Draft version March 22, 2022
Typeset using LaTeX default style in AASTeX631

Simulated Annealing

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1. INTRODUCTION

For this assignment, the objective is to utilize the technique of simulated annealing to tackle the problems below. Simulated annealing has to do with determining the most optimal solution to an optimization problem. This technique is best saved when dealing with discrete problems, in comparison to continuous problems. Simulated annealing can also be applied when analyzing multi-variable problems and determine an overall better solution. Annealing is the heating and cooling of an object with the purpose of removing internal deformities. This process is done by manipulating the internal structure or crystal of the object and changing its form. A relation between the two is found through the determination of an overall solution, which is similar to the heating and cooling of the object. Both methods are able to determine a general approximation of the solution.

2. FREE HANGING NECKLACE

The *Free Hanging Necklace* is a type of problem in which simulated annealing can be applied. Imagine a bead necklace which hangs from a ceiling. The parts of the necklace that are not attached to the ceiling will be pulled downward due to gravity. Assuming mass is equally distributed along the whole length of the necklace, a hyperbolic shape forms, when looking at two fixed points. This holds true when placing an *nth* number of beads, separated by equal distances, along the string. In this scenario, 20 beads will be placed equidistant from each other and can be dependent on 20 different states. Depending on the current state being observed, the potential energy of the bead can change. By lowering the bead to a lower discrete level, the potential energy of the bead decreases by one unit. Similarly, if the bead increases to a higher discrete level, then the potential energy of that bead will then increase by one unit. The change in potential energy of the beads also affects the surrounding beads. The spring constant of the neighboring beads increases proportionally to the square of the difference between levels. From this, the equilibrium energy can be determined as a function of the temperature.

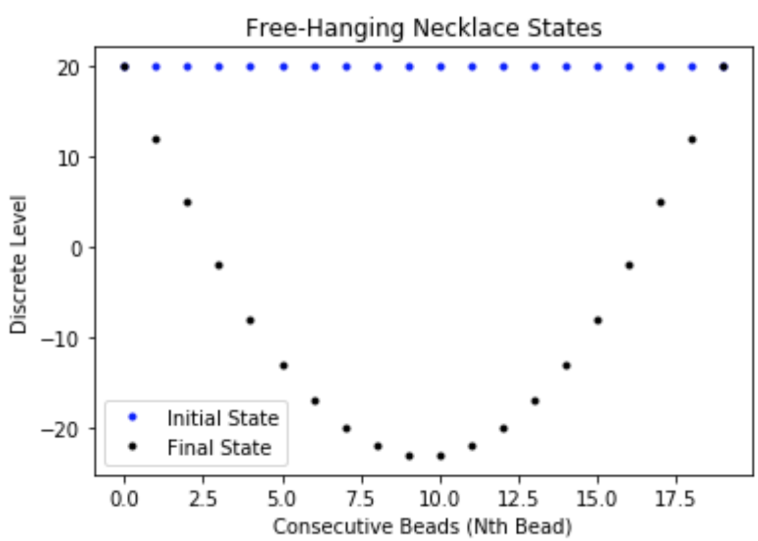

Figure 1. Plot of the initial and final states of the Free-Hanging Necklace Problem

Figure 1 is a plot that depicts the initial and final states that the necklace can take on. As it can be observed, the initial state is when all of the beads are all level with each other, and the final state is representative of the hyperbolic shape that forms when the first and last bead are fixed at the same level.

Figure 2 depicts the plots of the free-hanging necklace when it is at a random state in comparison to the final state possible. The random state is meant to be representative of the behavior of the beads as the functions progresses and is suddenly stopped at a random point in time.

