PYL435: Advanced Computational Physics

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Assignment: 1 (3D Ising Model)

Introduction

This Assignment required a Monte Carlo simulation of a 3D Ising model. 3D Spin systems were simulated at different temperatures, and using the 'Metropolitan Algorithm', a large number of states were sampled to take an average of measurables like Energy and Magnetization and their squares. Then, the spin systems' susceptibilities and specific heat capacities at different Temperatures were calculated. Eventually, all of these calculated quantities were plotted for varying temperatures.

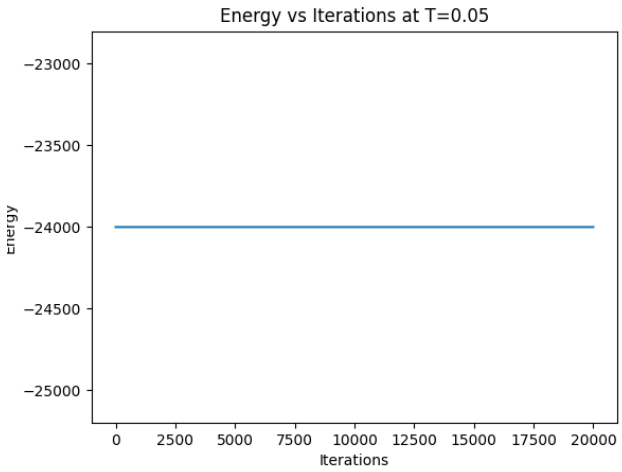
Simulation parameters

- Number of Spins, $N_{spins} = 8000$
- Coupling strength, $J = 1$
- Boltzmann constant,$k = 1$
- External Magnetic Field, $B = 0T$
- Temperatures $=0.05, 0.10, 0.15..., 10.0, 10.5, 11.0, 11.5, ..., 40.0$
- The initial spin configuration is that all spins are aligned. Thus, the lowest energy configuration.
- Number of Iterations, 20,000 for equilibriation, and 10,000 for sampling.

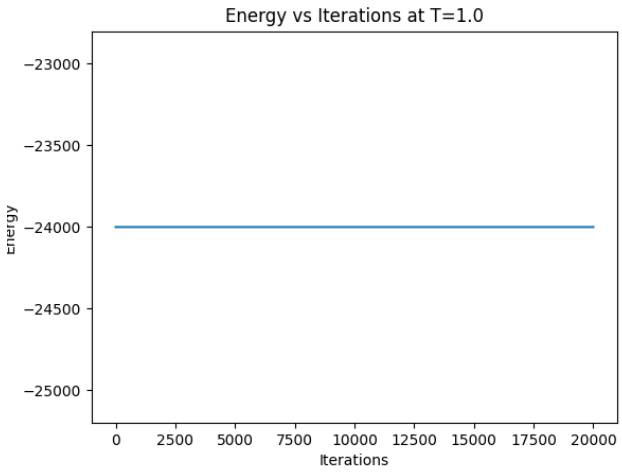
Plots

0.1 Equilibriation step

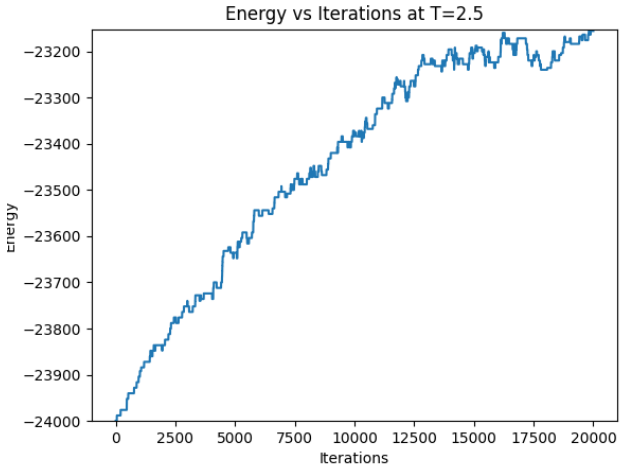
Energy of System versus Iteration count data are plotted here for a few temperatures.



