Journal Club 2018/10/5 Akiyama Shinichiro

# Coarse-graining renormalization by higher-order singular value decomposition Z. Y. Xie, J. Chen, M. P. Qin, J. W. Zhu, L. P. Yang, and T. Xiang Phys. Rev. B 86 045139 (2012)



Contents

### 1. Introduction

### 2. Tensor Network Method (Ex. 2D Ising model)

I) Construction of Tensor Network Representation

II) Higher-Order Tensor Renormalization Group

**3.** Conclusion



The "Tensor Network Method" discussed here consists of 2 steps :

① Convert the system on the real space into the "virtual" network by Singular Value Decomposition

2 Compress the network,

preserving relevant elements in the long-scale physics

### Step1 Move on to the TN representation

Ex) 2D classical Ising Model (with periodic boundary):  $\sigma_i = \pm 1$ 

$$H = -\sum_{\langle ij \rangle} \sigma_i \sigma_j =: \sum_{\langle ij \rangle} K(\sigma_i, \sigma_j)$$
$$Z = \sum_{\{\sigma\}} \exp[-\beta H] = \sum_{\{\sigma\}} \prod_{\langle ij \rangle} \exp[-\beta K(\sigma_i, \sigma_j)]$$

Singular value decomposition for the transfer matrix element :

$$\exp\left[-\beta K(\sigma_i,\sigma_j)\right] = \sum_l \sqrt{\lambda_l} U(\sigma_i,l) \sqrt{\lambda_l} U(\sigma_j,l) = \sum_l W(\sigma_i,l) W(\sigma_j,l)$$

→ Change of variables from  $\{\sigma\}$  to  $\{l\}$  (bond d.o.f.).

For each site in the real space, we define the 4-rank tensor :

$$T_{l_1 l_2 l_3 l_4} \coloneqq \sum_{\sigma_i = \pm 1} W(\sigma_i, l_1) W(\sigma_i, l_2) W(\sigma_i, l_3) W(\sigma_i, l_4)$$

One obtains the TN representation of the partition function :



Step2 Higher-Order Tensor Renormalization Group (HOTRG)



The basic idea of the transformation is

"2 local tensors  $\Rightarrow$  1 Coarse-grained tensor"

And we want to obtain accurate thermodynamic properties.

(i) Align 2 local tensors vertically and contract them :

*n*: # of iteration

 $T^{(n)}$ 

#### (ii) Let us define the block spin transformation! Unfolding M into matrices in two ways, consider $\mathcal{MM}^{\dagger}$ such that



and by the eigen value decomposition,

$$\sum_{(jkl)} \mathcal{M}_{x(jkl)} \mathcal{M}_{\tilde{x}(jkl)}^* = \sum_{i} U_{ix}^{\mathrm{L}} \Lambda_{i}^{\mathrm{L}} U_{i\tilde{x}}^{\mathrm{L}}$$
$$\sum_{(ikl)} \mathcal{M}_{x'(ikl)} \mathcal{M}_{\tilde{x}'(ikl)}^* = \sum_{j} U_{jx'}^{\mathrm{R}} \Lambda_{j}^{\mathrm{R}} U_{j\tilde{x}'}^{\mathrm{R}}$$

Here, diagonal elements of  $\Lambda's$  are arranged in the descending order. Corresponding vectors in U's are also done in the same way. (iii) Define the block spin transformation.

$$\epsilon_{\mathrm{L(R)}} \coloneqq \sum_{i > D_{\mathrm{cut}}} \Lambda_i^{\mathrm{L(R)}}$$

where  $D_{\text{cut}}$  is an integer we can choose freely.

$$\epsilon_{\mathrm{L}} < \epsilon_{\mathrm{R}} \implies U^{(n+1)} \coloneqq U^{\mathrm{L}}$$
  
 $\epsilon_{\mathrm{L}} > \epsilon_{\mathrm{R}} \implies U^{(n+1)} \coloneqq U^{\mathrm{R}}$ 

 $\Rightarrow$  Using a part of unitary matrix, we define the transformation

If one aligns 2 local tensors vertically, it is necessary to do horizontally in the next.



In this way, 2*N*-times HOTRG calculation gives the partition function on the  $2^N \times 2^N$  square lattice by

$$Z \approx \mathrm{Tr}\big[T^{(2N)}\big]$$

In the 2D HOTRG calculation,

memory  $\sim D_{cut}^4$ computational time  $\sim D_{cut}^7$ 





Replication Test (S.A.)



