テンソルくりこみ群による相転移・臨界現象の解析

Analysis of Phase Transitions and Critical Phenomena by Tensor Renormalization Group

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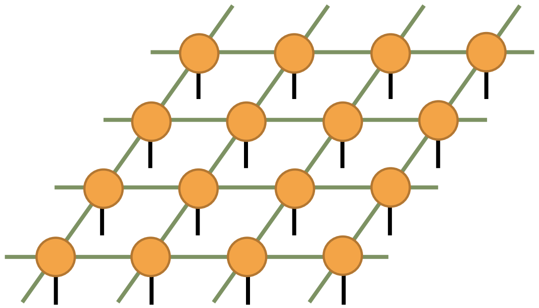
Tensor Networks in Physics

- **Hamiltonian approach**
  - Wave func. of many-body systems

$$|\psi\rangle = \sum_{i_1 \cdots i_N} C_{i_1 \cdots i_N} |i_1 i_2 \cdots i_N\rangle$$

$O(d^N)$ coefficients

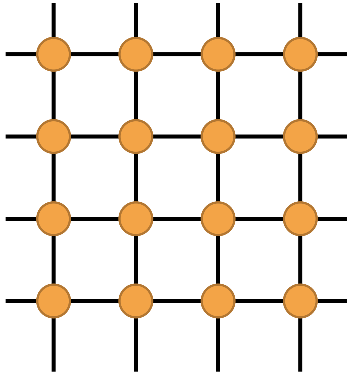


Approximation by TN

- **Lagrangian approach**
  - Partition function (Path integral)

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

$O(d^N)$ terms



Representation as contraction of TN

This talk

TeNeS
Tensor Network Solver for Quantum Lattice Systems

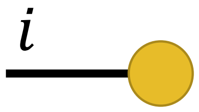
Motoyama, Okubo, Yoshimi, SM, Kato, and Kawashima, Comput. Phys. Commun. **279**, 108437 (2022)
https://www.pasums.issp.u-tokyo.ac.jp/tenes

Graph representations of tensor networks

- Bonds (edges) = indices of tensor

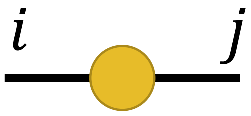
Scalar

x



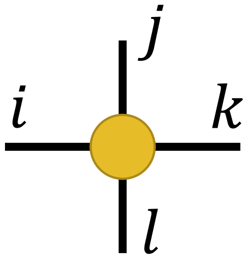
Vector

v_i



Matrix

M_{ij}

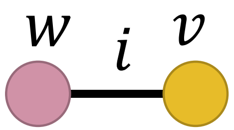


4-leg tensor

T_{ijkl}

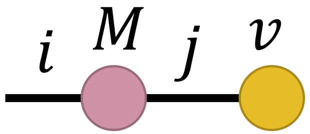
"Bond dimension"
= Dimension of index

- Bond connection = Contraction (sum up indices)



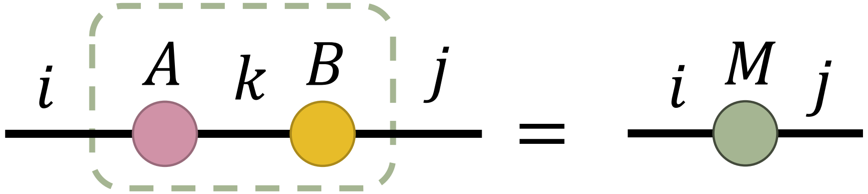
Inner product

$$\sum_i w_i v_i$$



Matrix-vector product

$$\sum_j M_{ij} v_j$$



Matrix product

$$\sum_k A_{ik} B_{kj} = M_{ij}$$

Outline

- Introduction
  - Transfer matrix method
- How to obtain TN representation of the partition function?
  - Three examples of TN representations
- How to approximate contraction of TN?
  - Real-space renormalization group approach
    - ✓ TRG, HOTRG, BWTRG, etc.
  - (Boundary MPS approach)
    - ✓ CTMRG, DMRG, TEBD, VUMPS, etc
- How to evaluate physical quantities?
  - Multi-impurity method with HOTRG and BWTRG
  - Finite-size scaling analysis
- Summary