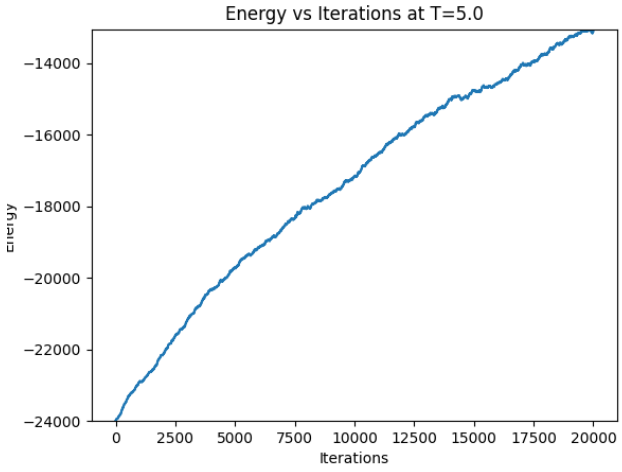
(a) T = 0.05 K



(b) T = 1 K

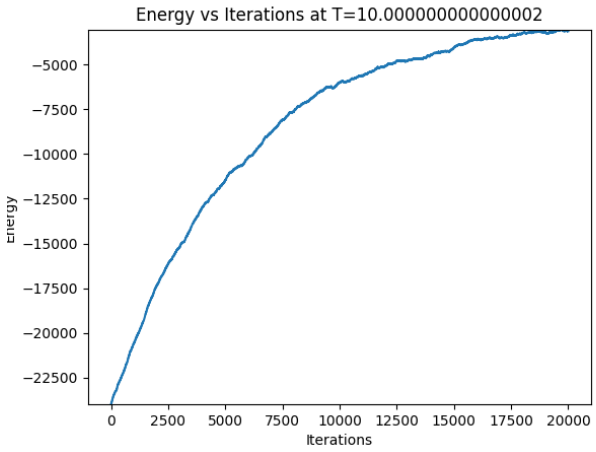


(c) T = 2.5 K

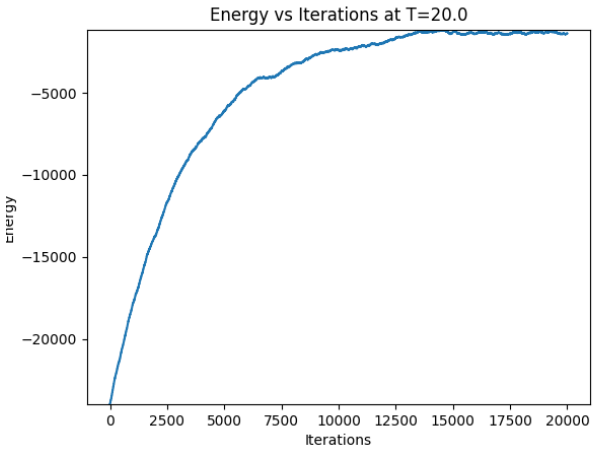


(d) T = 5 K

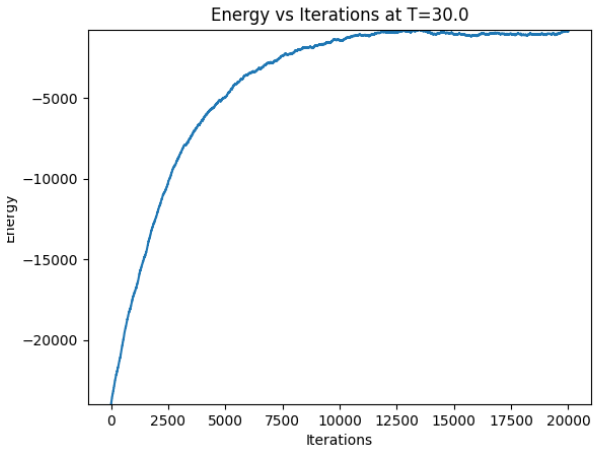
Figure 1: Energy vs Iterations



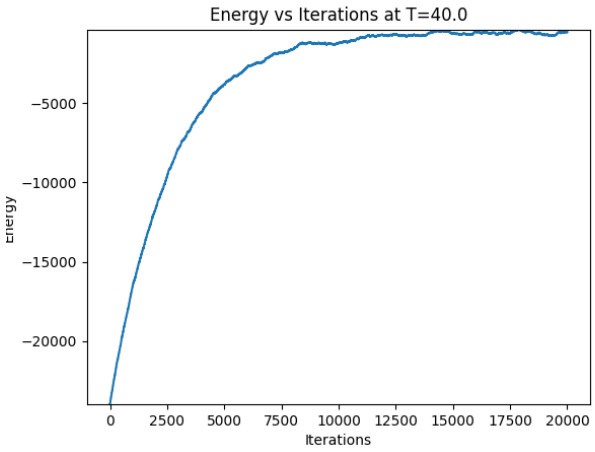
(a) T = 10 K



(b) T = 20 K



(c) T = 30 K



(d) T = 40 K

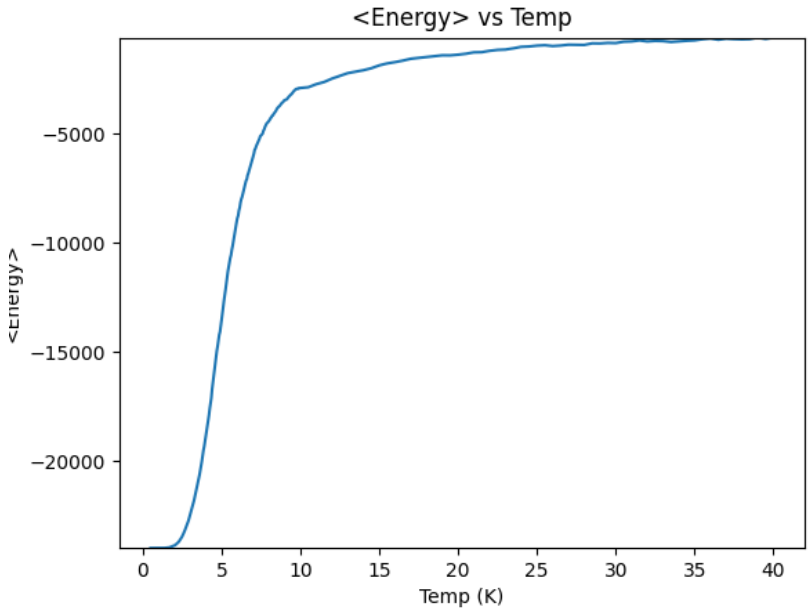
Figure 2: Energy vs Iteration

Remarks

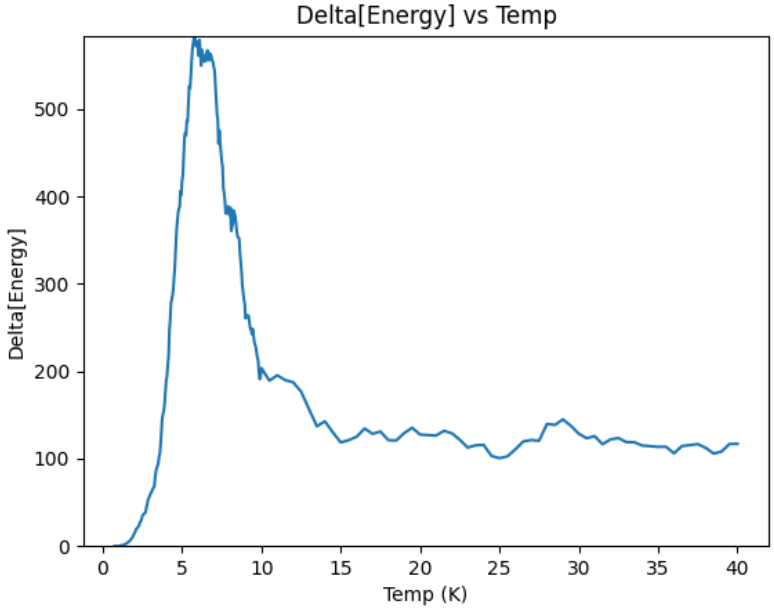
It can be seen that lower energy configurations are more probable at lower temperatures, and at higher temperatures, higher energy configurations are more probable. In these plots, the Iteration count acts as time; thus, these plots are similar to time evolution plots. Since all of the spin systems are initialized at the lowest energy configuration (i.e., all spins aligned parallel), all of the plots start from the lowest energy and increase after. For higher temperatures, the system reaches higher energy faster than at lower temperatures. The system then stabilizes around that energy state, which is most probable for that temperature.

Note that, In this simulation, the Initial distribution of the states is deterministic (since the system is initialized with the particular state where all spins point up and are parallel). Yet, the distribution of states eventually converges to Boltzmann distribution and then stays in it. This is one of the main features of the 'Metropolitan Algorithm', that the Boltzmann distribution persists once reached.