In the vicinity of  $T_c \approx 2.269$ , eigen values of  $\mathcal{MM}^{\dagger}$  decreases slowly.

Replication Test (S.A.)

## Conclusion

- HOTRG exploits a kind of block-spin transformation and it is easy to reach the thermodynamic limit.
- In principle, HOTRG can be applied for higher dimensional systems.
- However, large- $D_{cut}$  calculation in higher dimensional systems is computationally challenging.
- Research for the "finite-D<sub>cut</sub> scaling" is of great interest!

# APPENDICES

- "Phase Transitions of Ferromagnetic Potts Model on the Simple Cubic Lattice"
  - S. Wang, Z. Y. Xie, J. Chen, B. Normand, and T. Xiang Chin. Phys. Lett. 31, 070503 (2014)
- "A Multilinear Singular Value Decomposition"
  L. de Lathauwer, B. de Moor, and J. Vandewalle
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- "The density-matrix renormalization group"
  U. Schollwock
- Rev. Mod. Phys., 77, 259 (2005) ・「『密度行列繰り込み群』の変分原理」 西野友年, 奥西巧一, 引原俊哉
- 物性研究 (1997), 68(2), 133-155
- Lecture by H. Matsueda @ Chuo Univ. (2018/8/29~31)

q-state Ferromagnetic Potts Model on Cubic Lattice

$$H = -\sum_{\langle ij \rangle} \delta_{s_i s_j} \quad \text{where} \quad s_i \in \{0, 1, \cdots, q-1\}$$

 $q = 2 \implies$  Ising Model  $q = 3 \implies Z_3$  is the center symmetry of SU(3)

The initial local tensor is given by

$$Q(s_i, l) = e^{2\pi i l s_i/q} \sqrt{\frac{e^\beta - 1 + q\delta_{l,0}}{q}}$$



 $T_{xx'yy'zz'} \coloneqq \sum_{s_i} Q(s_i, x)Q^*(s_i, x')Q(s_i, y)Q^*(s_i, y')Q(s_i, z)Q^*(s_i, z')$ 

### HOTRG calculation

Contract 2 tensors vertically and one has to truncate the size of the tensor corresponding to the rest directions :



The partition function on the cube is given by

 $Z \approx \mathrm{Tr}\big[T^{(3N)}\big]$ 

After enough times of iteration, consider the  $D_{cut} \times D_{cut}$  matrix,

$$A_{zz'} \coloneqq \sum_{xy} T_{xxyyzz'}^{(n)}$$

the degeneracy of A plays a good indicator of the transition point

$$X \coloneqq \frac{(\mathrm{Tr}[A])^2}{\mathrm{Tr}[A^2]}$$

Ordered phase  $\Rightarrow$   $Z_3$  symmetry is broken spontaneously

The largest eigenvalue of A is 3-fold degenerated, X = 3

Disordered phase  $\Rightarrow$   $Z_3$  symmetry is preserved

The largest eigenvalue of A is unique, X = 1



 $\Rightarrow$  Distinguishable 2 phases are confirmed



$$E = -\frac{1}{V} \frac{\partial \ln Z}{\partial \beta}$$
$$C = \frac{\beta^2}{V} \frac{\partial^2 \ln Z}{\partial \beta^2}$$

#### $\Rightarrow$ Numerical derivative

$$M = \frac{1}{V} \sum_{i} \delta_{s_i,0}$$

- ⇒ Adding the source term to the Boltzmann weight, i.e. the initial tensor  $T^{(0)}$ .
- ⇒ Numerical derivative w.r.t. the magnetic field.

S. Wang, Z. Y. Xie, J. Chen, B. Normand, and T. Xiang (2014)

### Investigation of the $D_{cut}$ -dependence of $T_c$ , but ..... the lack of convergence !



S. Wang, Z. Y. Xie, J. Chen, B. Normand, and T. Xiang (2014)

#### Comparison of the estimated jump of internal energy and transition point S. Wang, Z. Y. Xie, J. Chen, B. Normand, and T. Xiang (2014)

Method	$\Delta E$	$T_c$
Series expansion (1979) [48]		1.7289(12)
Monte Carlo RG (1979) [14]		1.818
Monte Carlo (1982, $L = 8$ ) [45]	0.12	1.81
Pair approximation (1982) [45]	0.123	1.879
Monte Carlo (1987, $L = 16$ ) [46]	0.2222(7)	1.81618(7)
Monte Carlo (1991, $L = 36$ ) [47]	0.16062(52)	1.816455(35)
Monte Carlo (1997, $L = 36$ ) [18]	0.1614(3)	1.816316(33)
Monte Carlo (2007, $L = 50$ ) [5]	0.1643(8)	1.816315(19)
TPVA (2002) [19]	0.228	1.8195
HOTRG (this work)	0.2029	1.8166
	(D = 14)	(D = 21)

