CMMHw5

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November 30, 2024

1 2D Ising Model

The 2D Ising Model can be used to show the lattice configurations of magnetic materials and their alignments based on temperature. Each index of the matrix interacts with its nearest neighbors such that two lattice points with the same spin (those that are parallel) reduce the energy of the configuration. Neighbors with opposite spin (anti-parallel) increase the energy of the system. It is assumed that the energy of each interaction has a magnitude of J = 1.5 and that there is no external magnetic field. The Metropolis algorithm is used to relax the system. This algorithm is similar to Monte Carlo simulations.

The general setup of the two parts of this homework assignment is approached similarly. Generally, running the equilibration and subsequent steps for more runs will result in more accurate data. First, a lattice configuration of size nxn is created and filled with -1 or 1 randomly. The systems are allowed to equilibrate for some time determined by the number of steps the system takes. In each step, the energy change of switching the lattice element spin is calculated. If this value is less than 0, then the system will switch the lattice's spin. Alternatively, if the change in energy is greater than 0 and if a random number is generated and it falls within the range of 0 to $e^{\frac{-\Delta E}{kT}}$ where ΔE is the change in energy, and kT is used as the temperature then the system will switch the lattice's spin. Both parts of the problem used temperatures in the range of 0.1 to 10 with steps of 0.1. If neither condition is met, there will be no change in energy as the spin will not be changed. In part one of the homework, a lattice size of $n = 50$ is used and the focus of the problem is magnetization, M, as a function of temperature, T or kT. Once the system was equilibrated, another set of Monte Carlos or the Metropolis algorithm was run. Grouped by temperature, during each of these new runs, the magnetization was calculated of the lattice. The average of the magnetization was calculated by dividing by the number of steps after equilibration, and the magnetization was standardized by dividing by the size of the lattice configuration $N = nxn$.

Figure 1 represents the resulting graph of Magnetization vs. Temperature. This graph looks like a reverse sigmoid function, in that it starts with a magnitude of almost 1 and it drops down to a magnitude of 0. The critical temperature, T_c, is the temperature at which the magnet goes from being ferromagnetic

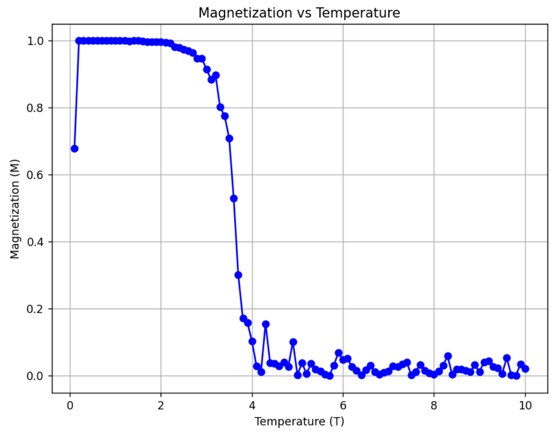

Figure 1: Magnitude vs. temperature graph at 100 iterations for equilibration and 100 iterations for average magnetization

to paramagnetic, possibly due to a phase transition. The T_c is between 3.3 and 3.4, as would be indicated by the inflection point.

Part two of the homework is a little more complicated. The sizes of the lattices are $n = 5, 10, 20, 30, 40, 50, 75, 100, 200, 500$. The following steps are repeated for every size: the system is allowed to equilibrate, after which the energy of each lattice configuration is noted and the average energy and average energy squared are calculated and used to find the specific heat. The specific heat is then divided by $N = nxn$ to get the specific heat per spin, $\frac{C}{N}$, and the maximum of $\frac{C}{N}$ is used to then plot $\frac{C}{N} vs.n$ (Figure 4) and $\frac{C}{N} vs.log(n)$ (Figure 5). The specific heat is calculated by using the formula:

$$C = \frac{(\Delta E)^2}{kT^2}$$

where C is the specific heat, $(\Delta E)^2$ is the variance of the energy, and kT^2 is the temperature. The variance of the energy is calculated by:

$$(\Delta E)^2 =< E^2 > - < E >^2$$

$$< E^2 >= \frac{1}{N} \sum_{\alpha} E_{\alpha}^2$$

$$< E >= \frac{1}{N} \sum_{\alpha} E_{\alpha}$$

where E_{α} is the energy and α is a configuration. This results in Figure 2 and Figure 3, which is a scatter plot of the specific heat as a function of temperature. It can be seen that running the code with longer equilibration and more steps makes the graphs more defined. Generally, a region can be seen in which the critical temperature would be found and it is implicated by a peak formation. The critical temperature was assumed to be the peak or where the specific heat per spin was the highest. This is more obvious for the size values found in Figure 2 than those in Figure 3.

