Transfer Matrix Spectrum of 2D Ising Model by Tensor Network

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ABSTRACT

We develop a scheme to compute the spectrum of transfer matrix of two dimensional Ising Model by using tensor network. The first step is to represent transfer matrix in terms of tensor network and then it is coarse grained by using Higher Order Tensor Renormalization Group. From the coarse-grained tensor, we obtain approximation of the transfer matrix and then it is diagonalized to get the eigenvalues and eigenvectors. Using the eigenvalues, several important quantities such as energy gap and free energy of finite system can be computed. Furthermore, by computing an impurity tensor network, quantum number of the energy state can be classified.

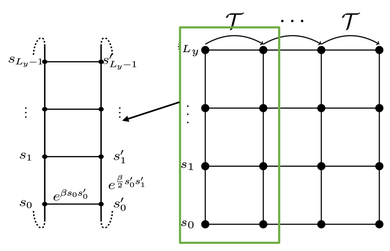
INTRODUCTION

- Transfer matrix method is a tool to evaluate the partition function
- The eigenvalues of transfer matrix can be used to compute the energy gap, correlation length, free energy, etc.
- The eigenvector is important to determine the quantum number of the energy spectrum.
- Direct diagonalization of transfer matrix is very hard because its dimension is equal to exponential of system size.
- One way to diagonalize transfer matrix is by using tensor network (TN) based algorithm i.e. Higher Order Tensor Renormalization Group (HOTRG) [2].
- This algorithm truncates the bond dimension of tensor into cutoff χ.
- With this technique, the dimension of transfer matrix is reduced into χ^2.

METHODS

To compute the approximate energy gap and quantum number by using transfer matrix formalism combined with tensor network algorithm , we follow the steps below:

1. Define 2D Ising Model in the transfer matrix formalism.



$$Z = \sum_{\{s\}} e^{-\beta H(\{s\})} = Tr\,(\mathcal{T}^{L_x})$$

Z is the partition function of 2D Ising system with volume $V = L_x \times L_y$

$$\mathcal{T}_{ss'} = \left(\prod_{i=0}^{L_{y-1}} e^{\beta s_i s_{i'}}\right)\left(\prod_{i=0}^{L_{y-1}} e^{\frac{\beta}{2}s_i s_{i+1} + \frac{\beta}{2}s'_i s'_{i+1}}\right)$$

$\mathcal{T}$ is transfer matrix , $s = \{+1, -1\}$, β is inverse of temperature

Figure 1. Transfer matrix formalism on 2D Ising Model. The transfer matrix $\mathcal{T}$ of the model contain the information of nearest neighbor interaction in x and y direction.

2. Find the tensor network (TN) representation of transfer matrix $\mathcal{T}$

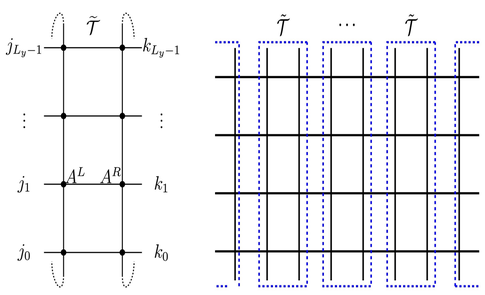


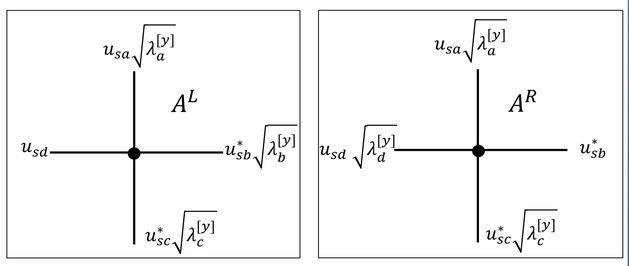
Figure 2. TN representation of transfer matrix

$$\widetilde{\mathcal{T}}_{jk} = \sum_{ss'} U^{\dagger}_{js}\mathcal{T}_{ss'}U_{s'k}$$

Unitary transformation of transfer matrix $\mathcal{T}$ into its TN representation $\tilde{\mathcal{T}}$

$$U_{js} = u_{j_0 s_0} u_{j_1 s_1} \dots u_{j_{L_y-1} s_{L_y-1}}$$

U is global unitary matrix
u is local unitary matrix



Rank−4 tensor of each lattice site in TN representation of transfer matrix

$e^{\beta s_i s_{i'}}$ (interaction in x direction) can be decomposed into:

$$e^{\beta s_i s_{i'}} = \sum_{s_i} u^{\dagger}_{s_i k_i}\lambda^{[x]}_{k_i}u_{k_i s_i}$$

$$u_{s_i k_i} = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}$$

$$\lambda^{[x]}_{k_i} = \begin{bmatrix}2\cosh\beta & 0\\ 0 & 2\sinh\beta\end{bmatrix}$$