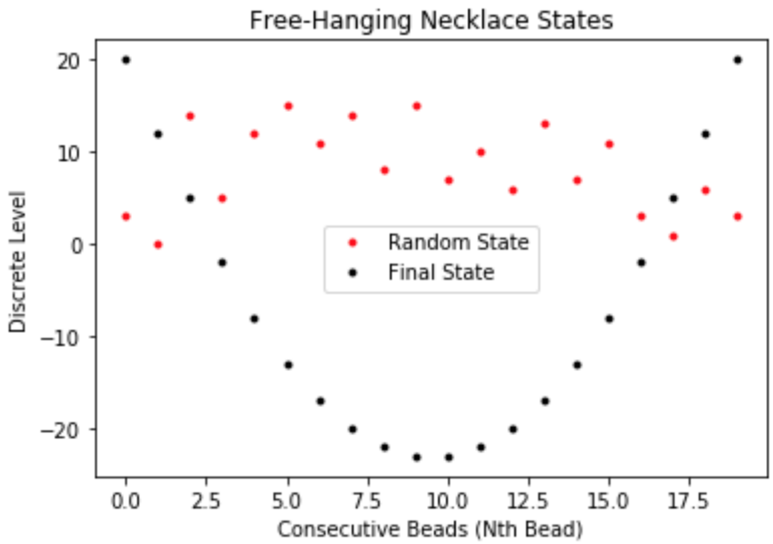

Figure 2. Plot of the Free-Hanging Necklace which compares a random state to the final state.

Figure 3 is a depiction of the three previous states all in one plot. The disorder of the random state is more apparent when compared to the behavior of the beads at the initial and final states.

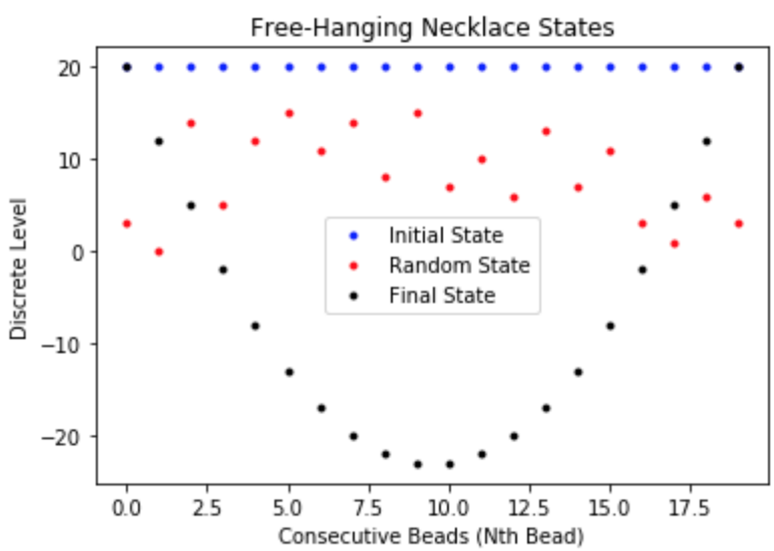

Figure 3. Plot of all three previous plots.

Figure 4 is a visual representation of the hyperbolic cosine, which was utilized to model the theoretical shape of the free-hanging necklace.

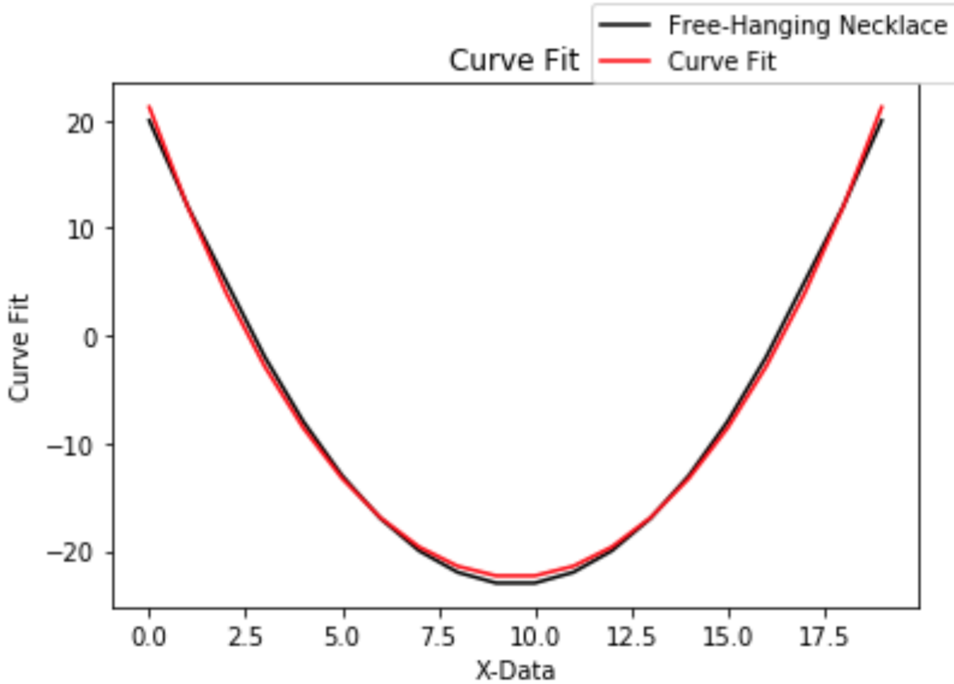

Figure 4. Plot of the theoretical shape of the free-hanging necklace.

