Homework 8: Introduction to Ising Model

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Introduction

Here, we are simulating a 2-D Ising model. In simulating this, we are concerned with the phase transition form ferromagnetic to paramagnetic.

Method

We use a 10×10 lattice to represent the model with spins -1 and +1. The spins have periodic boundary conditions and an exchange constant of $J = 1$.

For a larger lattice, the phase transition occurs at the point where spanning clusters of spins are no longer found. However, because we are limited to such a small lattice, we instead define the phase transition as the point of inflection in the plot for average spin energy $\langle E \rangle$ or average spin magnetization $\langle m \rangle$ with respect to temperature.

An even better approach (since points of inflection are often not so obvious), we recognize that the peak of the plot for the specific heat, the derivative of energy with respect to temperature (much easier to pinpoint than a point of inflection), occurs at the critical temperature. While we could use such a derivative (as done in Figure 10), we can also use the following equation (as done in Figure 9):

$$C_P = \frac{\langle E^2 \rangle - \langle E \rangle^2}{(k_b T)^2}. \tag{1}$$

For this simulation, we use $k_b = 1$ for convenience; hence, we are working with fundamental temperature when we refer to "temperature".

Verification of program

As expected, the lattice becomes much more noisy following the critical temperature; likewise, the points of inflections for $\langle E \rangle$ and $\langle m \rangle$ as well as the peak for specific heat all occur at critical temperature. The figures shown here are comparable to those shown in the textbook.

Data

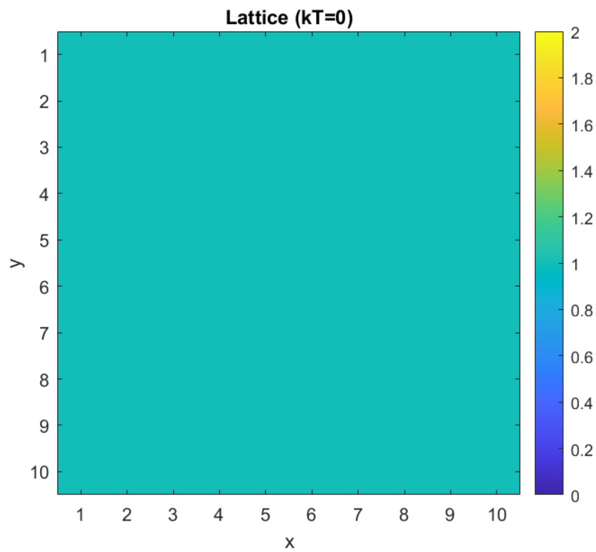

Figure 1: 10×10 lattice at $kT = 0$ (before T_C). Here, the lattice is ferromagnetic.

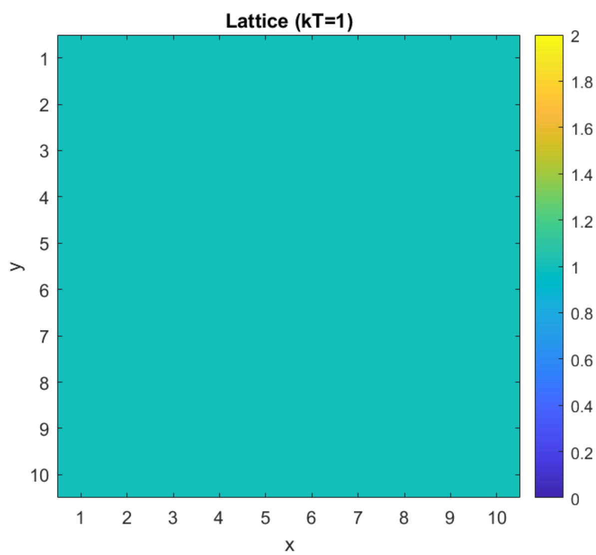

Figure 2: Lattice at $kT = 1$ (before T_C).

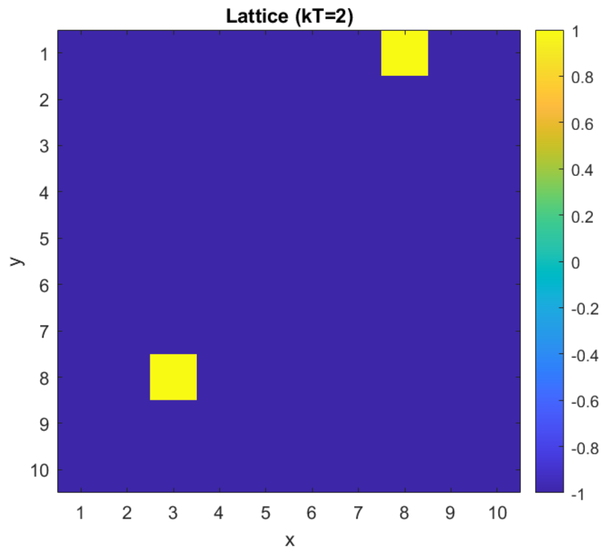

Figure 3: Lattice at $kT = 2$ (before, but close to T_C).

