Numerical Approaches to 1D and 2D Ising Model with Periodic Boundary Condition

Chun-Tse, Yang

December 2025

1 Thermodynamic Relations

In statistical mechanics, macroscopic thermodynamic behavior emerges from the collective properties of microscopic states.

For a system with discrete energy, the probability p_i for it to stay at i^{th} state is the Boltzmann factor $e^{-\beta E_i}$, normalized by partition function Z

$$p_i = \frac{e^{-\beta E_i}}{Z}, Z = \sum_i e^{-\beta E_i}, \beta = \frac{1}{k_B T} \tag{1}$$

The internal energy is the ensemble average of the energy

$$U = \langle E \rangle = \sum_i p_i E_i = \frac{1}{Z} \sum_i E_i e^{-\beta E_i} = -\frac{\partial \ln Z}{\partial \beta} \tag{2}$$

The entropy is given by the Gibbs entropy

$$S = -k_B \sum_i p_i \ln p_i = k_B \sum_i p_i (\beta E_i + \ln Z) = \frac{U}{T} + k_B \ln Z \tag{3}$$

The Helmholtz free energy H measures how much useful work a system can perform under isothermal condition.

$$H = U - TS = U - T\left(\frac{U}{T} + k_B \ln Z\right) = -k_B T \ln Z \tag{4}$$

The heat capacity C_V characterizes the system's response to temperature changes and quantifies energy fluctuations in thermal equilibrium.

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V = T\left(\frac{\partial S}{\partial T}\right)_V = -T\left(\frac{\partial^2 F}{\partial T^2}\right) \tag{5}$$

2 1D Site

For a periodic boundary 1D Ising model of particle amount N, nearest-neighbor coupling H, and external field h, the Hamiltonian $\mathcal{H}$ is

$$\mathcal{H} = -J \sum_{i=1}^{N} s_i s_{i+1} - h \sum_{i=1}^{N} s_i, s_i = \pm 1 \tag{6}$$

Its Boltzmann factor at temperature T is

$$e^{-\beta \mathcal{H}} = e^{\beta\left(J \sum_{i=1}^{N} s_i s_{i+1} + h \sum_{i=1}^{N} s_i\right)} = \left(\prod_i^N e^{\beta J s_i s_{i+1}}\right) \cdot \left(\prod_i^N e^{\beta h s_i}\right), \beta = \frac{1}{k_B T} \tag{7}$$

By summing up the Boltzmann factors, we can get the partition function Z, since the coupling is only between adjacent spins, we have

$$Z = \sum e^{-\beta \mathcal{H}} = \sum \prod_{i}^{N} w(s_i, s_{i+1}) \tag{8}$$

Where $w(s_i, s_{i+1})$ is the Boltzmann weight function

$$w(s_i, s_{i+1}) = \exp\left[\beta J s_i s_{i+1} + \frac{\beta h}{2}(s_i, s_{i+1})\right] = \begin{cases} e^{\beta(J \pm h)}, s_i = \pm 1, s_{i+1} = \pm 1 \\ e^{-\beta J}, s_i = \pm 1, s_{i+1} = \mp 1 \end{cases} \tag{9}$$

By putting the four combinations into the matrix, we obtained the transfer matrix W

$$W = \begin{bmatrix} e^{\beta(J+h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} \end{bmatrix} \tag{10}$$

With the transfer matrix W, we are able to calculate the partition function Z_L for L site

$$Z_L = \mathrm{Tr}\,(W^L) = \lambda_+^L + \lambda_-^L \tag{11}$$

Where $\lambda_\pm$ is the eigenvalues of W

$$\lambda_\pm = e^{\beta J}\cosh \beta h \pm \sqrt{e^{2\beta J}\cosh^2(\beta h) - 2\sinh^2(\beta J)} \tag{12}$$

The Helmholtz free energy F_L can thus be obtained

$$F_L = -\frac{1}{\beta}\ln Z_L = -\frac{1}{\beta}\ln(\lambda_+^L + \lambda_-^L) \tag{13}$$

And the free energy per site is

$$F_L = -\frac{1}{\beta N}\ln Z_L = -\frac{1}{\beta N}\ln(\lambda_+^L + \lambda_-^L) \tag{14}$$