0.2 Energy-Temperature Statistics



(a) Average Energy vs Temperature

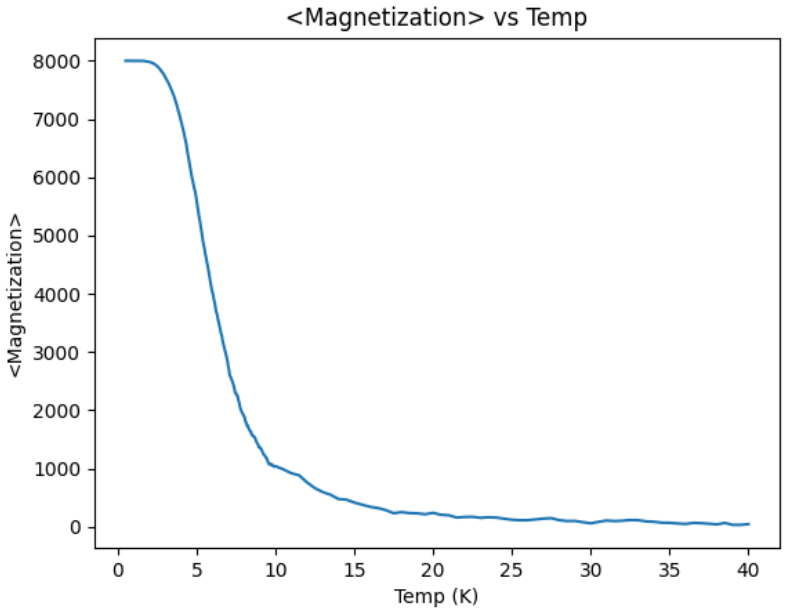


(b) Standard deviation of Energy vs Temperature

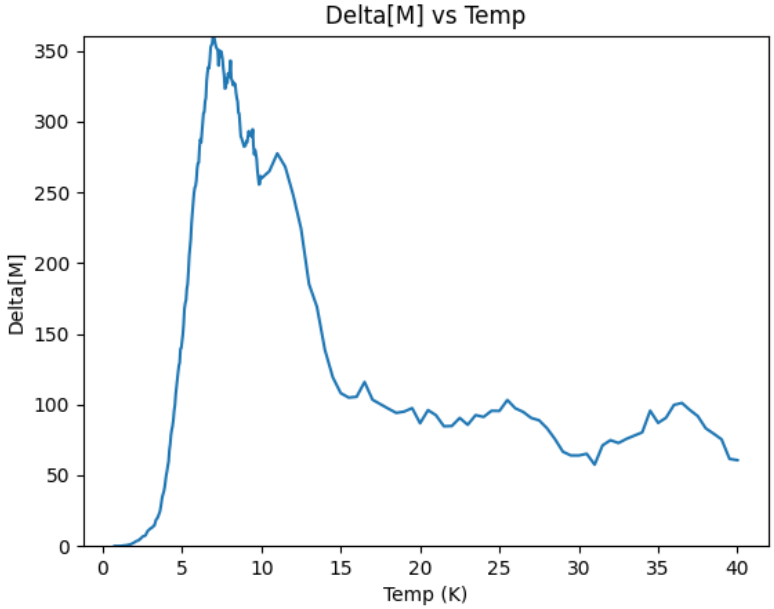
Remarks

As expected, average energy increases with temperature. But the rate of increase seems to be decreasing with increasing temperature. And there's also a fast increase in Average energy near the critical temperature ($3K - 10K$).
The deviation from mean energy also rises rapidly near the critical temperature, reaches a maximum, decreases, and then appears to remain constant at some non-zero value for high temperatures.

0.3 Magnetisation-Temperature Statistics



(a) Average Magnetisation vs Temperature



(b) Standard deviation of Magnetisation vs Temperature

Remark

Since by mean field approximation of 2D Ising model, the critical temperature, where mean magnetization abruptly rises and a 2nd order discontinuity is seen at the temperature point, is related as $< M >= \frac{JD}{2K_b}$, we can try to get a rough estimate of critical temperature value to be, $T_c = 3K$, by putting $J = 1$,$K_b = 1$ and $D = 6$(for 3D, six nearest neighbors). In the graph, a similar abrupt $< M >$ change is seen in the temperature range $T = 3K$ to $T = 10K$. The observation is nearly in agreement with Mean field approximation theory, and the 2nd-order discontinuity is apparent in this graph.

Standard deviation of Magnetization w.r.t. temperature is similar to that of Energy w.r.t. temperature and appears nearly constant for higher temperatures.