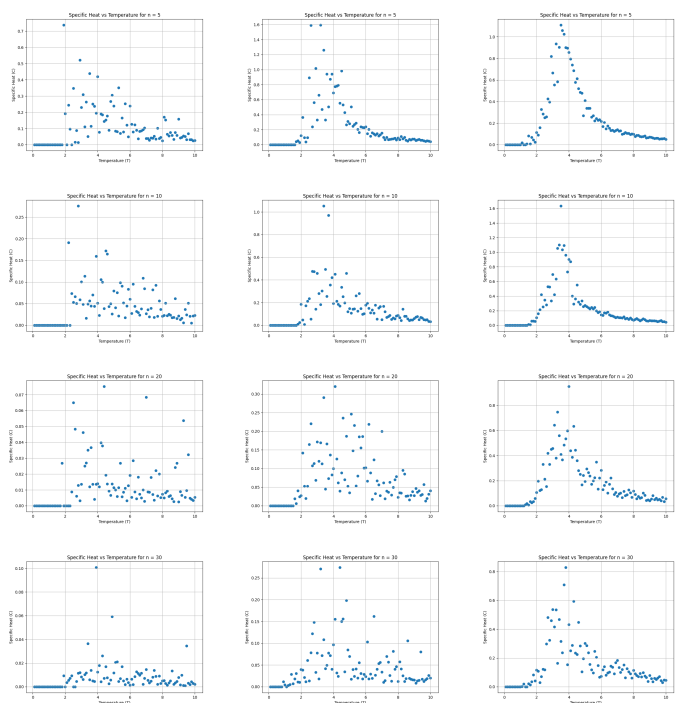

Figure 2: Specific heat vs. temperature for n = 5(top), 10(middle-top), 20(middle-bottom), 30(bottom) for 100(left), 1000(middle), and 10000(right) iterations

Figures 4 and 5 are used to try to identify a correlation between the specific heat per spin and the size of the lattice. When plotted against the normal size and against the logarithmic scale of the graph, it could be seen that neither of these could be used to linearly predict the specific heat per spin of a new lattice size. Thus, it is inconclusive whether the specific heat per spin is proportional to the size of the lattice or the logarithm of the lattice. To check if this would be the case, the model should be run for more iterations such as 1000 or 10000. This was not done for the larger values due to time constraints, however, given that Figure 2 has more defined peaks when the number of iterations increases, it is assumed the same would hold for larger lattice sizes.

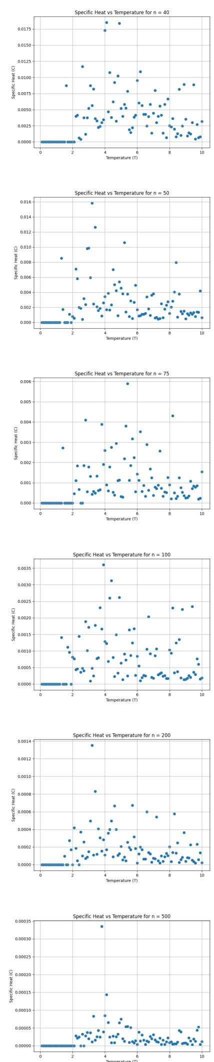

Figure 3: Specific heat vs. temperature for n = 40(top left), 50(top middle), 75(top right), 100(bottom left), 200(bottom middle), 500(bottom right) for 100 iterations

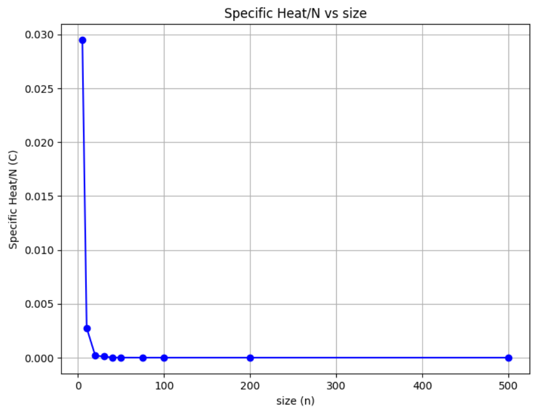

Figure 4: Specific heat per spin vs. size

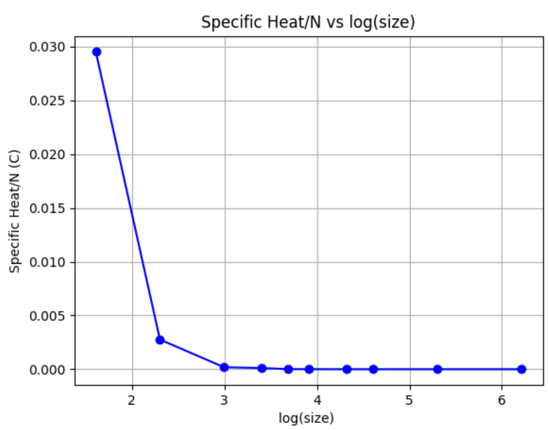

Figure 5: Specific heat per spin vs. log(size)