3. THE ISING MODEL

The Ising model deals with ferromagnetism, which also falls within the section of discrete math. To better understand this idea, it is important to revisit a magnetic dipole and a dipole moment. A magnetic dipole is a closed loop of magnetic field lines that stem from two poles. A dipole moment is a value utilized to measure the interaction between a dipole and an external magnetic field. This is usually expressed as a vector. With this in mind, a ferromagnetic material is a substance that becomes attracted to another material, due to the polarization of the atoms within it. In comparison, an anti-ferromagnetic material does not have this attractive characteristic due to the internal structure of the atoms being aligned and later re-shaping into an nonparallel pattern, which eliminates the magnetic field and makes the external magnetic field impossible to determine. The Hamiltonian equation below (Equation 1) describes ferromagnetic and anti-ferromagnetic materials in two dimensions in the two state approximation:

$$H = -J \sum_{\vec{ij}} s_i s_j - \mu \sum_i h_i s_i \tag{1}$$

Within this equation, H is representative of the Hamiltonian, J is the intensity of the interaction between two particles, s_i are the two possible polarized states. The magnetic moment is denoted as μ, h_i is the external magnetic field. The first sum (left-hand side) covers the neighboring atoms while the second one (right-hand side) covers all of the atoms. When the J value is positive, it is applied towards ferromagnetic materials and when it is negative, it is applied to anti-ferromagnetic materials. When J is equivalent to 0, it is applied to non-interacting materials.

Figure 5 depicts the plot of the average as a function of temperature. As the plot displays, as the temperature increases, so does the average energy. While difficult to pinpoint exactly, the inflection point of this plot appears to be at $T = 240$ at which there appears to begin leveling off of the energy. This is an expected observation as at high temperatures, kinetic energy is higher and collisions between particles are more frequent. The leveling off is indicative that the temperature is approaching equilibrium.