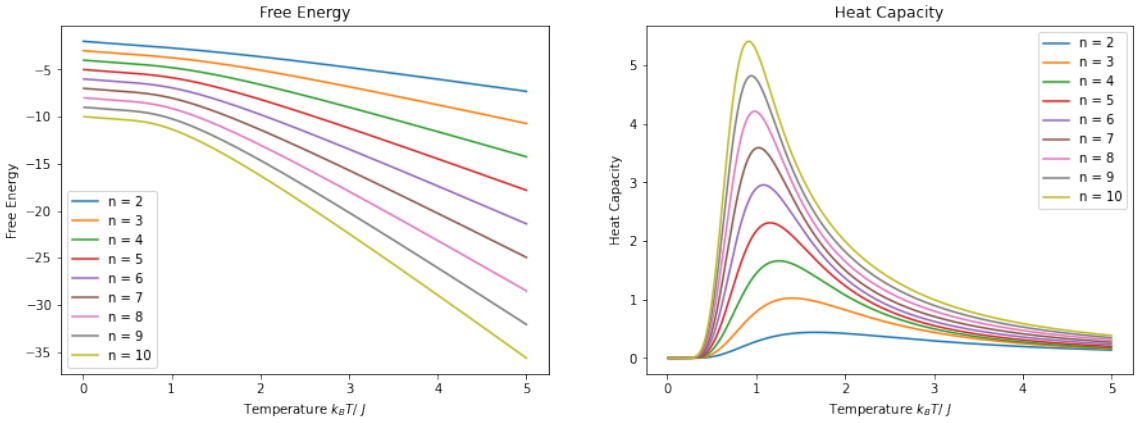


Figure 1: 1D Ising Model Simulation Result (1000 points)

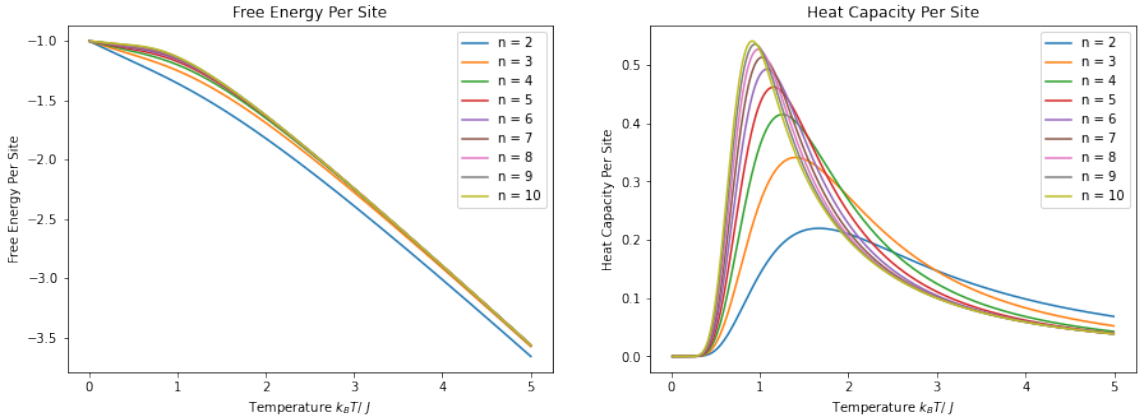


Figure 2: 1D Ising Model Simulation Result (Per Site, 1000 points)

3 2D Site

For the 2D site, the energy of spin is not only affected by the neighbors at left and right but also up and down. To obtain the result, we have to further expand the previous 2 'legs' transfer matrix W into a 4 'legs' tensor $\mathcal{T}$ connecting to all four adjacent spins.

To do this, we first have to extract the matrix M representing each leg from W using Cholesky decomposition

$$W = MM^T = PAP^T \rightarrow M = P\sqrt{A} = \sqrt{A}P^T \tag{15}$$

Where A is a diagonal matrix constructed by the eigenvalues and P is a matrix constructed by the eigenvectors

Connecting the 4 legs, we obtain the transfer tensor $\mathcal{T}$

$$\mathcal{T}_{ijkl} = \sum M_{si} M_{sj} M_{sk} M_{sl} \tag{16}$$

With this transfer tensor, two algorithms are deployed to obtain the solution

3.1 Einstein Summation

The first approach is to simply use Einstein summation `np.einsum` to combine the adjacent and boundary legs