0.4 Average Susceptibility vs Temperature

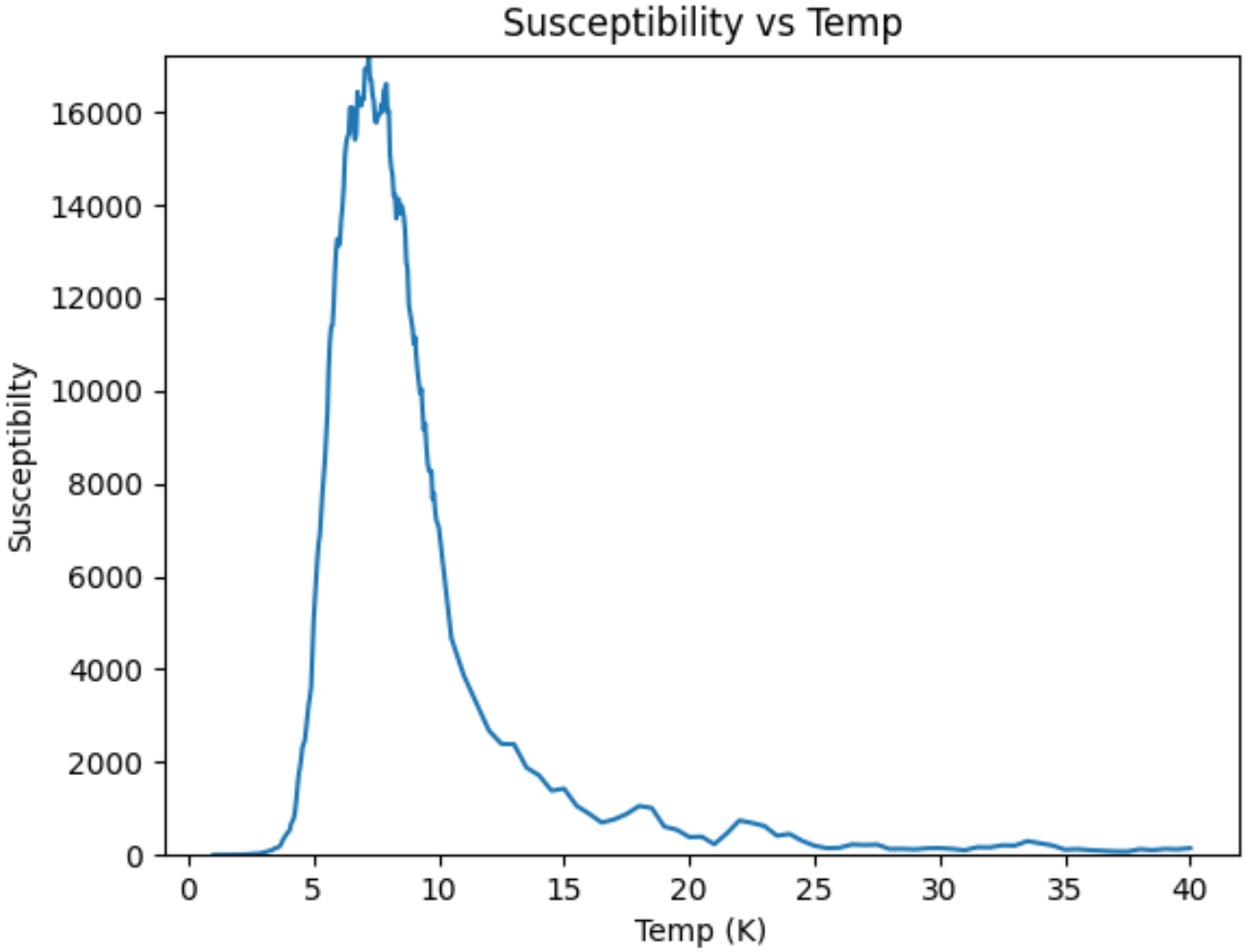


Figure 5: Average Susceptibility vs T

Remarks

The Susceptibility resembles the results of analytical solutions of the 2D Ising model. Right skewed and nearly zero in near zero temperature range. Then, it increases quickly around the critical temperature, reaches the maximum, and then goes down slower than it increased. Susceptibility is nearly zero at higher temperatures ($T > 30K$, from the graph).