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q = 2 Potts Model  $\Leftrightarrow$  Ising Model

$$H = -J \sum_{\langle ij \rangle} \delta_{s_i, s_j} - h \sum_i \delta_{s_i, 1} \quad \text{where} \quad s_i \in \{0, 1\}$$

Regarding  $s_i=0$  as  $\sigma_i=-1$  and  $s_i=1$  as  $\sigma_i=+1$  ,

$$\delta_{s_i,s_j} = \frac{1 + \sigma_i \sigma_j}{2} \qquad \delta_{s_i,1} = \frac{1 - \sigma_i}{2}$$

hold.

That is, the Hamiltonian of 2-state Potts Model can be written as

$$H = -\frac{J}{2} \sum_{\langle ij \rangle} \sigma_i \sigma_j + \frac{h}{2} \sum_i \sigma_i + \text{Const.}$$

This is nothing but the Ising model.

### Singular Value Decomposition (SVD)

For any complex  $I_1 \times I_2$  -matrix A can be written as the product  $A = U^{(1)}SU^{(2)}^{\dagger}$ 

where

- 1.  $U^{(1)}$  is an  $I_1 \times I_1$  unitary matrix.
- 2.  $U^{(2)}$  is an  $I_2 \times I_2$  unitary matrix.
- 3. *S* is an  $I_1 \times I_2$ -matrix such that
  - (i) Pseudo-diagonality :  $S = \text{diag}(\sigma_1, \sigma_2, \cdots, \sigma_{\min(I_1, I_2)})$

(ii) Ordering : 
$$\sigma_1 \ge \sigma_2 \ge \cdots \ge \sigma_{\min(I_1, I_2)} \ge 0$$

 $\sigma_i$ 's are singular values of A and the *i*-th column vectors of  $U^{(1)}$  and  $U^{(2)}$  are, resp., *i*-th left and right singular vector.

### SVD introduces virtual dof

Consider the system consisting of subsystems *X* and *Y*. Setting the pure state of the total system as

$$|\psi\rangle = \sum_{x \in X} \sum_{y \in Y} \psi(x, y) |x\rangle \otimes |y\rangle$$

If  $\psi(x, y) = u(x)v(y)$ , then the state is separable. Actually,

$$|\psi\rangle = \left(\sum_{x \in X} u(x)|x\rangle\right) \otimes \left(\sum_{y \in Y} v(y)|y\rangle\right)$$

### SVD introduces virtual dof

Regarding  $\psi(x, y)$  as a matrix element. By SVD,

$$\psi(x,y) = \sum_{l=1}^{N} u_l(x)\sigma_l v_l(y)$$

If N > 1, the state is not pure. However, as a matrix,

$$\psi = U\Sigma V^{\dagger} = (U\Sigma^{1/2})(V\Sigma^{1/2})^{\dagger} =: \widetilde{U}\widetilde{V}^{\dagger}$$

This looks very similar with  $\psi(x, y) = u(x)v(y)$ .

### Higher-Order Singular Value Decomposition (HOSVD)

Any complex  $I_1 \times I_2 \times \cdots \times I_n$ -tensor A can be written as the product

$$A_{i_1 i_2 \cdots i_n} = \sum_{j_1 j_2 \cdots j_n} S_{j_1 j_2 \cdots j_n} U_{j_1 i_1}^{(1)} U_{j_2 i_2}^{(2)} \cdots U_{j_n i_n}^{(n)}$$

where

1.  $U^{(k)}$  is a unitary  $I_k \times I_k$  -matrix.