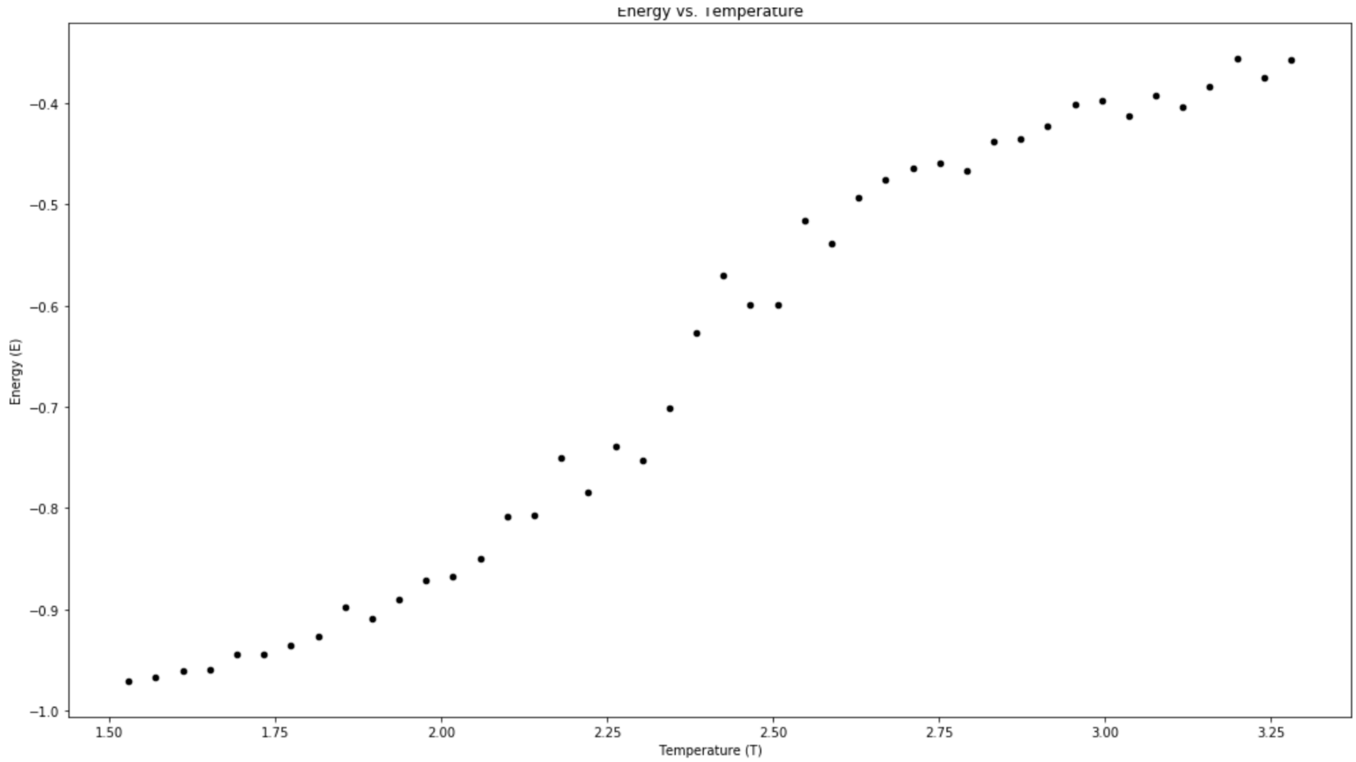

Figure 5. Plot of the average energy vs temperature

The next plot, *Figure 6*, displays the average magnetization as a function of time. As it can be observed, the magnetization decreases exponentially as the temperature increases. The inflection point appears to be at approximately $T = 245$. Again, this plot is in complete agreement with our expectations as we have previously mentioned that at high temperatures, particles lose their aligned structure and their polarization gets affected.

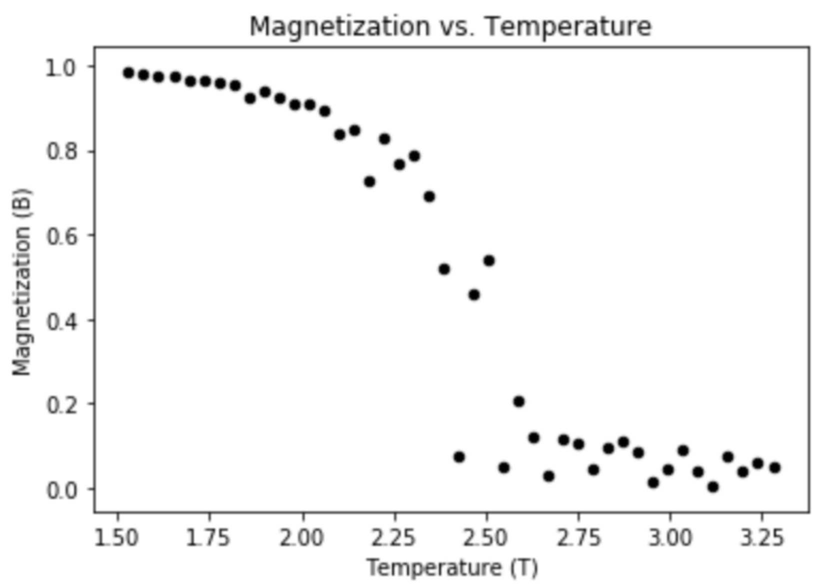

Figure 6. Plot of average Magnetization vs Temperature

The spin susceptibility of the material can also be plotted as a function of time. *Figure 7* depicts the behavior of the plot as the temperature increases. As temperature increases, the spin susceptibility remains constant and experiences a jump before decreasing shortly after to a lower equilibrium. This jump occurs at approximately the same temperature range that has been pointed out before with the previous plots.