$e^{\frac{\beta}{2}s_i s_{i+1}}$(interaction in y direction) can be decomposed into:

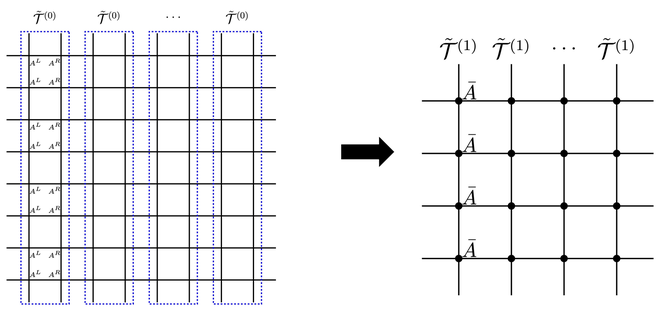
$$e^{\beta s_i s_{i+i}} = \sum_{s_i} u^{\dagger}_{s_i k_{i+i}}\lambda^{[y]}_{k_{i+1}}u_{k_{i+1} s_i}$$

$$\lambda^{[y]}_{k_i} = \begin{bmatrix}2\cosh\frac{\beta}{2} & 0\\ 0 & 2\sinh\frac{\beta}{2}\end{bmatrix}$$

$$A_L = \sqrt{\lambda^{[y]}_a\lambda^{[x]}_b\lambda^{[y]}_c}\sum_s u_{sa}u^*_{sb}u^*_{sc}u_{sd}$$

$$A_R = \sqrt{\lambda^{[y]}_a\lambda^{[x]}_d\lambda^{[y]}_c}\sum_s u_{sa}u^*_{sb}u^*_{sc}u_{sd}$$

3. Full Contraction of TN



Initial TN Representation

Figure 3: Full contraction of initial TN before coarse graining

Diagonalization of the coarse grained tensor $\tilde{\mathcal{T}}^{(n)}$

$\tilde{\mathcal{T}}^{(n)} = W\lambda' W^{\dagger}$
λ' =Eigenvalues
W = Eigenvector

4. Coarse grain the tensor network by using HOTRG algorithm

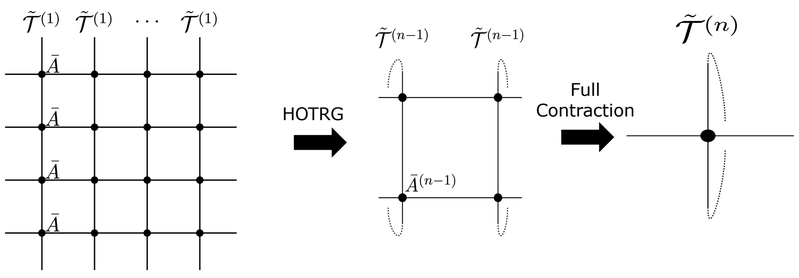


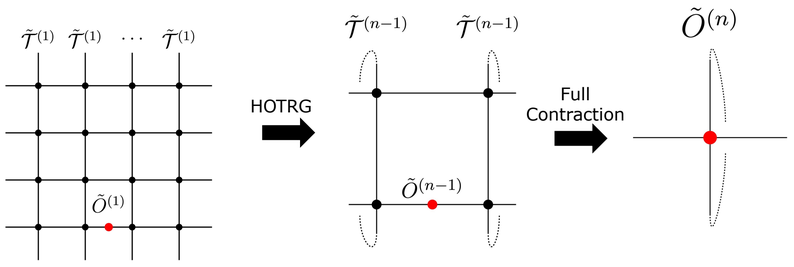
Figure 4: Coarse graining of TN with HOTRG