2. *S* is a complex  $I_1 \times I_2 \times \cdots \times I_n$ -tensor such that

(i) Fixing the k-th index of S, say  $S_{i_k=\alpha}$ , and if  $\alpha \neq \beta$ , then

$$\sum_{i_1 i_2 \cdots i_n} S_{i_1 i_2 \cdots i_{k-1} \alpha i_{k+1} \cdots i_n} S_{i_1 i_2 \cdots i_{k-1} \beta i_{k+1} \cdots i_n} = 0$$

(ii) Ordering :

$$\|S_{i_k=\alpha}\| \coloneqq \sqrt{\sum_{i_1i_2\cdots i_n} S_{i_1i_2\cdots i_{k-1}\alpha i_{k+1}\cdots i_n} S_{i_1i_2\cdots i_{k-1}\alpha i_{k+1}\cdots i_n}}$$

$$||S_{i_k=1}|| \ge ||S_{i_k=2}|| \ge \dots \ge ||S_{i_k=I_k}|| \ge 0$$

### TRG VS HOTRG

"Tensor Renormalization Group"

M. Levin and C. P. Nave, Phys. Rev. Lett. 99 120601 (2007)

In TRG, SVD for  $T_{xx'yy'}$  itself is a key in compressing the network.

$$T_{xx'yy'} \approx \sum_{l=1}^{D_{\text{cut}}} \sqrt{\lambda_l} U_{x'y,l} \sqrt{\lambda_l} V_{y'x,l} \quad \text{or} \quad T_{xx'yy'} \approx \sum_{l=1}^{D_{\text{cut}}} \sqrt{\lambda_l} U_{xy,l} \sqrt{\lambda_l} V_{x'y',l}$$

![](_page_28_Figure_5.jpeg)

### TRG VS HOTRG

On the other hand, HOTRG exploits HOSVD of  $M = \sum TT$ , so T itself is not decomposed.

Ex) 2D Ising model

![](_page_29_Figure_3.jpeg)

Z. Y. Xie, J. Chen, M. P. Qin, J. W. Zhu, L. P. Yang, and T. Xiang (2012)

Density Matrix Renormalization Group (1/9)

DMRG is a kind of variational method in which **one optimizes the variational wave function expressed by the matrix product of a part of a unitary matrix, which diagonalizes a density matrix**.

The ground state and its energy of the 1D quantum systems can be obtained with high accuracy!

**Fundamental Fact** 

For any projection operator P, such that  $P^2 = P$  and  $\text{Tr}P = \chi$ the inequality,  $\text{Tr}\rho \geq \text{Tr}P\rho$ 

holds.

Density Matrix Renormalization Group (2/9) Ex) 1D N-site S = 1/2 Heisenberg Model Subsystem *l* Subsystem r M sites N - M sites  $\widehat{H} = \sum_{i=1}^{N-1} \vec{S}_i \cdot \vec{S}_{i+1}$ 

The matrix representation of  $\widehat{H}$  is given by  $2^N \times 2^N$  symmetric matrix.

Density Matrix Renormalization Group (3/9)

 $\{|lr\rangle\}$ : the basis of the Hilbert space for the total system

$$H_{lrl'r'} \coloneqq \left\langle lr \big| \widehat{H} \big| l'r' \right\rangle$$

For the density matrix  $\hat{\rho} = e^{-\beta \hat{H}}$ , the element  $\rho_{lrl'r'}$  describes the following development:

![](_page_32_Figure_4.jpeg)

Density Matrix Renormalization Group (4/9)

$$Z = \mathrm{Tr}\hat{\rho} = \mathrm{Tr}_{\mathrm{L}(\mathrm{R})}\hat{\rho}^{\mathrm{L}(\mathrm{R})}$$

Let us compress  $2^M \times 2^M$  matrix  $\hat{\rho}^L$  into  $m \times m$  matrix  $\tilde{\rho}$ . Since  $\hat{\rho}^L$  is symmetric,

$$\exists \hat{Q} = \begin{bmatrix} \vec{q}_1, \vec{q}_2, \cdots, \vec{q}_{2^M} \end{bmatrix} \quad \text{s.t.} \quad \hat{Q}^{\mathrm{T}} \hat{\rho}^{\mathrm{L}} \hat{Q} = \mathrm{diag}(\lambda_1, \lambda_2, \cdots, \lambda_{2^M})$$

Assuming the diagonal elements are arranged in the descending order,

$$\tilde{Z} \coloneqq \sum_{i=1}^{m} \lambda_i$$

gives the best approximation of Z. So, we choose  $m \times m$  matrix  $\tilde{\rho}$  as

$$\tilde{\rho} = \operatorname{diag}(\lambda_1, \lambda_2, \cdots, \lambda_m)$$

Density Matrix Renormalization Group (5/9)

This selection is equally expressed by the transformation

$$\tilde{\rho} \coloneqq \tilde{Q}^{\mathrm{T}} \hat{\rho}^{\mathrm{L}} \tilde{Q}$$
$$\tilde{Q} = [\vec{q}_1, \vec{q}_2, \cdots, \vec{q}_m]$$

The matrix  $\tilde{Q}$  truncates the size of  $\hat{\rho}^{L}$ . Defining  $P \coloneqq \tilde{Q}\tilde{Q}^{T}$ , this transformation is expressed by

$$\tilde{Z} = \mathrm{Tr}_{\mathrm{L}} P \hat{\rho}^{\mathrm{L}}$$

The projection *P* can be seen as a block spin transformation from the original system to the coarse-grained system.