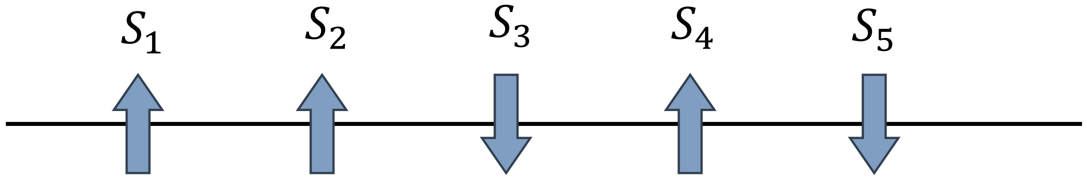
Transfer matrix method

- 1D Ising chain $H = -J \sum_{i=1}^{L} S_i S_{i+1}$ $\qquad S_i = +1$ or -1

  up down

Partition function

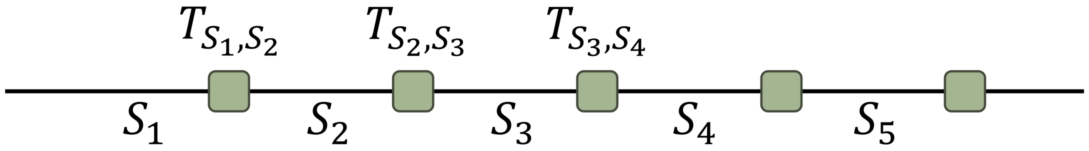
$$Z = \sum_{\{S_i\}} e^{\beta J \sum_i S_i S_{i+1}}$$



Transfer matrix

$$T = \begin{array}{cc} & \begin{array}{cc} S_{i+1} = 1 & \quad -1 \end{array} \\ & \begin{pmatrix} e^{K} & e^{-K} \\ e^{-K} & e^{K} \end{pmatrix} \begin{array}{l} S_i = 1 \\ S_i = -1 \end{array} \end{array}$$

$K \equiv \beta J$



$Z = \langle \boldsymbol{v}_L | T^{L-1} | \boldsymbol{v}_R \rangle$ (open/fixed boundary)

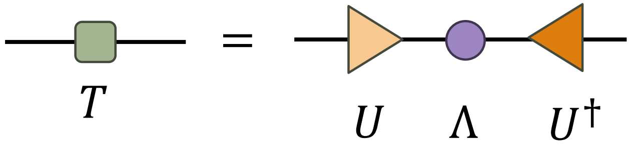
$Z = \mathrm{Tr}\ T^L$ (periodic boundary)

- ✓ Matrices are located between spins.
- ✓ Index of matrix corresponds to spin direction.

Evaluation of Z

◘ Eigenvalue decomposition of transfer matrix

$$T = U\Lambda U^\dagger$$

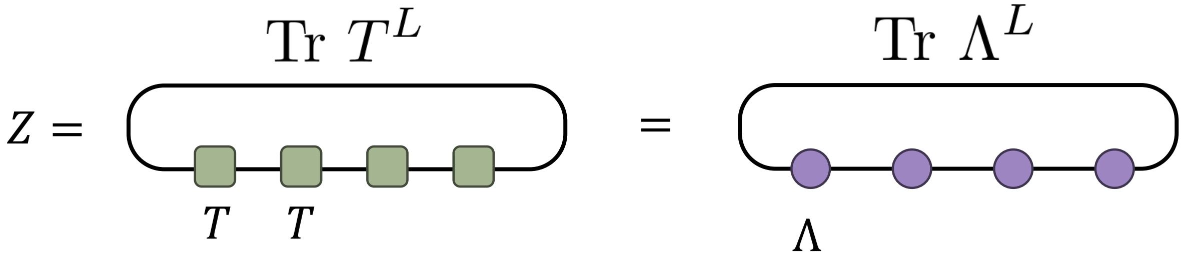


$$\Lambda = \begin{pmatrix} 2\cosh K & 0 \\ 0 & 2\sinh K \end{pmatrix}$$

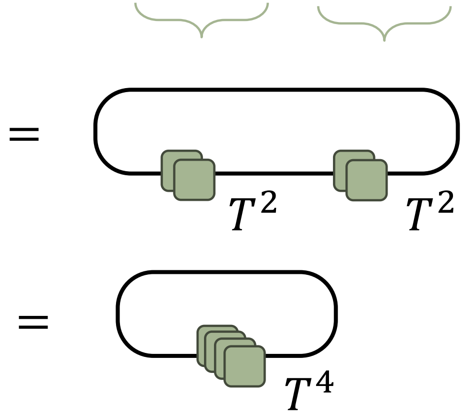
$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

