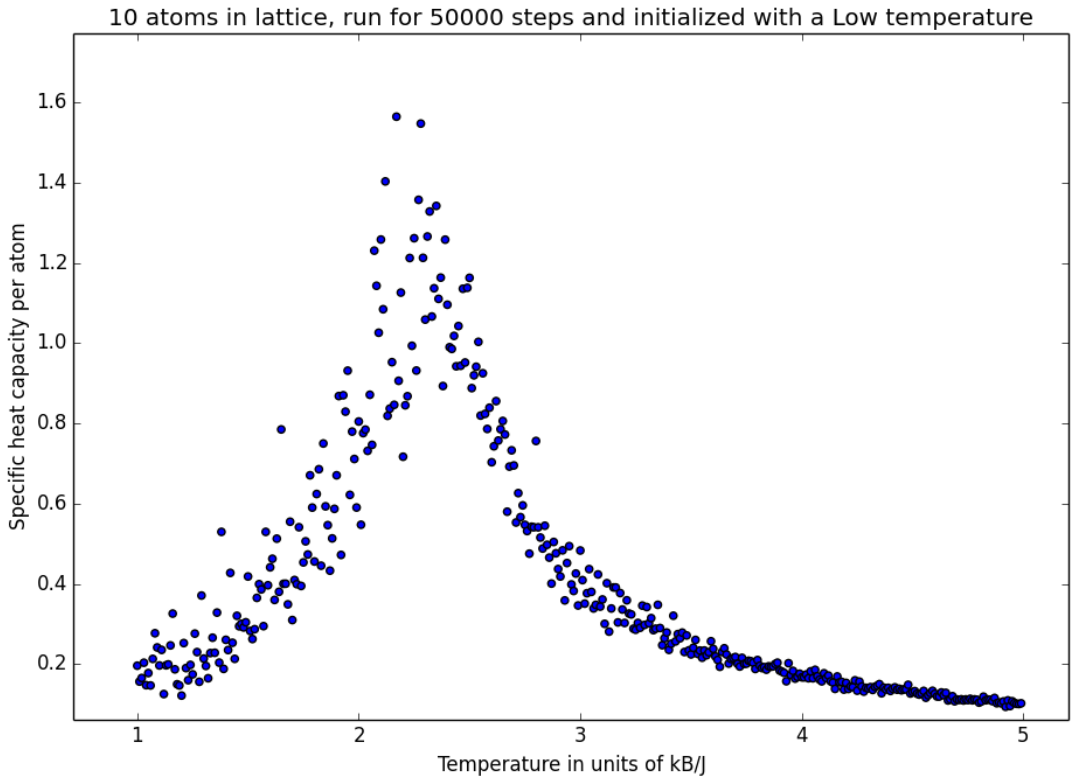

Figure 13

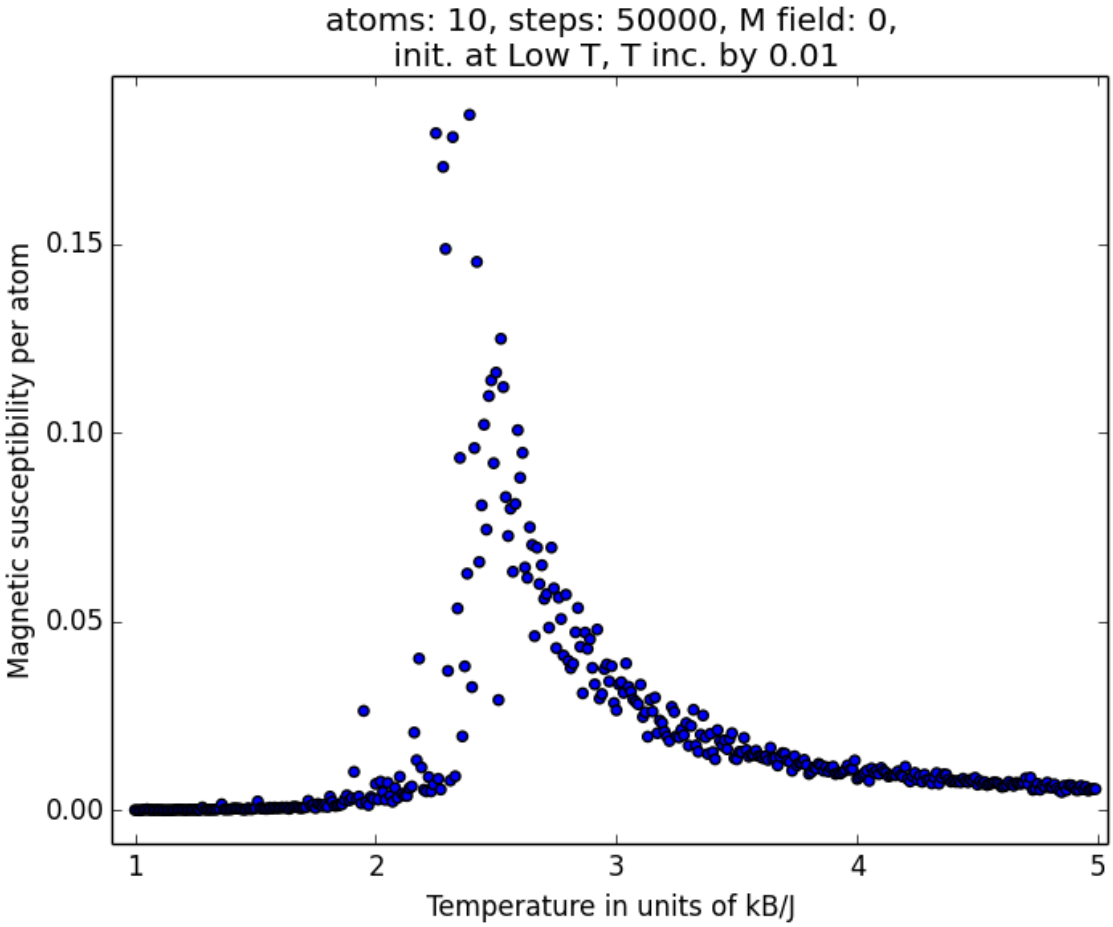

Figure 14

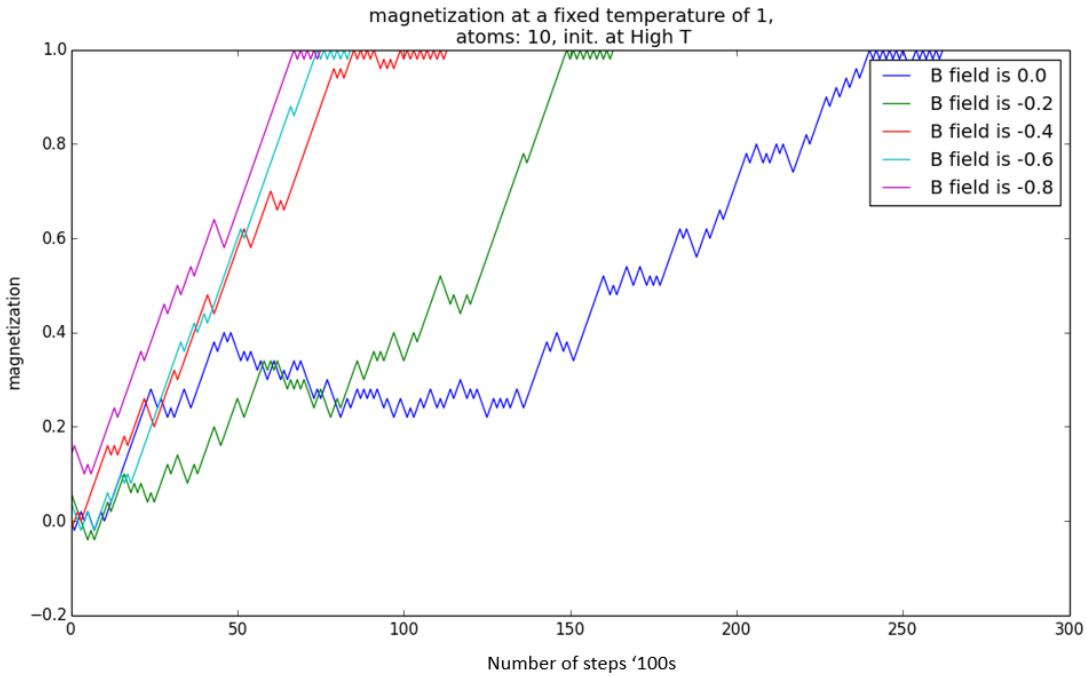

Figure 15

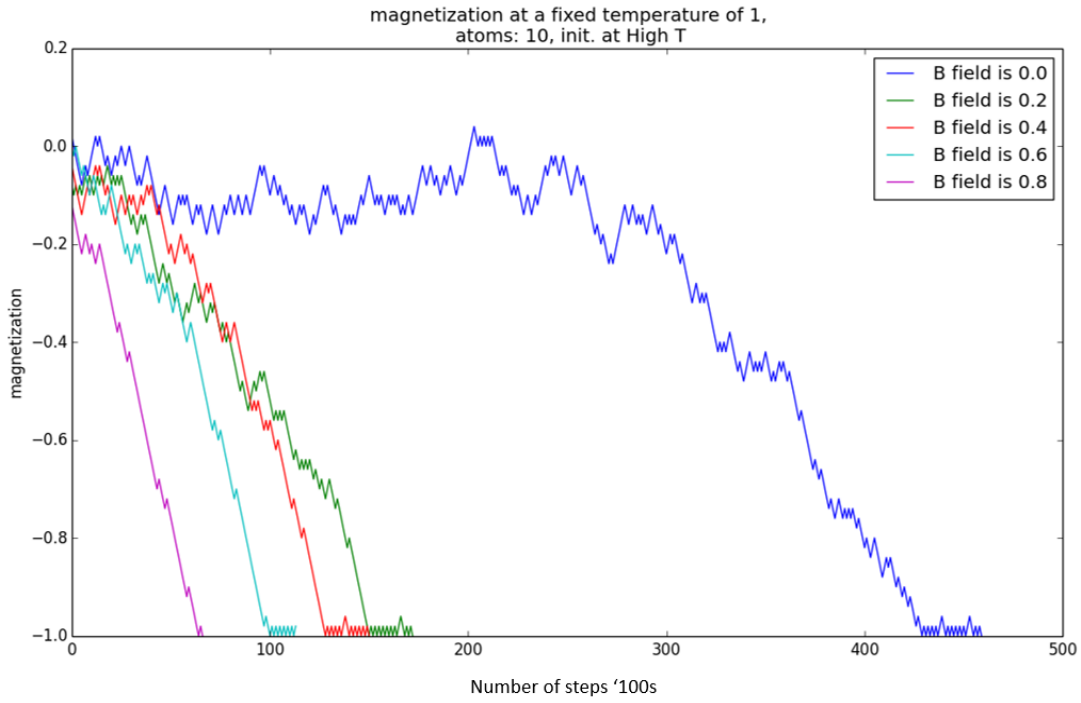

Figure 16

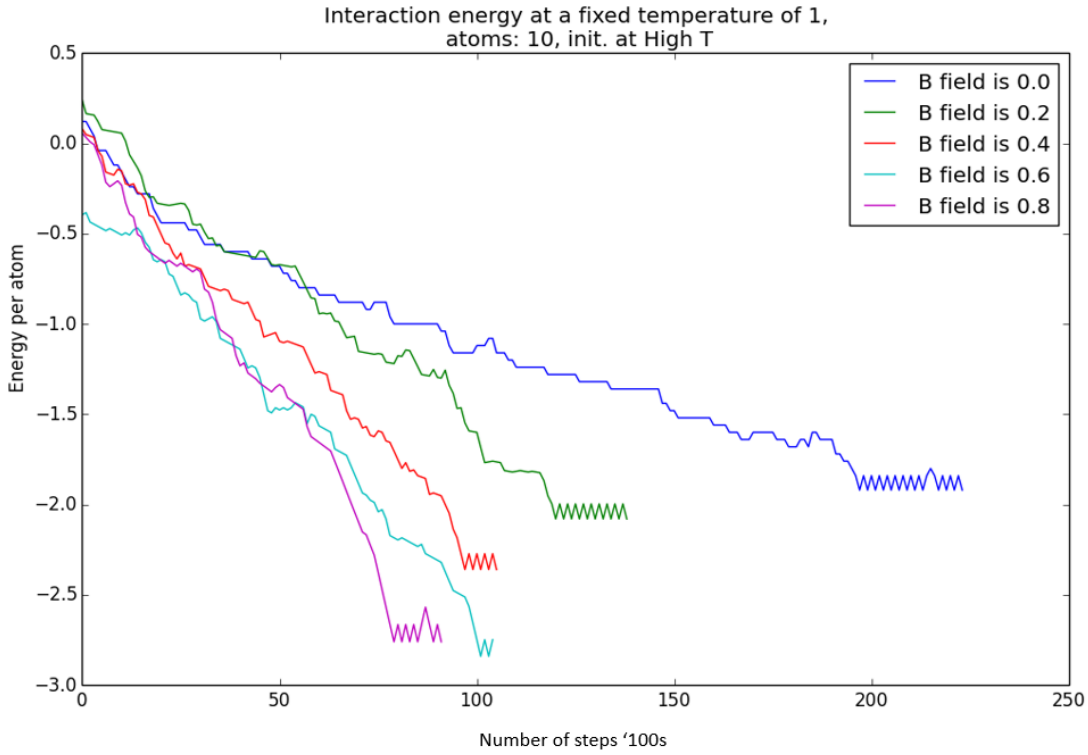

Figure 17

Figure 18

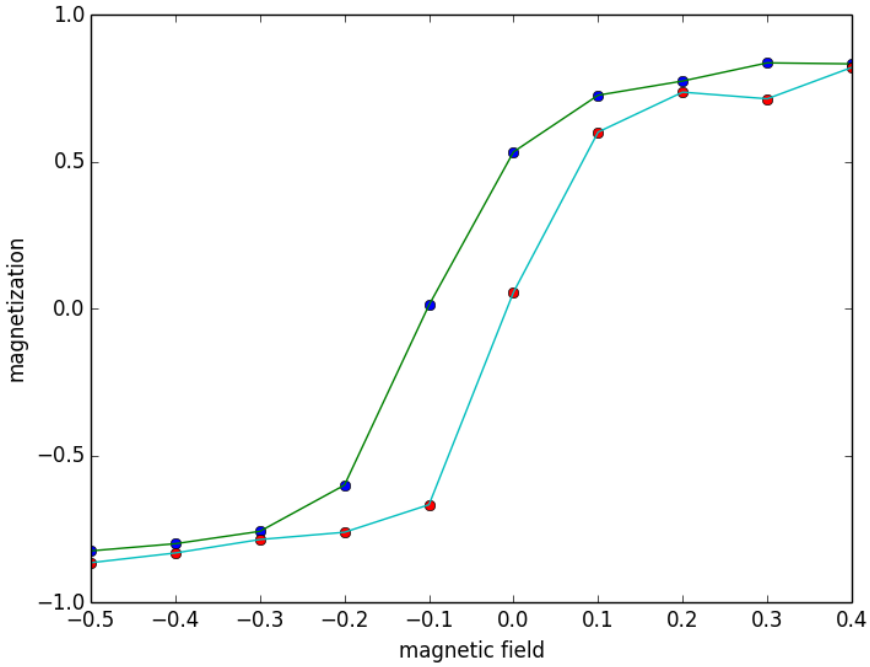

Figure 19 – hysteresis loop lattice equilibrated at T=1

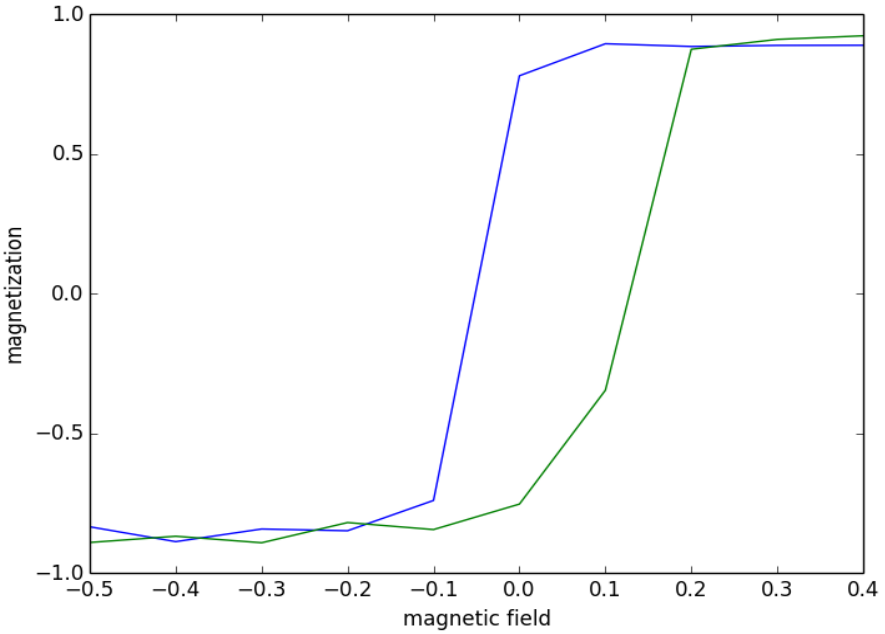

Figure 20 hysteresis loop, lattice equilibrated at T=0.5