0.5 Average Specific Heat Capacity vs Temperature

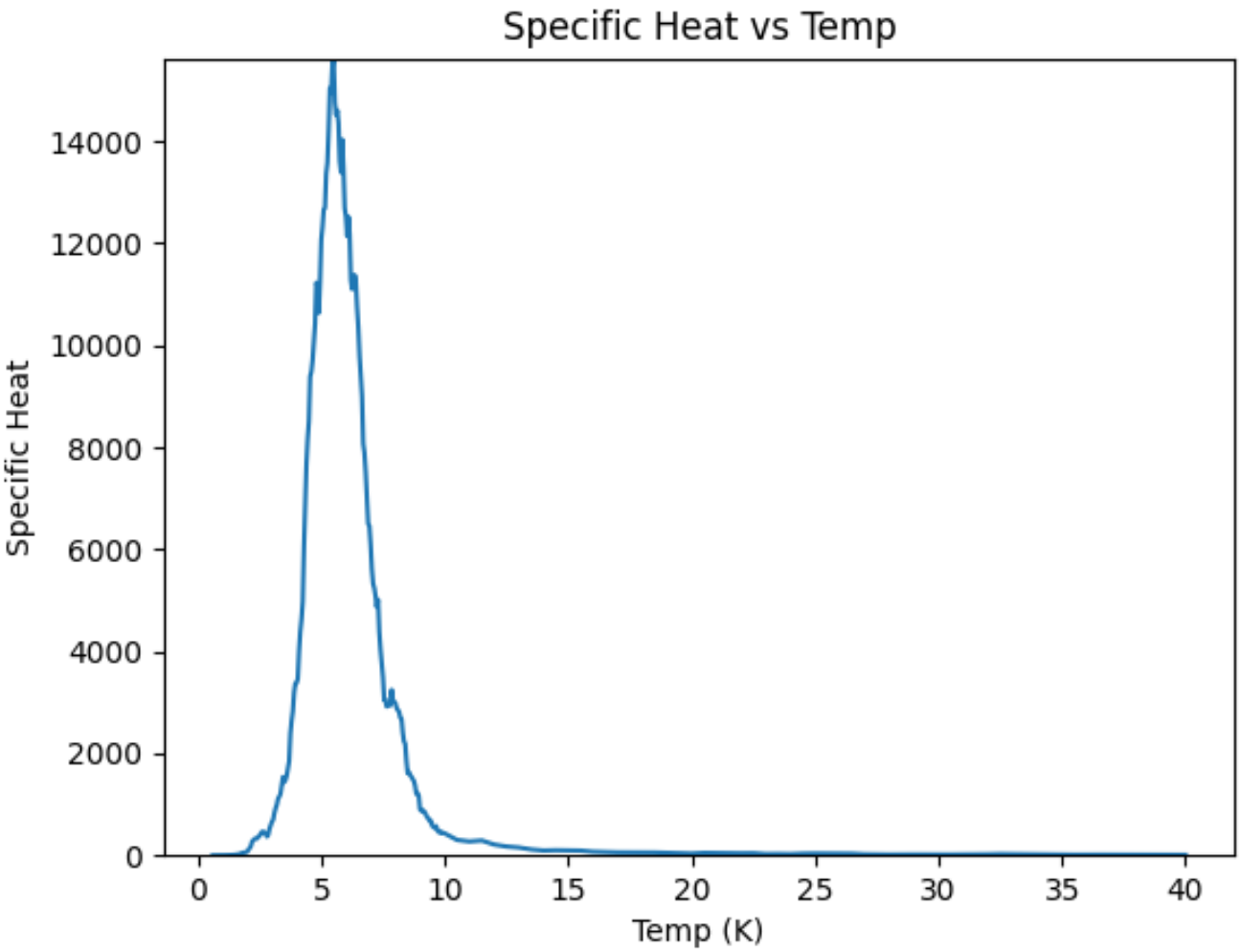


Figure 6: Average Specific Heat Capacity vs T

Remarks

The plot has relatively low skewness and appears to be nearly symmetric. The behavior around the critical temperature appears to be similar to the susceptibility plot.

Conclusion

The simulation gave good results that nearly matched the analytical solutions of the 2D Ising Model. But some improvements in the simulation algorithm could be,

- redefining the moveset to be more energy change informed. The moveset used here involved all those possible spin configurations that differ from the current spin configuration at only a single spin, which could have maximum energy difference of $12J(= 2 * J * max(spin) * max(\sum neighbouringspins) = 2 * J * 1 * 6)$ for near neighbour interaction in 3D, which is significant for small number of spins. Rather, choosing uniformly randomly among those moves that differ slightly in energy from the current configuration would be better. The consecutive data points would be closer in terms of energy, and the state evolution plots (like Energy vs iterations plots) would be more accurate. However, this causes an increase in the number of computations done in simulations which would be large for large systems.
- So, other way could be to increase the number of spins so that the maximum energy difference ($12J$) would be relatively small in magnitude compared to the magnitude of net energy of most of the states of the system. This can be efficiently done to avoid a lot of unnecessary computation. The bottleneck is still to evaluate the net energy and magnetisation in the beginning of simulation, but all of the iteration that follow could use that computed value of energy and magnetisation to calculate new energy and magnetisation in constant time. Thus, saving a lot of computation and so the system can be scaled comfortably without much increase in simulation duration.

Code

For the code, visit here
For plots at all specified temperature values, click here