Unitary matrix

$UU^\dagger = I$



$$= (2\cosh K)^L + (2\sinh L)^L$$



coarse-graining

Free energy per site in thermodynamic limit

$$-\beta f = \lim_{L\to\infty} \frac{1}{L} \ln Z = 2\cosh K$$

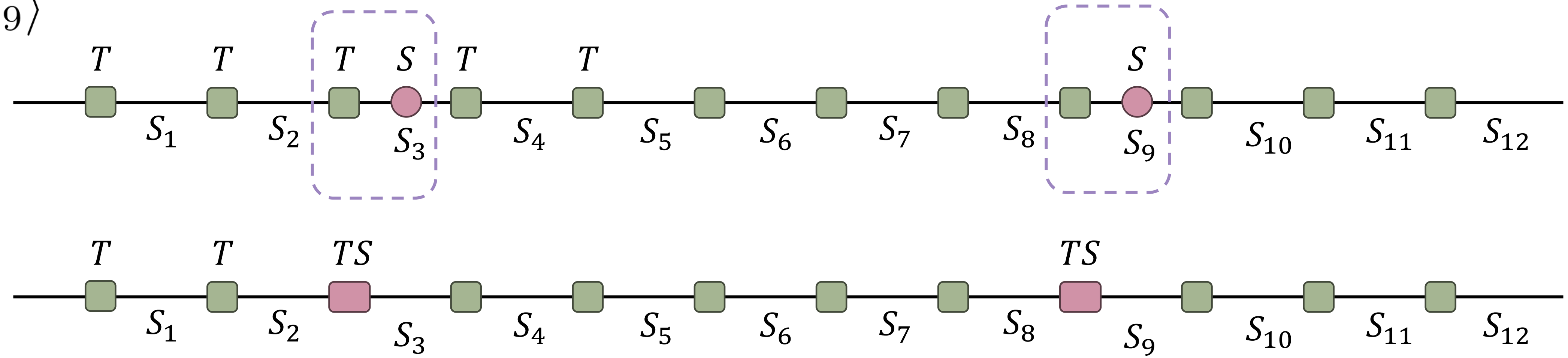
Spin-spin correlation function

$$\langle S_i S_{i+r} \rangle = \frac{\sum_{\{S_j\}} S_i S_{i+r} e^{-\beta H}}{Z} = \frac{\mathrm{Tr}\ T^i\, S\, T^r\, S\, T^{L-i-r}}{\mathrm{Tr}\ T^L} = (\tanh K)^r$$

$$S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Exponential decay for $K < \infty$
No magnetic order

$\langle S_3 S_9 \rangle$



Some tensors are replaced by other tensors corresponding to physical observables.

“impurity method”