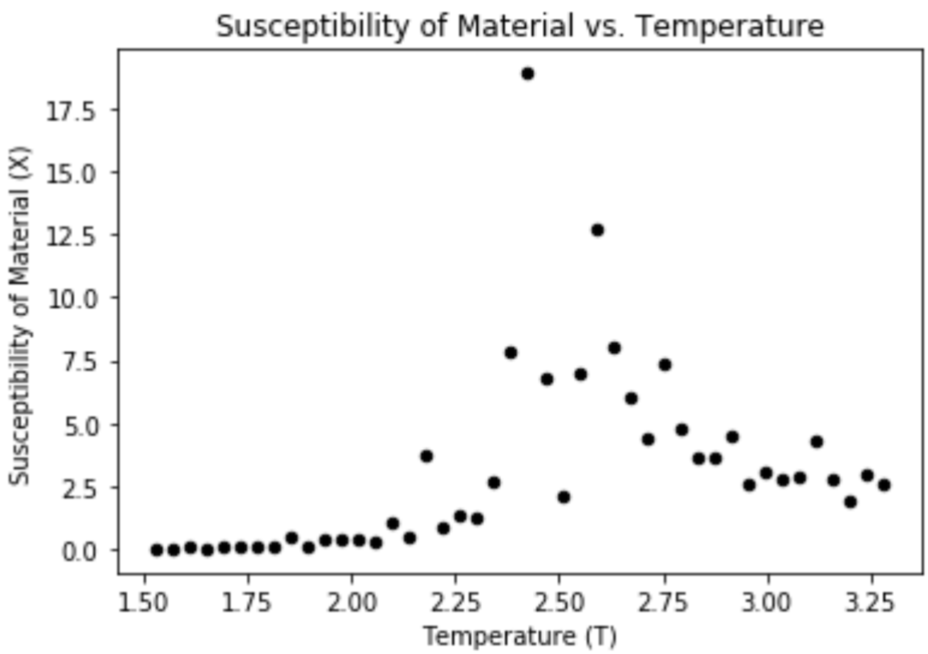

Figure 7. Plot of susceptibility of the material against temperature

Another property that can be plotted is the specific heat as a function of time. We expect the behavior of this plot to generally mimic the behavior of the spin susceptibility of the material. *Figure 8* depicts the specific heat plot. As evidenced by the plot, the specific heat rises at a constant rate and later decreases at a constant rate. However, what is interesting is that the switch in the behavior of the plot occurs at the same temperature range that caused the spin susceptibility to experience a sudden jump.

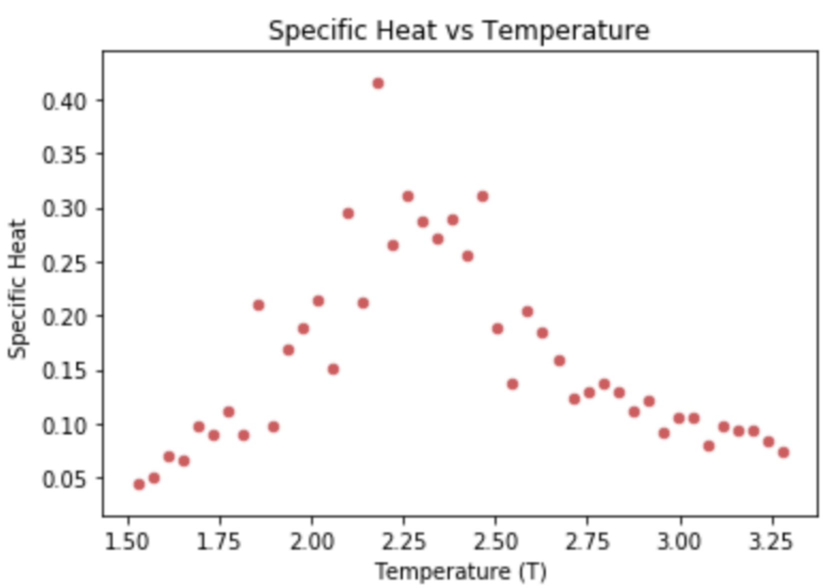

Figure 8. Plot of specific heat against temperature.

What if an external magnetic field were not present? When this is the case, the equation below (Equation 2) can be solved to determine the temperature of the transition phase, T_c.

$$1 = sinh\frac{2J}{k_B T_c} \tag{2}$$

When solved, $T_c = 2.269185\ \frac{J}{k_B}$. The following plots confirm that $h_i = 0$.