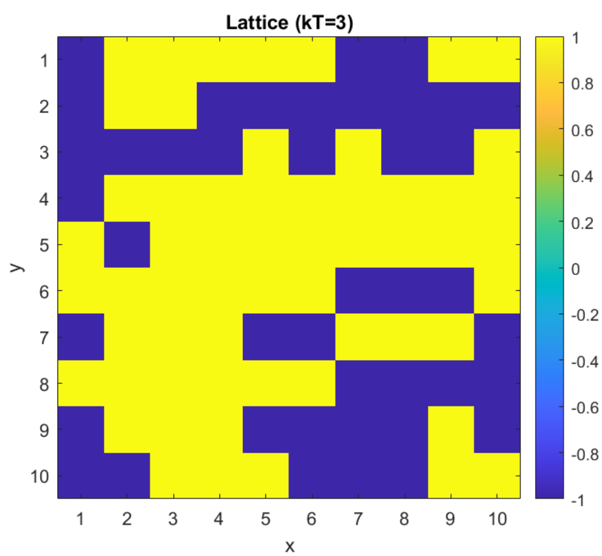

Figure 4: Lattice at $kT = 3$ (after T_C). Now, the lattice has transitioned to be paramagnetic, though spanning clusters still exist due to the small size of the lattice.

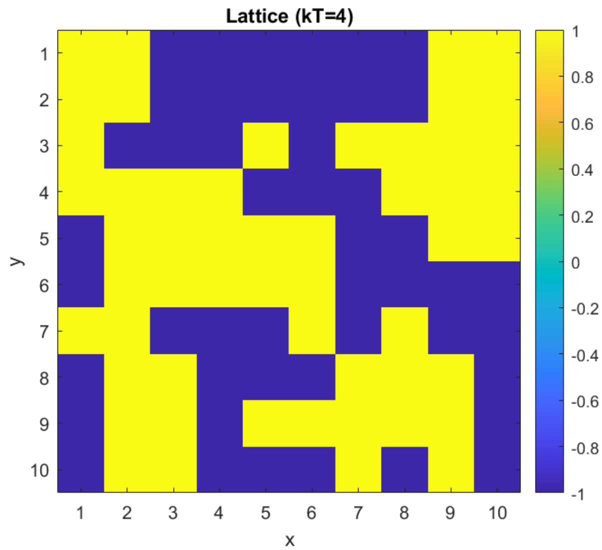

Figure 5: Lattice at $kT = 4$ (after T_C).

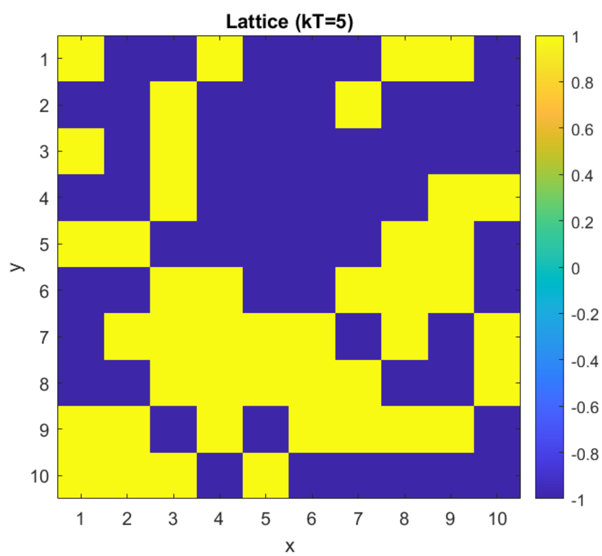

Figure 6: Lattice at $kT = 5$ (after T_C). Note that there are no longer any spanning clusters.

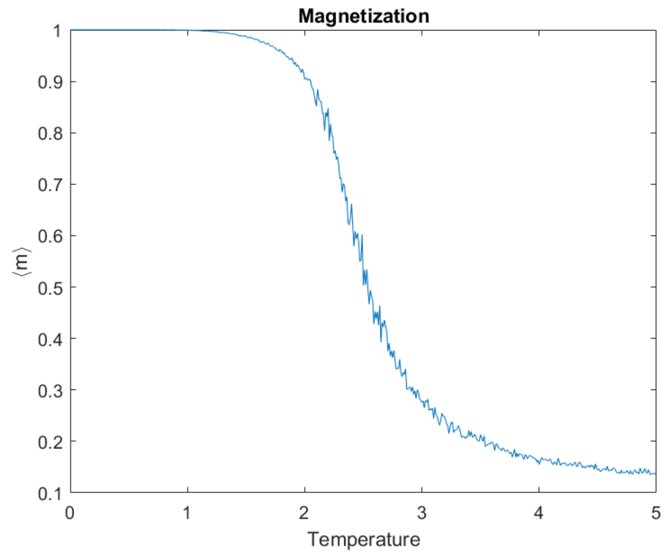

Figure 7: Plot of average magnetization of spins.