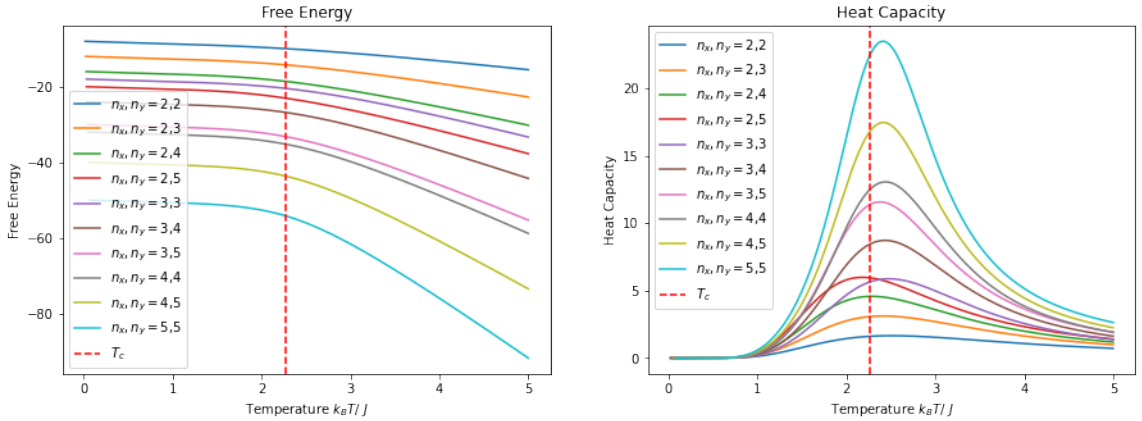


Figure 3: Einstein summation method simulation result (1000 points)

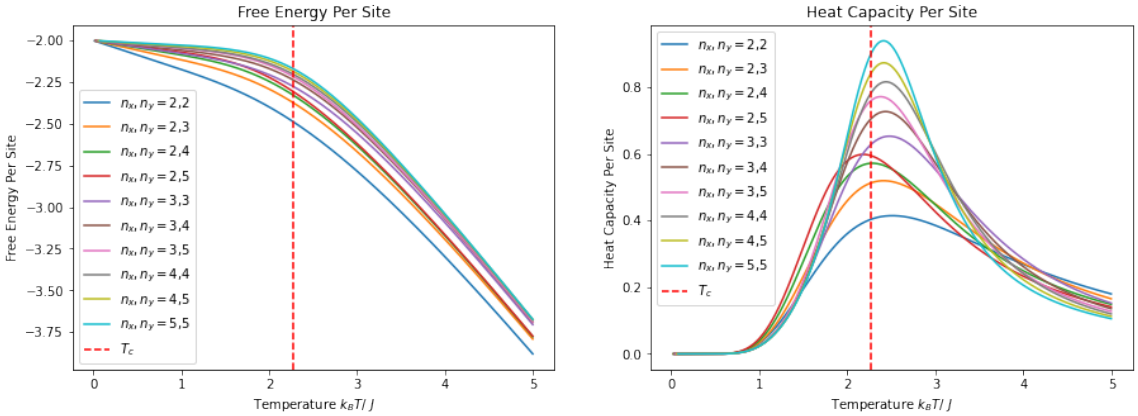


Figure 4: Einstein summation method simulation result (Per Site, 1000 points)

3.2 TRG

The TRG algorithm reduce the size of the site by separating each transfer tensor into two via SVD decomposition and re-merging them