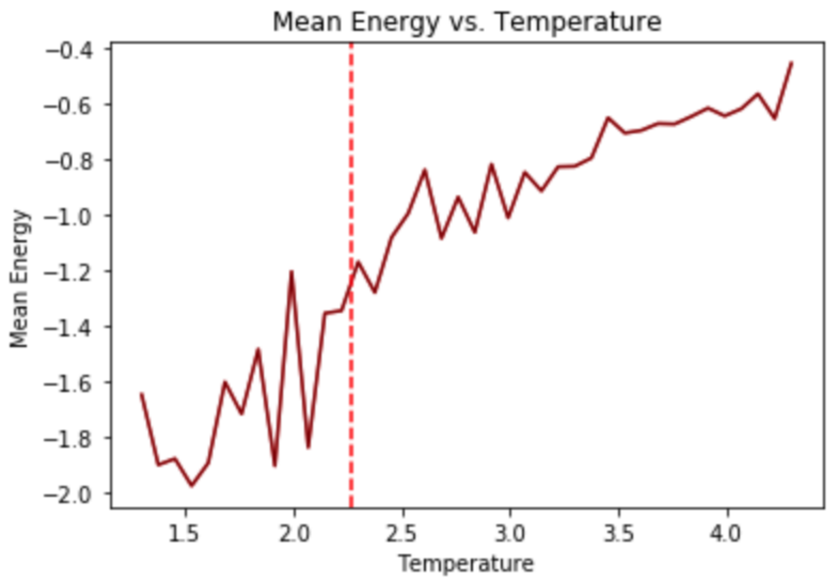

Figure 9. Average Energy vs Temp.

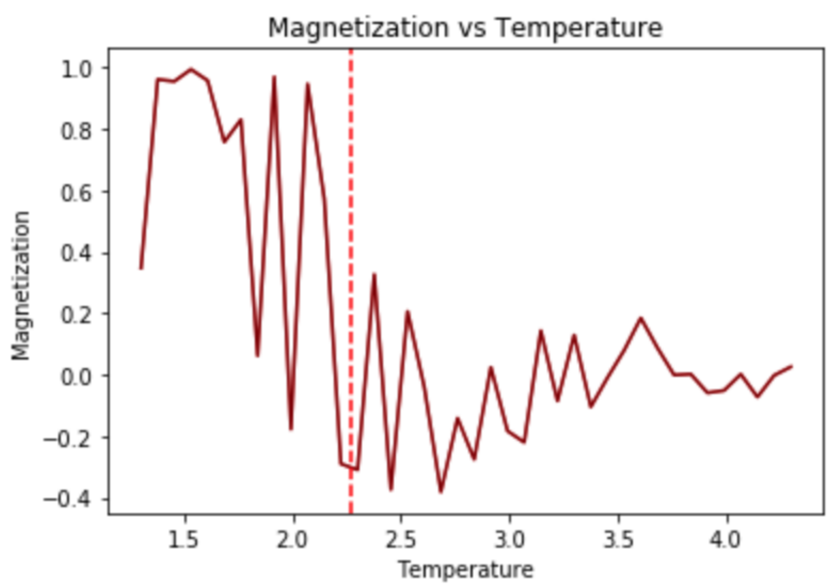

Figure 10. Magnetization vs Temp.

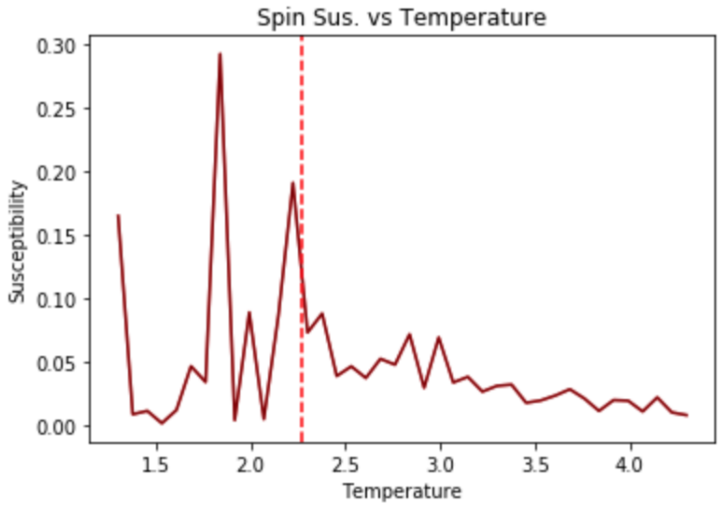

Figure 11. Spin susceptibility vs vs Temp.

Figure 12 represents a snapshot of the spin state of the material. Due to the seemingly random spin states, it can be said that thermal agitation is currently occurring. More specifically, it can be deduced that the level of thermal agitation is above the critical point due to the non-existing alignment that is present. If it were below this value, then some alignment would be present.

