Ising 1D

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1 Introduction

Here we have used Metropolis Monte Carlo Simulation for an 1 dimensional Ising Model in this report and calculated some equilibrium observables of this system. We have also calculated these observables analytically and have compared the numerical results to the analytical ones.

For each temperature, we have used the initial state as the one in which all spins are $+1$. We have then let each of them to relax upto 1000 Monte Carlo time steps. We record the evolution of the magnetization for these steps and take an ensemble average over 200 to compute the characteristic timescales (τ) for the relaxation of this initial state to the equilibrium.

The evolution of the magnetization is plotted below:

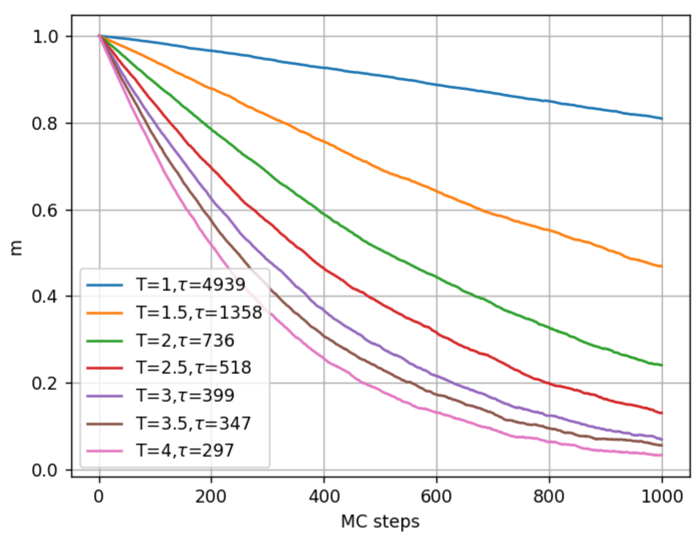


Figure 1: magnetization vs # of MC steps

For the simulation purposes, we have used these τ values to determine approximately the number of MC steps after which the system equilibrates (we have chosen $t_{equilibrium} = 15\tau$). The parameters chosen are $k_B = 1$, $J = 1$ and $N = 256$.

2 Magnetization

The Hamiltonian of the system is given as:

$$H(\{s_i\}) = -J\sum_{i=1}^{N} s_i s_{i+1}$$

The equilibrium probability associated to a state of the ensemble is given by:

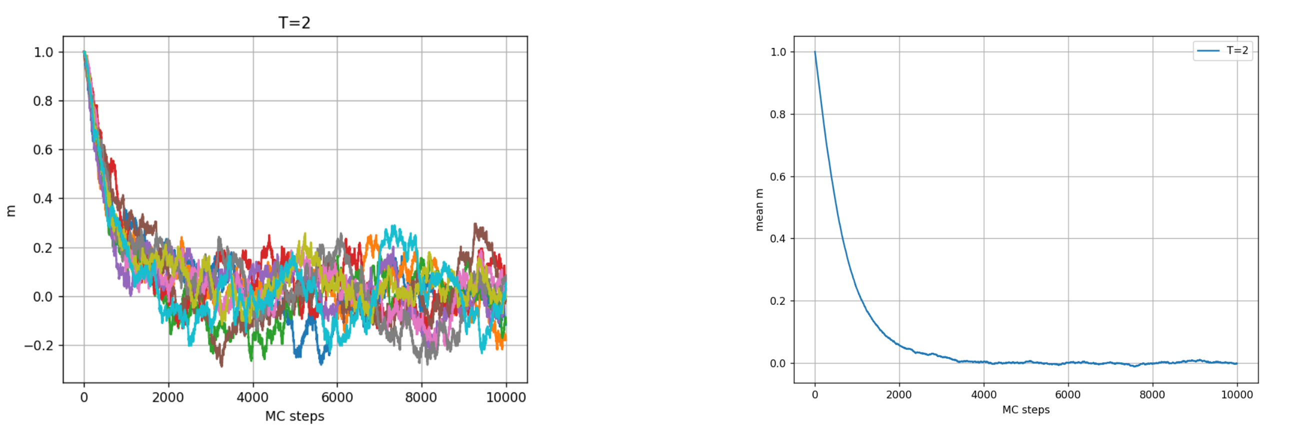
$$P(\{s_i\}) = \frac{e^{-\beta H(\{s_i\})}}{Z}$$

where $Z = \sum_{\{s_i\}} e^{-\beta H(\{s_i\})}$

The expected magnetization is calculated as follows:

$$\begin{aligned}
\langle m \rangle &= \frac{1}{N}\langle \sum_j s_j \rangle \\
&= \frac{1}{N}\sum_j \langle s_j \rangle \\
&= \frac{1}{N} N \langle s_0 \rangle \\
&= \frac{1}{Z}\sum_{\{s_i\}} s_0 e^{-\beta H(\{s_i\})} \\
&= \frac{1}{Z}\sum_{s_0} s_0 T^N_{s_0,s_0} \\
\implies \langle m \rangle &= \frac{1}{Z}\left(T^N_{1,1} - T^N_{-1,-1}\right) = 0
\end{aligned}$$