$$\mathcal{T} = U_1 \Sigma_1 V_1^T = \mathcal{U}_1 \mathcal{V}_1 \tag{17}$$

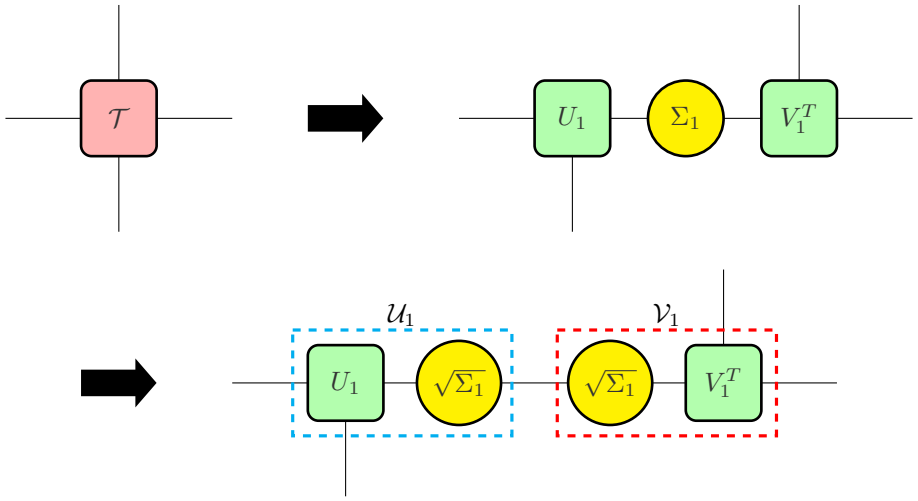


Figure 5: schematic of SVD decomposition

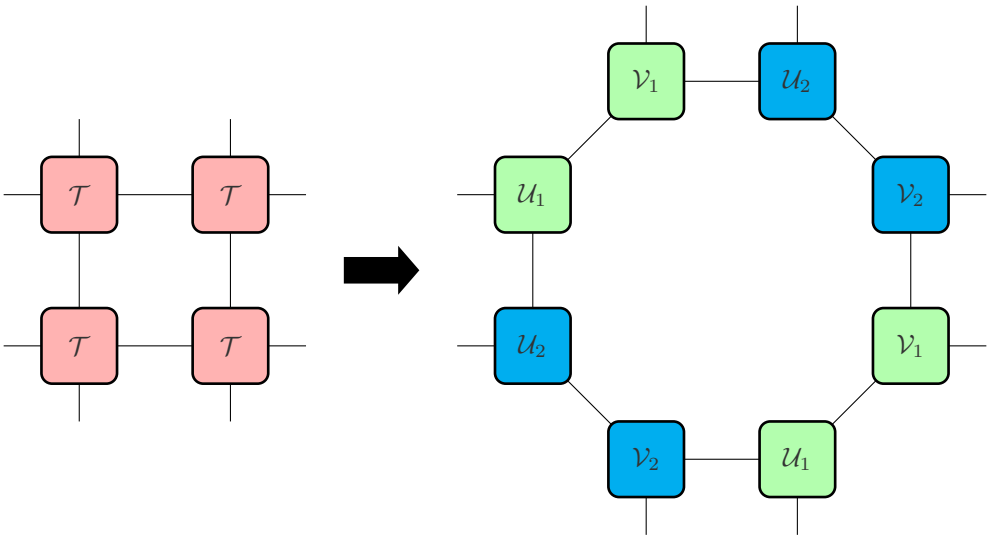


Figure 6: Schematic of separation

To merge it, we sum the tensor legs with their neighbors and obtain a new transfer tensor $\tilde{\mathcal{T}}$ with 'longer' leg that is $\sqrt{2}$ original one

$$\tilde{\mathcal{T}}_{URDL} = \sum \{\mathcal{V}_2\}_{\alpha\beta U}\{\mathcal{U}_1\}_{\alpha\gamma R}\{\mathcal{U}_2\}_{\gamma\delta D}\{\mathcal{V}_1\}_{\beta\delta L} \tag{18}$$