Correlation function in TN representation of transfer matrix

$$\langle\tilde{O}(\tau)\tilde{O}(0)\rangle = \frac{Tr\left[\tilde{O}\tilde{\mathcal{T}}^{\tau}\tilde{O}^{\dagger}\tilde{\mathcal{T}}^{L_x-\tau}\right]}{Tr\left[\tilde{\mathcal{T}}^{L_x}\right]}$$

$$Tr\left[\tilde{O}\tilde{\mathcal{T}}^{\tau}\tilde{O}^{\dagger}\tilde{\mathcal{T}}^{L_x-\tau}\right] = Tr\left[\widetilde{W}^{\dagger}\tilde{O}\widetilde{W}\lambda^{\tau}\widetilde{W}^{\dagger}\widetilde{O^{\dagger}}\widetilde{W}\lambda^{L_x-\tau}\widetilde{W}\right] = Tr\left[\tilde{B}\lambda^{\tau}\tilde{B}^{\dagger}\lambda^{L_x-\tau}\right]$$

5. Compute impurity matrix by HOTRG to find quantum numbe



To classify quantum number, compute:

$$\tilde{B} \approx \lambda'^{-1/2}W^{\dagger}\tilde{O}^{(n)}W\lambda'^{-1/2}$$

$\lambda' \approx \lambda^{L_x}$, approximate eigenvalues
W = approximate eigenvector
$\tilde{O}^{(n)}$ =impurity tensor after coarse graining

Figure 5: Coarse graining of TN representation of impurity matrix $\tilde{O}$, where $\tilde{O} = U^{\dagger}OU$ is unitary transformation of arbitrary operator O.

RESULTS

As the first step, we compute the eigenvalues of transfer matrix of 2D Ising model of finite system sizes. From the eigenvalues λ', the energy gap ω_a and its relative error $\delta\omega_a$ can be obtained by using the following equations

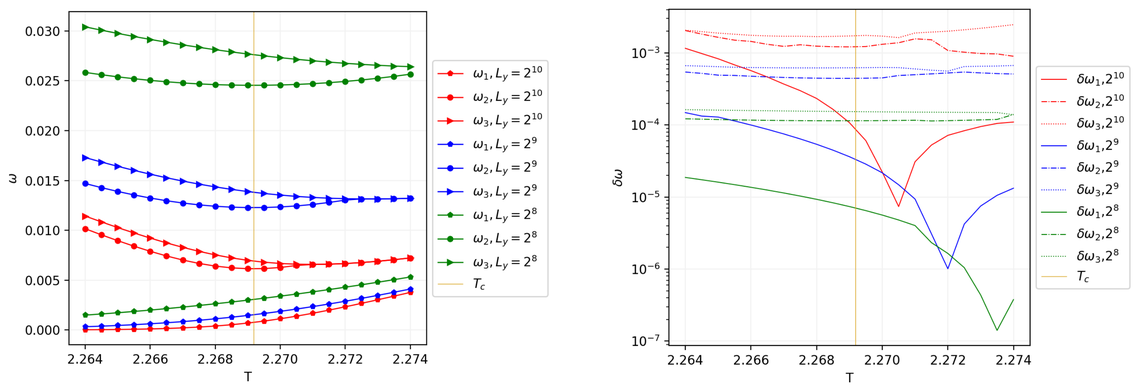
$$\omega_a = E_a - E_0 \approx -\frac{1}{L_x}\ln\frac{\lambda'_a}{\lambda'_0}$$

E_a = Energy of state a
E_0 = Ground state energy

$$\delta\omega_a = \frac{|\omega_a^{HOTRG} - \omega_a^{exact}|}{|\omega_a^{exact}|}$$

ω_a^{exact} =exact energy gap [1]

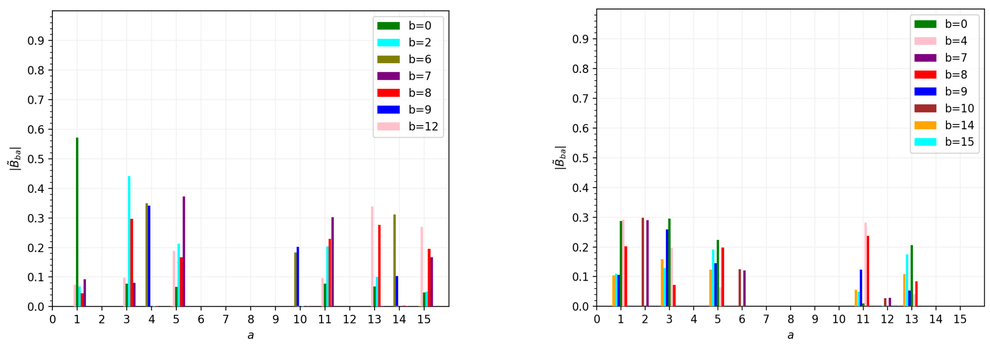
- **Three lowest energy gap $\omega_1, \omega_2, \omega_3$ over several system size and the relative error**



(a) (b)

Figure 6. (a). Three lowest energy gap for system wth linear size on y $L_y = 2^8$, 2^9, and 2^{10} computed by HOTRG with $\chi = 100$. It can be seen that when system size gets larger, ω_1 below T_c gets closer to zero which means the first energy state and ground state degenerate. (b) The relative error of three lowest energy gap over several linear size L_y. The error is getting larger when system size is getting larger.