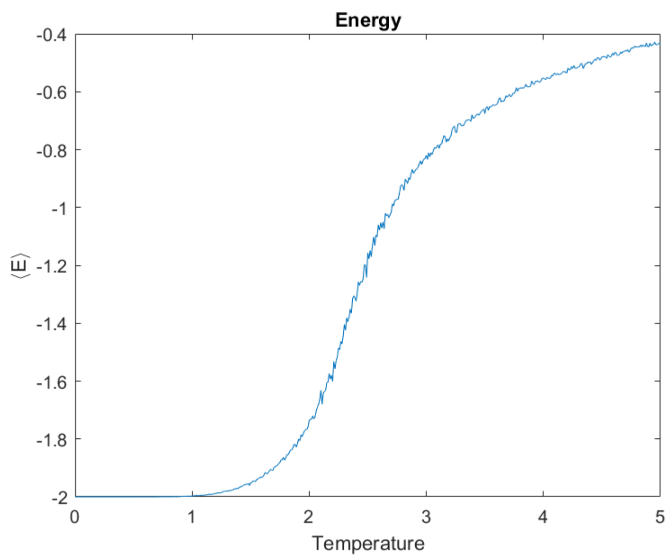

Figure 8: Plot of average energy of spins.

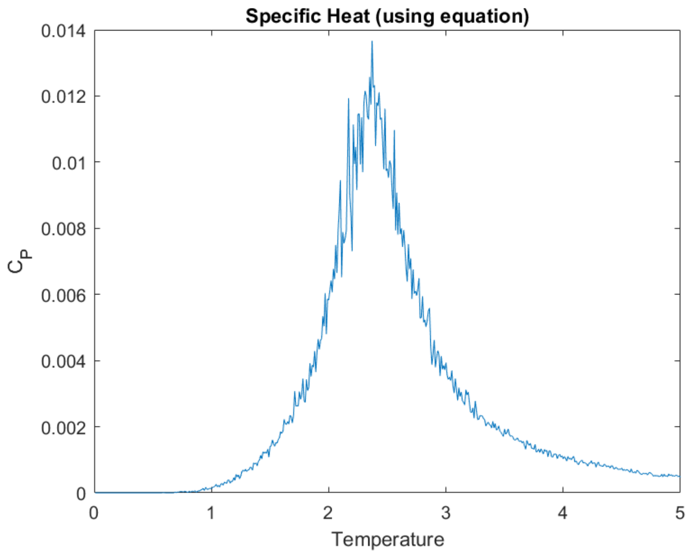

Figure 9: Specific heat as found using equation (1). We find that the peak occurs around critical temperature $T_C = 2.35 \pm 0.05$.

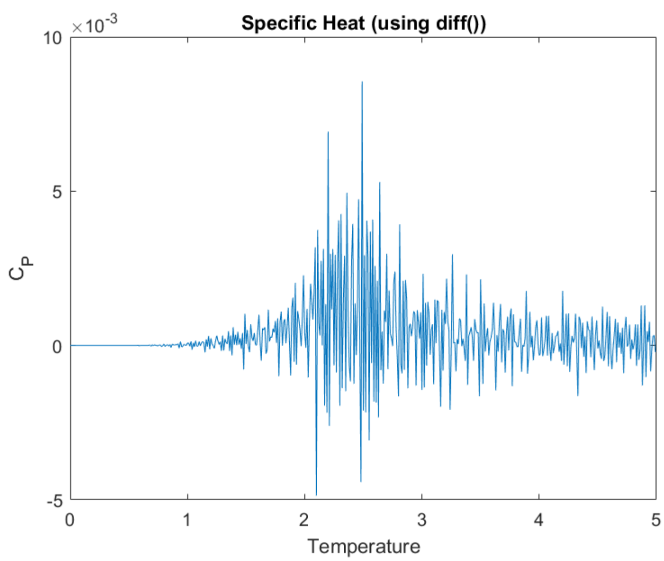

Figure 10: Specific heat as found using derivative of energy with respect to temperature. We once again find that the peak occurs around critical temperature $T_C = 2.35 \pm 0.05$.

Analysis

We find that the critical temperature for our lattice is $T_C = 2.35 \pm 0.05$. Regarding Figures 9-10, the differences in these plots are expected. This is due to the larger fluctuations of energy observed in Figure 8. Hence, the derivative of energy is greatly fluctuating between positive and negative values, although the magnitude stays relatively the same, thus explaining Figure 10. We should expect that if only the magnitude of Figure 10 were plotted, it would much closer resemble Figure 9.

Critique

In a large lattice, spanning clusters should not exist after the critical temperature is reached; however, because our lattice is so small, these clusters still continue to span. Nonetheless, Figures 7-10 as well as the general noisiness of Figures 4-6 despite the existence of some spanning clusters will show that a phase transition as in fact occurred past critical temperature $T_C = 2.35 \pm 0.05$.