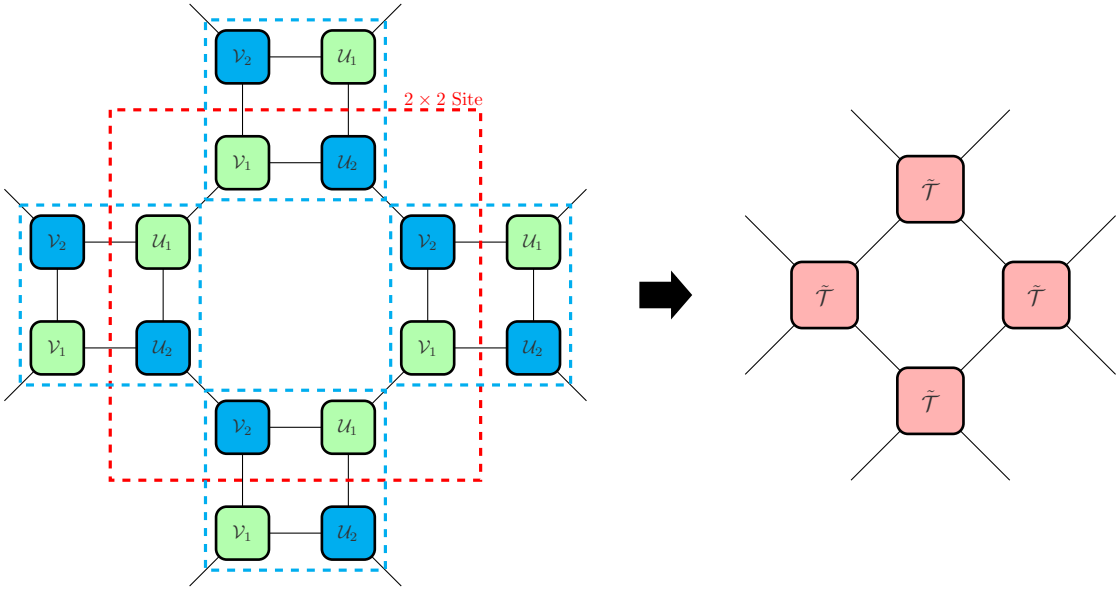


Figure 7: Schematic of the merging process

However, this takes a lot of time and binary due to the growth of the tensor size, and thus we apply low-rank approximation (Eckart–Young–Mirsky theorem) for lowering the dimension of the tensor to reduce the computational costs

The amount of the elements to be kept is denoted as `chi`

We first tested the code by calculating the free energy per site at critical temperature $k_B T_c/J = 2/\ln\left(1+\sqrt{2}\right) \approx 2.27$

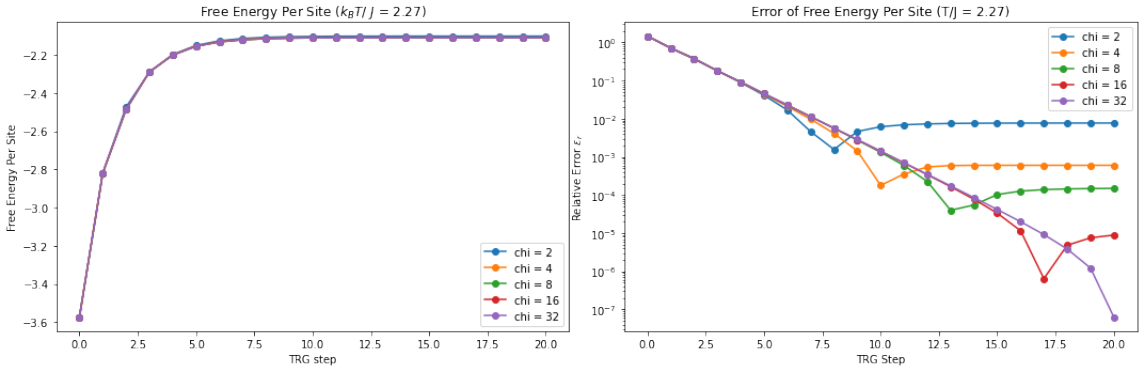


Figure 8: Free energy per site under different TRG step (iteration)