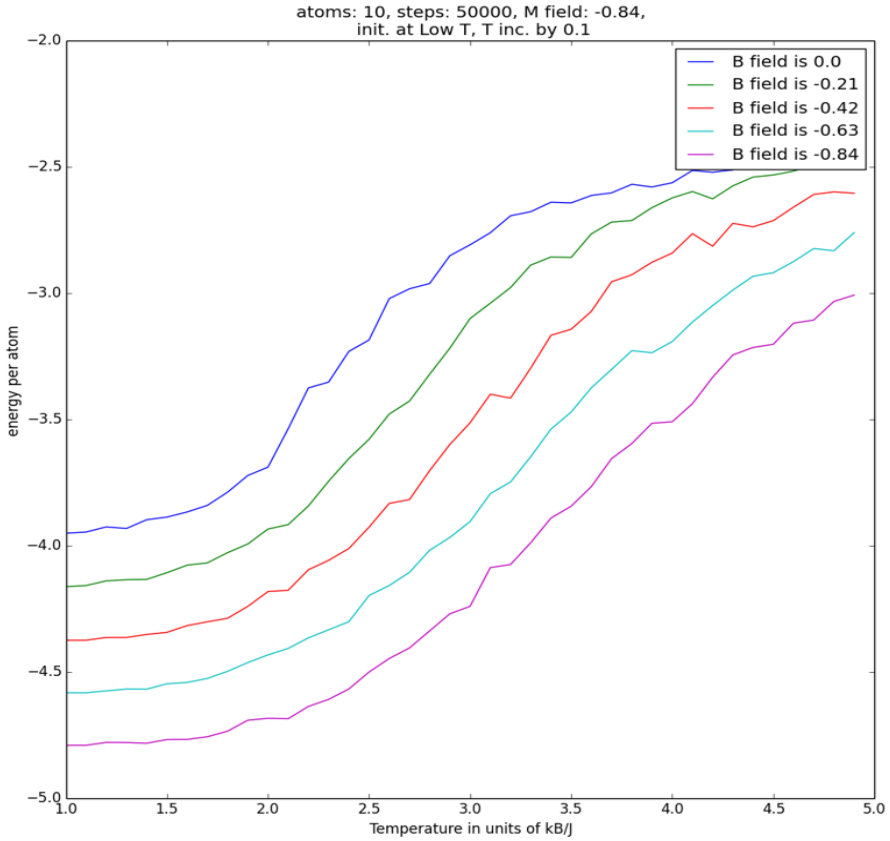

Figure 21

Conclusion

The temperature at the peaks of the magnetic susceptibility and specific heat capacity plots was calculated to be $T = 2.3\frac{J}{k_b} \pm 0.1$ $(\text{units of } \frac{J}{k_b})$. The theoretical value for the critical temperature of the 2D Ising model is $T = 2.27\ \frac{J}{k_b}$ [4]. Therefore, the analytical result compares well with the experimental