Density Matrix Renormalization Group (6/9)

Let us consider the following example

![](_page_35_Figure_2.jpeg)

Starting the case M = 2 and  $\hat{\rho}^{L}$  is diagonalized iteratively.

Density Matrix Renormalization Group (7/9)

Finally, we approach the total  $\hat{\rho}$  and

 $(QRSTU)^{\mathrm{T}}\hat{\rho}(QRSTU) = \mathrm{diag}(\mathrm{e}^{-\beta E_{0}}, \mathrm{e}^{-\beta E_{1}}, \cdots)$ 

This indicates that the energy eigen state is given by

$$\Psi^{\nu}_{s_1 s_2 s_3 s_4 s_5 s_6} = \sum_{\xi \zeta \eta \mu} Q_{s_1 s_2, \xi} R_{\xi s_3, \zeta} S_{\zeta s_4, \eta} T_{\eta s_5, \mu} U_{\mu s_6, \nu}$$

which satisfies

$$\widehat{H}\Psi^{\nu} = E_{\nu}\Psi^{\nu}$$

Density Matrix Renormalization Group (8/9)

Now the eigen state is expressed by the unitary matrix product

$$\Psi^{\nu}_{S_1 S_2 S_3 S_4 S_5 S_6} = \sum_{\xi \zeta \eta \mu} Q_{S_1 S_2, \xi} R_{\xi S_3, \zeta} S_{\zeta S_4, \eta} T_{\eta S_5, \mu} U_{\mu S_6, \nu}$$

In the zero-temperature limit, one expects

$$\widetilde{\Psi}^0_{s_1s_2s_3s_4s_5s_6} = \sum_{\xi\zeta\eta\mu} \widetilde{Q}_{s_1s_2,\xi} \widetilde{R}_{\xi s_3,\zeta} \widetilde{S}_{\zeta s_4,\eta} \widetilde{T}_{\eta s_5,\mu} \widetilde{U}_{\mu s_6,0}$$

gives a good approximation of  $\Psi^0$ !

Density Matrix Renormalization Group (9/9)

The real DMRG algorithm starts with the ansatz: the ground state of the 1D quantum many-body system is given by

$$\widetilde{\Psi}^0_{s_1s_2s_3s_4s_5s_6\cdots} = \sum_{\xi \zeta \eta \mu \cdots} \widetilde{Q}_{s_1s_2,\xi} \widetilde{R}_{\xi s_3,\zeta} \widetilde{S}_{\zeta s_4,\eta} \widetilde{T}_{\eta s_5,\mu} \widetilde{U}_{\mu s_6,\nu} \cdots$$

This is called "Matrix Product State" ansatz.

Here, the all elements of the tilde matrices play the role of variational parameters. The goal of DMRG is to minimize

$$\langle E \rangle = \frac{\left\langle \widetilde{\Psi}^{0} \middle| \widehat{H} \middle| \widetilde{\Psi}^{0} \right\rangle}{\left\langle \widetilde{\Psi}^{0} \middle| \widetilde{\Psi}^{0} \right\rangle}$$

### Finite $-\chi$ scaling (semi-infinite 1D quantum chain)

In the numerical analysis of critical phenomena, we have to care the correction originating from finite size and finite  $\chi$  (# of states). Ground state energy is modified by these corrections as

$$E = E_0 + \frac{A}{\xi^2} + \frac{B}{\xi}\epsilon(\chi)$$

The second term is the finite-size correction and the third term is the finite- $\chi$  correction:

$$\epsilon(\chi) = \sum_{i=\chi+1}^{\infty} \lambda_i$$

Finite  $-\chi$  scaling (semi-infinite 1D quantum chain)

Focusing on the finite- $\chi$  correction, it is known that  $\chi$ -dependence of the entanglement entropy is given by

$$S \sim \frac{1}{\sqrt{\frac{12}{c} + 1}} \log \chi =: \frac{c\kappa}{6} \log \chi$$

For the semi-infinite 1D chain, the Calabrese-Cardy formula says

$$S \sim \frac{c}{6} \log \xi$$

From these,

$$\xi \sim \chi^{\kappa}$$