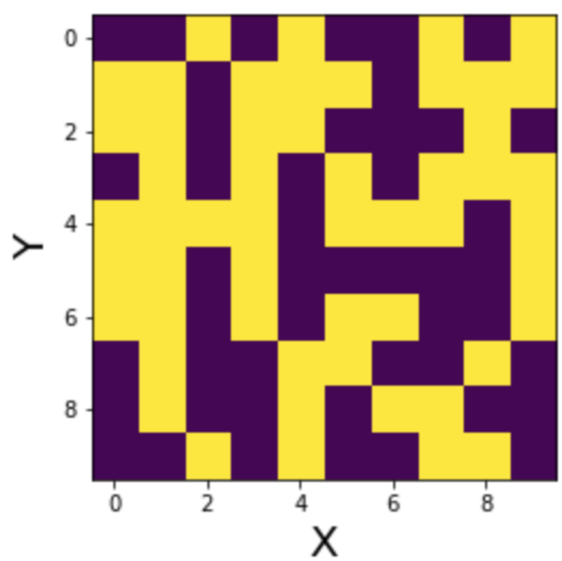

Figure 12. Spin Grid.

An interesting idea that was explored is the magnetic hysteresis which is modeled in *Figure 13*. The idea behind this is how permanent magnetism comes to be. This occurs when an external magnetic field is introduced to a ferromagnetic material. Alignment of the dipoles occurs with this magnetic field to the point where, if the field were to be removed, a part of the alignment is still present. Thus the material would stay magnetized. The untraceability of the plot adds on this fact.

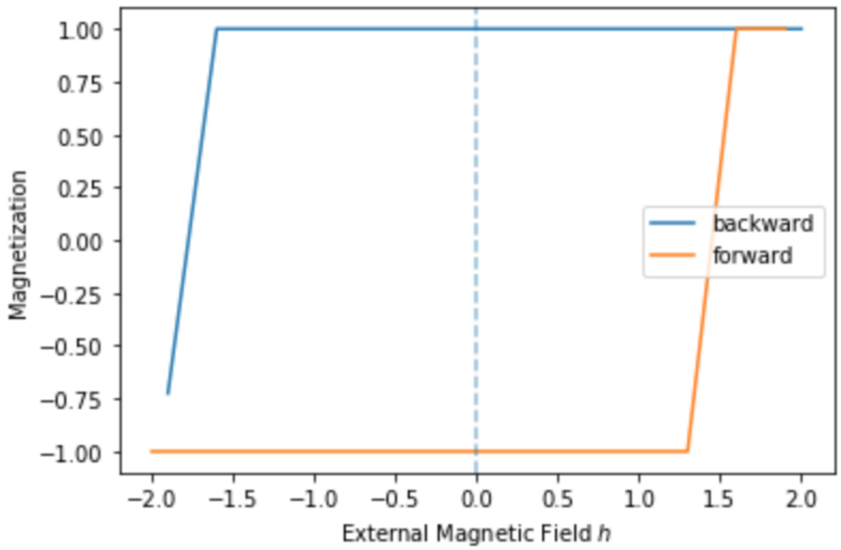

Figure 13. Magnetic hysteresis

4. THE TRAVELING SALESMAN

Another type of problem that utilizes simulated annealing to determine the most optimal outcome is the *Traveling Salesman Problem.* A salesman has many cities he must go to and must find the most optimal path, a.k.a the shortest path possible. This is where simulated annealing comes in to save the day. Further restrictions are that the salesman can only visit each city once and must end at the city that he/she started at.

Figure 14 depicts the initial solution that simulated annealing deemed as optimized. In this model, the optimized path was a total distance of 43.22. However, upon inspection, it is easy to tell that the path is actually not as optimized as can be. Doing so, would greatly reduce the total distance the salesman would have to walk.