We simulate the evolution of magnetization and plot below:



(a) m evolution for each state in the ensemble

(b) ensemble average of m evolution over 500 instances

Figure 2: magnetization evolution with time

Here we compare the simulated mean magnetization (ensemble size = 3000000) to the analytical magnetization:

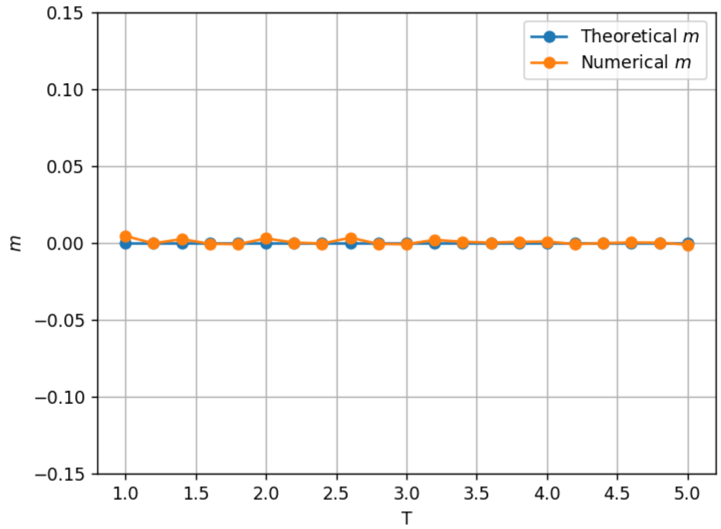


Figure 3: Caption

3 Energy

We wish to analytically calculate the expected Energy at thermal equilibrium (at β). We proceed as follows:

$$\begin{aligned}\langle E\rangle &= \frac{1}{Z}\sum_{\{s_i\}} H(\{s_i\})e^{-\beta H(\{s_i\})} \\ &= -\frac{1}{Z}\frac{\partial Z}{\partial \beta} \\ &= -\frac{\partial ln(Z)}{\partial \beta}\end{aligned}$$

Now,

$$\begin{aligned}Z &= \sum_{\{s_i\}} e^{-\beta H(\{s_i\})} \\ &= \sum_{\{s_i\}} e^{\beta J \sum_{i=0}^{N-1} s_i s_{i+1}}\end{aligned}$$

We define the matrix T as:

$$T = \begin{bmatrix} e^{\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} \end{bmatrix}$$

Hence we have,

$$Z = Tr\left(T^N\right)$$

We calculate the eigenvalues and eigenstates of T to compute T^N. The eigenvalues are given by:

$$\lambda_+ = 2cosh(\beta J)$$

$$\lambda_- = 2sinh(\beta J)$$

corresponding to the eigenstates $\lambda_+ = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ and $\lambda_- = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$.

Therefore we have,

$$T^N = 2^{N-1} \begin{bmatrix} cosh^N(\beta J) + sinh^N(\beta J) & cosh^N(\beta J) - sinh^N(\beta J) \\ cosh^N(\beta J) - sinh^N(\beta J) & cosh^N(\beta J) + sinh^N(\beta J) \end{bmatrix}$$

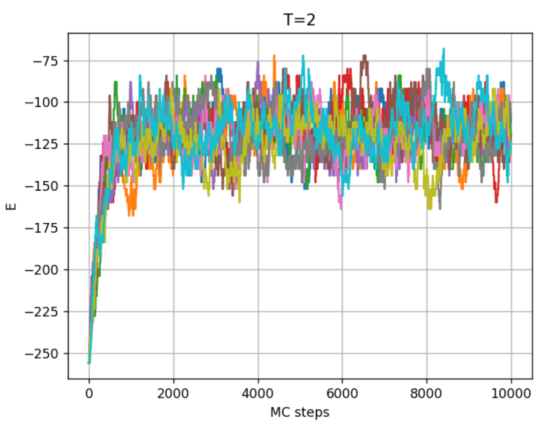
Hence,

$$\begin{aligned} Z &= Tr(T^N) \\ &= 2^N(cosh^N(\beta J) + sinh^N(\beta J)) \\ \implies Z(N \to \infty) &\approx 2^N cosh^N(\beta J) \end{aligned}$$