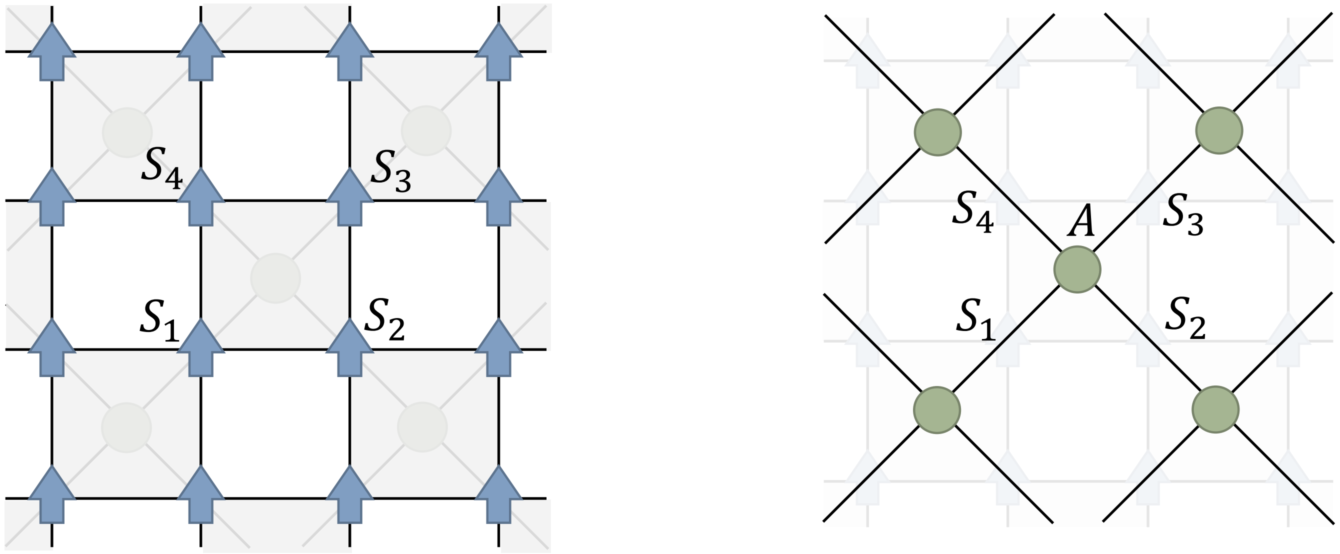
TN approach for 2D models

1. TN representations of partition function
2. Contraction of TN
3. Evaluation of physical quantities

TN representation of the partition function

$$Z = \sum_{\{\sigma_i\}} \prod_{ij} e^{K\sigma_i\sigma_j} = \mathrm{tTr}\left(\bigotimes_{x=1}^{N} A\right)$$

Sum over states   Tensor contraction



Ising model $A_{S_1S_2S_3S_4} = e^{K(S_1S_2+S_2S_3+S_3S_4+S_4S_1)}$

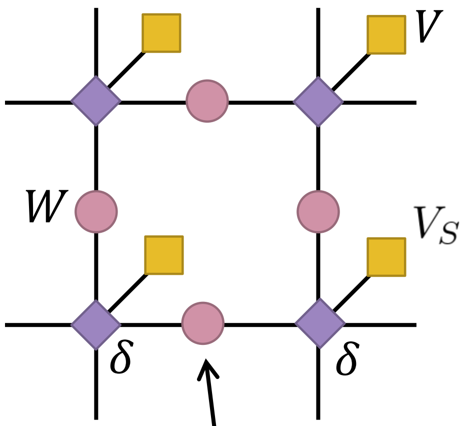
- Tensor index corresponds to spin direction.
- One tensor contains two spin.
- In higher dimensional systems, a tensor has many indices (=2^d).

TN representation of the partition function

$$H = \sum_{\langle ij \rangle} h_2(S_i, S_j) + \sum_{i=1}^{N} h_1(S_i)$$

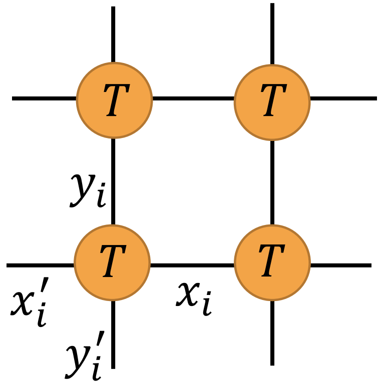
$$Z = \sum_{\{S_i\}} \prod_{\langle ij \rangle} W_{S_i, S_j} \prod_{i=1}^{N} V_{S_i} = \mathrm{tTr} \prod_{i=1}^{N} T_{x_i y_i x_i' y_i'}$$

Sum over states Tensor cont.