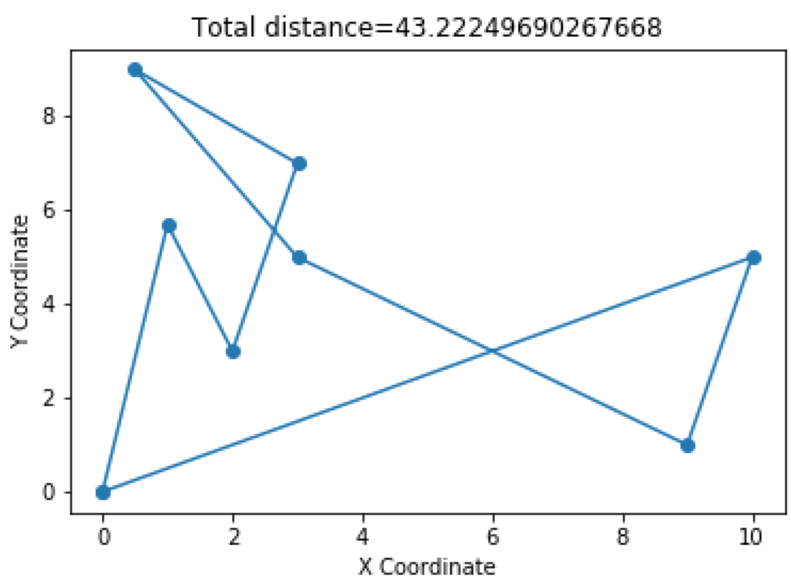

Figure 14. Initial optimized answer

Figure 15 depicts the most optimal solution that simulated annealing could come up with. There is no better path that the salesman could take that would reduce the total distance they must walk. In this model, the most optimal solution was deemed to be 34.95840. This path is much better than the initial solution from the previous plot. However, it is still imperative to check our solution.

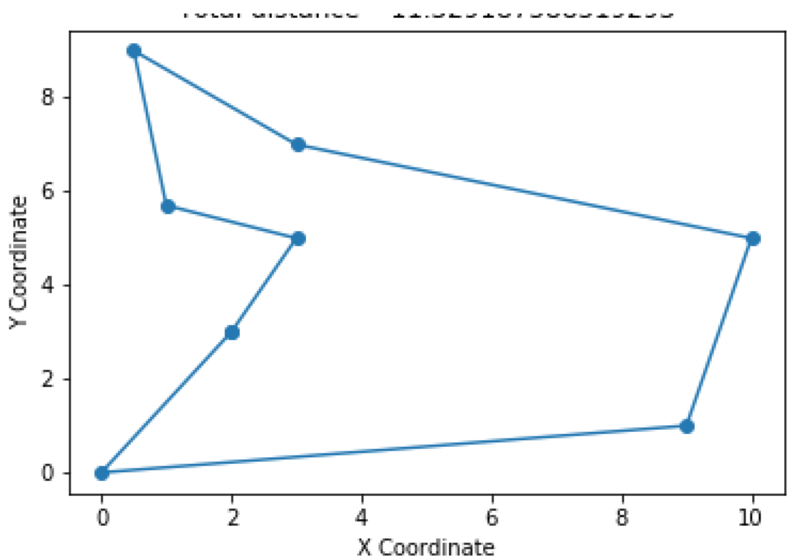

Figure 15. Most optimal solution to the salesman problem.

Figure 16 displays the same problem, but the solution was determined through the Brute Force method. The Brute Force method does the process as simulated annealing, however it is very limited when it comes to the number of iterations allowed. This is due to the fact that after a certain number of iterations, the method would have to go through a high number of permutations. For this problem, the Brute Force method determined 34.95840 to be the most optimal path. This number is in agreement with the most optimal path that simulated annealing and thus, assures us that this value is the best solution.

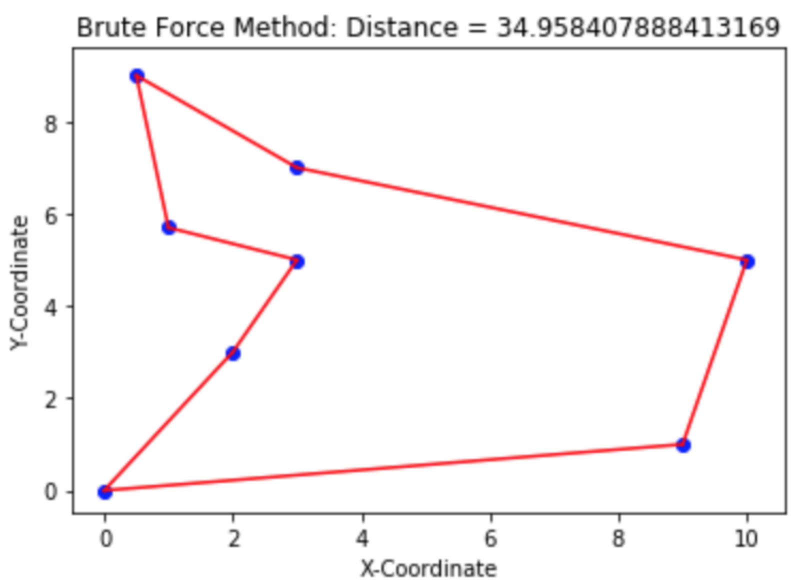

Figure 16. Brute Force in action.

5. CONCLUSION

The objective of this assignment was to apply simulated annealing to various situations. Regardless of the situation, simulated annealing was utilized to determine the most optimal general solution.