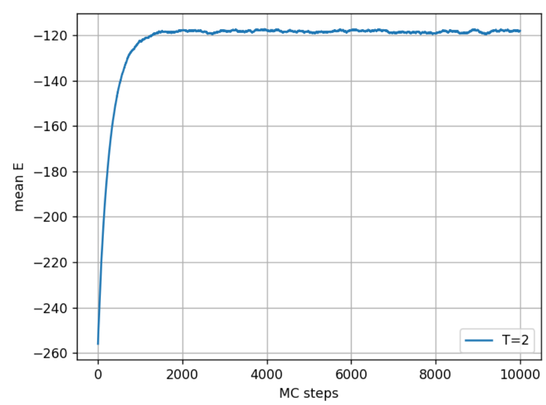
Hence for a big enough Ising chain, we get the expected energy as:

$$\begin{aligned} \langle E \rangle &= -\frac{\partial ln(Z)}{\partial \beta} \\ \implies \langle E \rangle &= -JNtanh(\beta J) \end{aligned} \tag{1}$$

We plot the simulated Energy evolution:



(a) E evolution for each state in the ensemble



(b) ensemble average of E evolution over 500 instances

Figure 4: Energy evolution with time

Here we compare the simulated mean energy (ensemble size = 3000000) to the analytical expected energy (obtained using the above formula) :

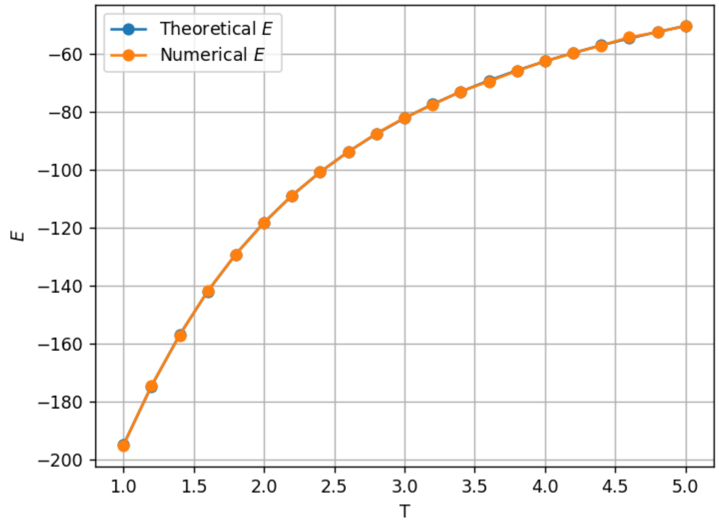


Figure 5: Energy vs Temperature

4 Specific Heat

The specific heat of this system is defined as:

$$\begin{aligned} C_v &= \frac{\partial \langle E \rangle}{\partial T} \\ \implies C_v &= -\frac{1}{k_B T^2} \frac{\partial \langle E \rangle}{\partial \beta} \\ \implies C_v &= \frac{J^2 N}{k_B T^2} (1 - tanh^2(\beta J)) \qquad (2) \end{aligned}$$

Here we compare the simulated mean specific heat (ensemble size = 3000000) to the analytical specific heat (obtained using the above formula):

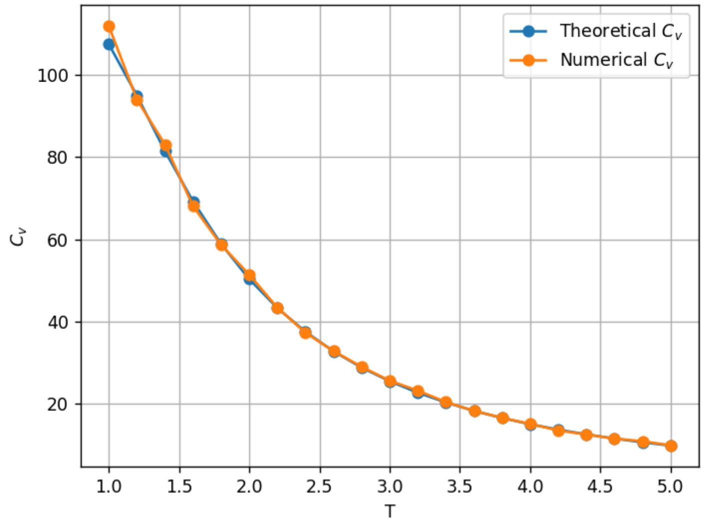


Figure 6: Specific heat vs Temperature

5 Correlation Function

We define the Correlation Function as:

$$\begin{aligned} C(r) &= \langle s_0 s_r \rangle - \langle s_0 \rangle \langle s_r \rangle \\ &= \langle s_0 s_r \rangle \\ &= \frac{1}{Z} \sum_{\{s_i\}} s_0 s_r e^{-\beta H(\{s_i\})} \\ &= \frac{1}{Z} \sum_{\{s_i\}} s_0 s_r e^{\beta J \sum_{i=1}^{N} s_i s_{i+1}} \\ &= \frac{1}{Z} \sum_{s_0, s_r} s_0 s_r T^r_{s_0, s_r} T^{N-r}_{s_r, s_0} \\ &= \frac{2}{Z} \left(T^r_{1,1} T^{N-r}_{1,1} - T^r_{1,-1} T^{N-r}_{1,-1} \right) \end{aligned}$$

$$\begin{aligned} \implies C(r) &\approx \frac{2^N}{Z} \left(tanh^r(\beta J) cosh^N(\beta J) + coth^r(\beta J) sinh^N(\beta J) \right) \\ \implies C(r) &\approx tanh^r(\beta J) \qquad (3) \end{aligned}$$

We plot the Simulated Correlation function for a range of temperatures below:

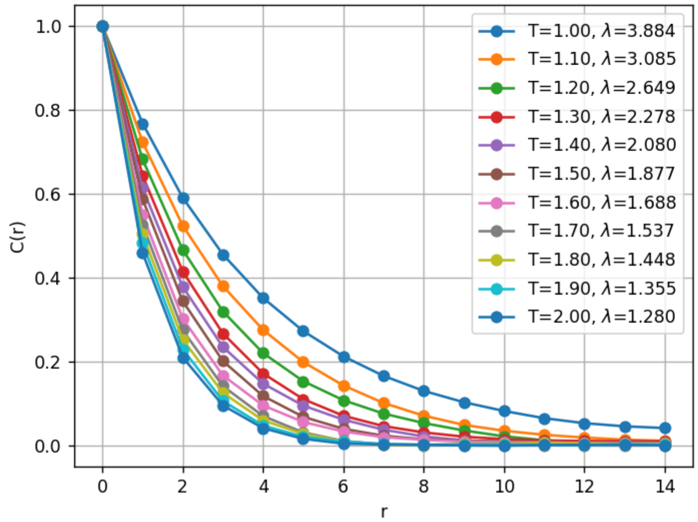


Figure 7: Correlation function vs separation distance (λ is the correlation length defined below)

We observe that,

$$
\begin{aligned}
C(r) &= tanh^r(\beta J) \\
&= \left(e^{-|ln(tanh(\beta J))|}\right)^r \\
&= e^{-\frac{r}{\lambda}}
\end{aligned}
$$

where, we have λ as the correlation length defined as,

$$
\lambda = \frac{1}{|ln(tanh(\beta J))|} \tag{4}
$$

We plot the simulated Correlation length vs Temperature and compare it with the analytical value (calculated using above formula) below :

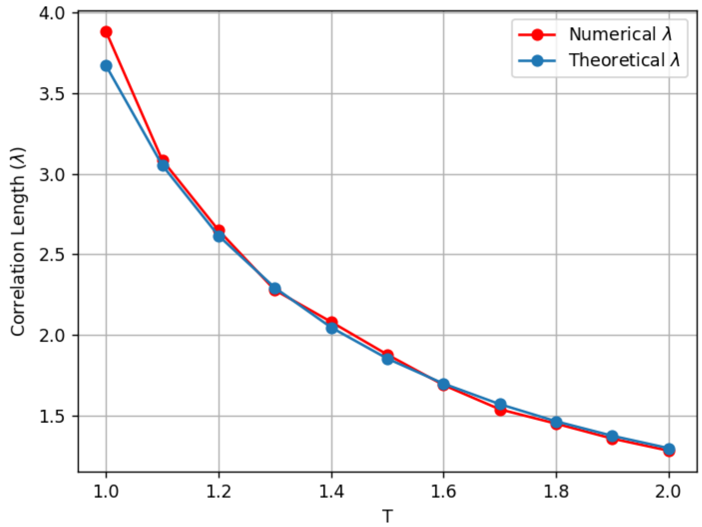


Figure 8: Correlation length vs Temperature

6 Conclusion

We have analytically calculated some observables of a 1D Ising Model and compared them to the simulated values (using the Metropolis Monte-Carlo algorithm).