result. The data had a lot of noise, perhaps more averages had to be taken. The quality of the data was mainly limited by the constraints on computational power. Python is not a dynamically compiled language. It is inefficient compared to compiled languages such as C or C++. As a result, the size of the lattice and time steps had to be kept relatively small. The results are strongly affected by the time steps and size of the lattice. The analytical derivation for $T_{critical}$ assumes an infinite lattice, however only a 10x10 lattice was used. As a result, some deviation from the expected result should be expected. In practice physics research facilities run programs on supercomputers for a very long time to obtain reliable data.

Word Count: 2206

Bibliography:

1. Robert Kingham, Imperial College London, 2014 3rd year project script for Computational Physics.
2. Michael Mansfield, Colm O'Sullivan. (2011), *Understanding Physics Second Edition.* Wiley.
3. Hyper Physics (2011), *Hysteresis in magnetic materials*. Retrieved 20th December 2014 from: http://hyperphysics.phy-astr.gsu.edu/hbase/solids/ferro.html
4. DAVID CIMASONI AND HUGO DUMINIL-COPIN, University of Geneva, *THE CRITICAL TEMPERATURE FOR THE ISING MODEL ON PLANAR DOUBLY PERIODIC GRAPHS*. Retrieved 20th December 2014 from: https://www.unige.ch/~duminil/publi/Kac%20Ward.pdf