Then, we tested it on different temperature

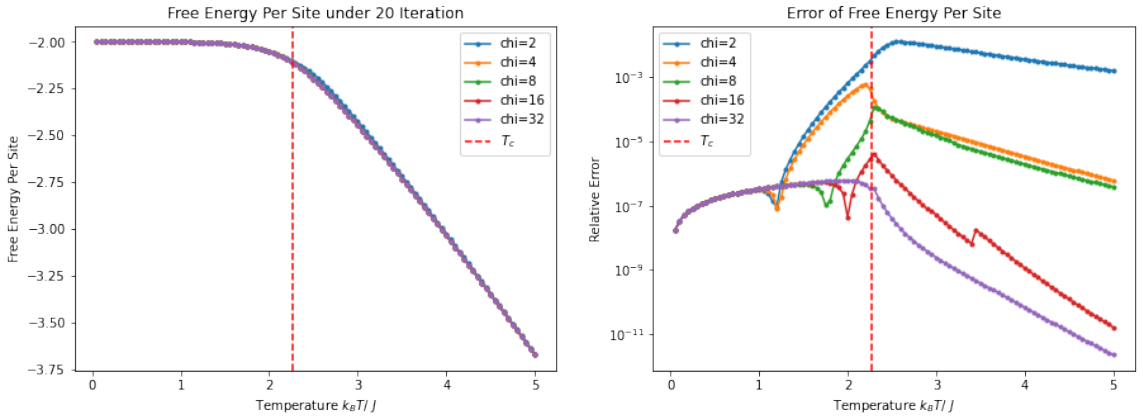


Figure 9: Free energy per site under different temperature (step = 20, 100 points)

We also calculate the heat capacity using central finite difference

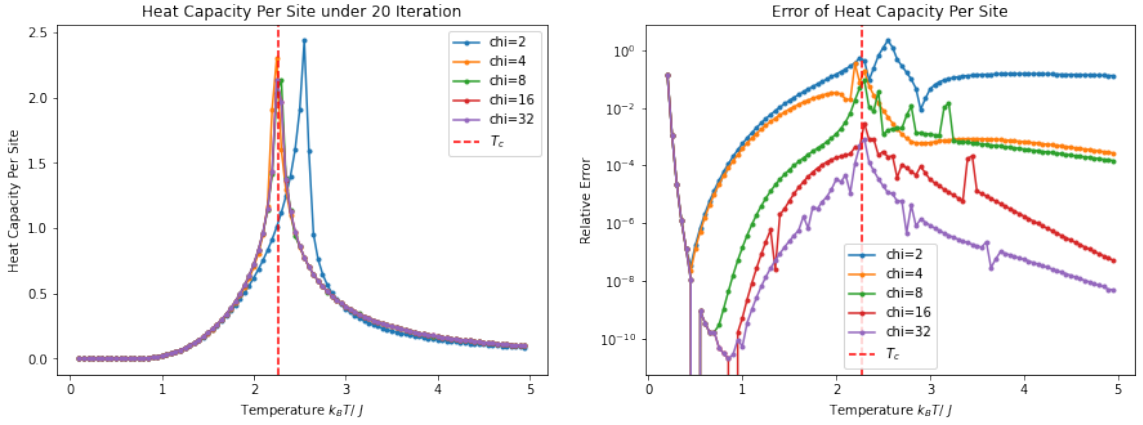


Figure 10: Heat capacity under different temperature (step = 20, 100 points)

To observe a more detailed peak behavior, we run 100 points simulation within $2 \leq k_BT/J \leq 3$

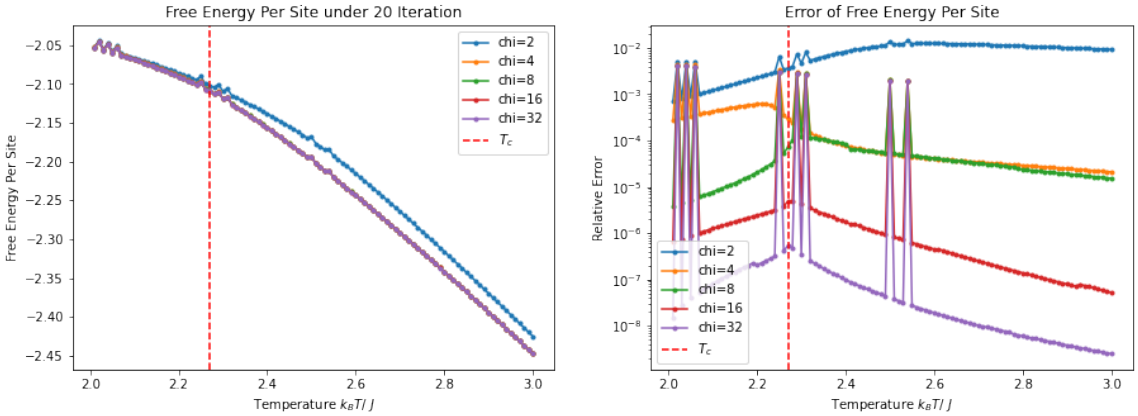
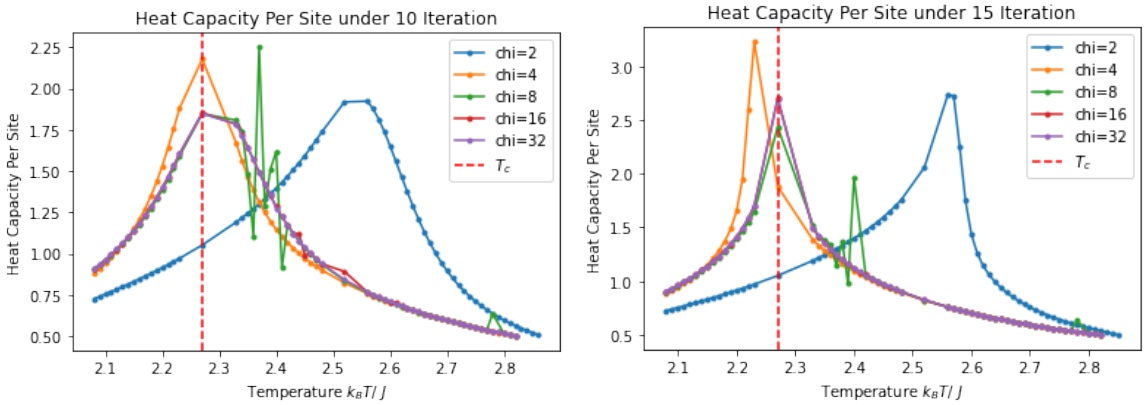