- **$|\widetilde{B}_{ba}|$ elements to determine quantum number of eigenstates at $T = 2.264 < T_c$ and $T = 2.274 > T_c$ and $L_v = 2^{10}$**



(a) (b)

Figure 7. First sixteen elements of matrix $\tilde{B}$ for system at $T = 2.264$ (a), and (b) $T = 2.274$. State a with nonzero $|\tilde{B}_{ba}|$ shows the state has quantum number $q = (-)$.

The matrix element is given by $\tilde{B}_{ba} = \langle a|s|b\rangle$, s is spin operator with quantum number $(-)$. The ground state which is given by $b = 0$ always has quantum number $q = (+)$. Thus $\tilde{B}_{0a}$ is equal to zero if state a has quantum number $q = (+)$ because $\tilde{B}_{0a} = \langle +|-|+\rangle = 0$. Therefore, from Fig.7 it can be deduced that for system with $L_y = 2^{10}$ at $T = 2.264$ state $a = 0,2,6,7,8,9,12$ have quantum number $q = (+)$. This result is summarized and compared with exact quantum number in Table 1.

T \ a		0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
2.264	Exact	+	−	+	−	−	−	+	+	+	+	−	−	+	−	−	−
	HOTRG	+	−	+	−	−	−	+	+	+	+	−	−	+	−	−	−
2.274	Exact	+	−	−	−	+	−	−	+	+	+	+	−	−	−	+	+
	HOTRG	+	−	−	−	+	−	−	+	+	+	+	−	−	−	+	+

Table 1. Comparison of exact and approximate quantum number. The exact quantum number is computed by following formula derived by [1].

- **Relative error of free energy of finite system**

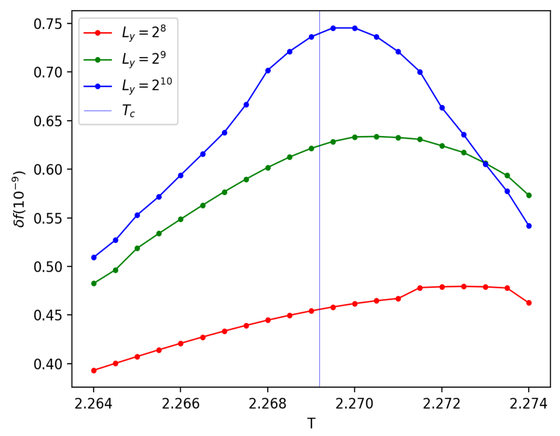


Figure 8. Relative error of free energy of finite system with size $L_x \times L_y = 2^{10}\times 2^{10}$, $2^9\times 2^9$, $2^8\times 2^8$, computed by HOTRG with $\chi = 100$

The relative error of free energy is

$$\delta f = \frac{|f_{HOTRG} - f_{exact}|}{|f_{exact}|}$$

Where f_{HOTRG} is the approximate free energy computed with HOTRG algorithm with $\chi = 100$ and f_{exact} is computed by following formulation in [1].

The relative error is around $\sim 10^{-9}$. The error is getting slightly larger when system size is larger because of coarse graining.

Furthermore, the error near $T_c = \frac{2}{\log(1+\sqrt{2})}$ is getting significant at larger system.

CONCLUSION

- The numerical result with $\chi = 100$ shows that error of the approximate energy spectrum is relatively small. However the error gets larger as the system size increases.
- The quantum number computed from HOTRG at at $T = 2.264$ and $T = 2.274$ shows good agreement with the exact result up to first 16 eigenvalues for $L_y = 2^{10}$.
- The quantum number accuracy highly depends on the error of the energy gap. When the error of the energy gap is large, energy gap of each state can not be distinguished. Thus, quantum number of those indiscernible approximate energy gap are not able to be judged correctly.

REFERENCES

[1] B. Kaufman, Phys. Rev. 76(8), 1232-1252, (1949)
[2] Z. Y. Xie, J. Chen, M. P. Qin, J. W. Zhu, L. P. Yang, and T. Xiang, Phys. Rev. B 86, 045139, (2012)