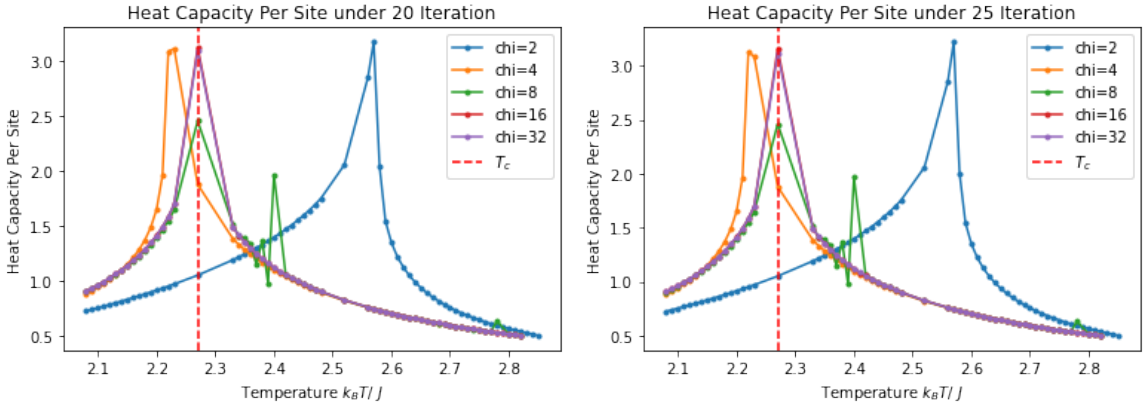
Figure 11: Free energy per site for $2 \leq k_BT/J \leq 3$ (100 points)

And the heat capacity is (data points exhibiting abnormally large fluctuations were removed)



(a) step = 10

(b) step = 15



(c) step = 20

(d) step = 25

Figure 12: Peak behavior of heat capacity

4 Conclusion

In this project we explore different numerical approach to simulate Ising model with transfer matrix.

For 1D site, we simply take trace of the powered matrix to obtain the partition function, while two different methods are deployed for 2D site.

The Einstein summation method calculates the partition function by combining the adjacent 'legs' of transfer tensor, and can be applied to square, rectangle, and other shapes. However, despite its simplicity, the method fails for large system sizes.

The TRG method instead calculating the partition function by splitting and merging the tensor though iteration, which enable it to obtain results for large site efficiently. However, the method can be only applied to square sites.

After obtaining the partition function, we derive the Helmholtz free energy and heat capacity. Assuming isotropic coupling, the heat capacity of the square lattice exhibits a pronounced peak near the critical temperature $T_c = 2J/k_B \ln(1 + \sqrt{2})$ This peak becomes increasingly sharp as the system size increases.

5 Reference

https://tensornetwork.org/trg/
https://github.com/pcchen/11410PHYS401200.git