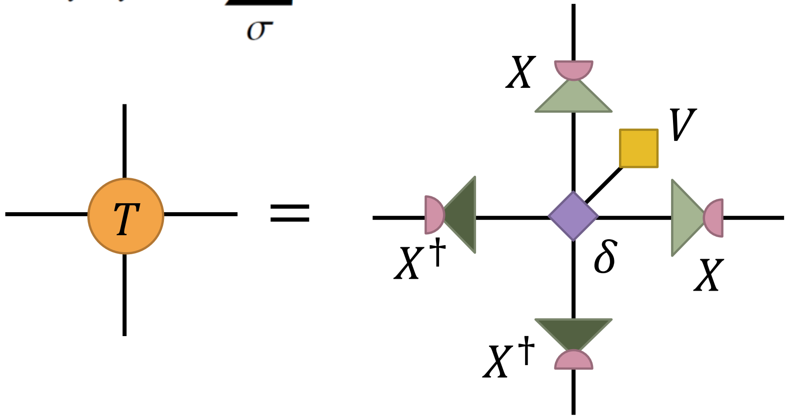


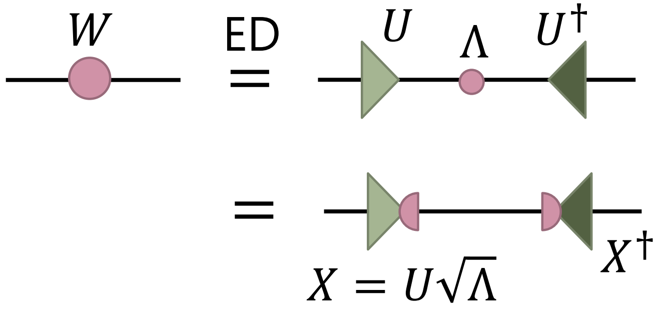
$V_S = e^{-\beta h_1(S)}$

$W_{S,S'} = e^{-\beta h_2(S,S')}$



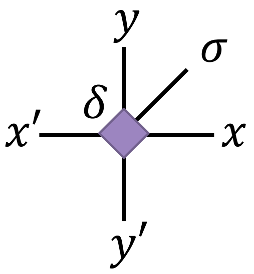
$$T_{xyx'y'} = \sum_{\sigma} X_{\sigma x} X_{\sigma y} X^*_{\sigma x'} X^*_{\sigma y'} V_\sigma$$





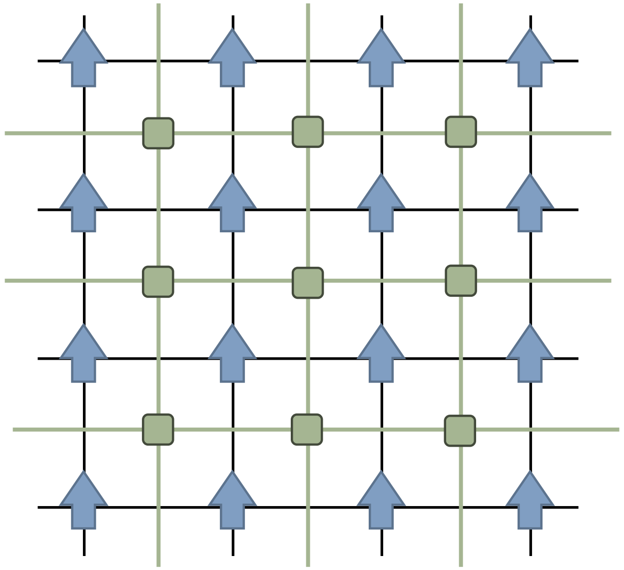
Kronecker's delta

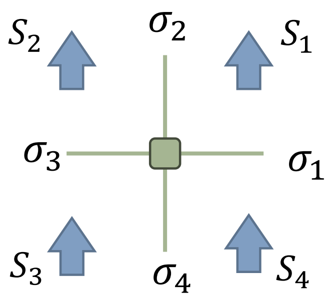
$$\delta^{\sigma}_{xyx'y'} = \delta_{\sigma x} \delta_{\sigma y} \delta_{\sigma x'} \delta_{\sigma y'}$$



- TN structure is the same as original lattice.
- Bond index is index of eigenvalue.
- Spin is already traced out.
- # of indices is $2d$ in a d-dimensional system.

TN representation on dual lattice (dual representation)





$$= \delta_{\sigma_1\sigma_2\sigma_3\sigma_4,1}\ e^{K(\sigma_1+\sigma_2+\sigma_3+\sigma_4)/2} = T_D$$

$\sigma_1 = S_1 S_4,$
$\sigma_2 = S_1 S_2, \ldots$

$$\sigma_1\sigma_2\sigma_3\sigma_4 = (S_1S_2S_3S_4)^2 = 1$$

Kramers-Wannier duality

$$Z \propto Z_D$$

$$Z = \sum_{\{n_i\}} \prod_{\langle i,j\rangle} \underline{f(n_i - n_j)}$$

Fourier transformation

$$Z_D = \sum_{\{m_k\}} \prod_{\langle k,l\rangle_D} \underline{\tilde{f}(m_k - m_l)}$$

original rep.

dual rep.

original rep.

$$Z = \frac{q^N}{q^{N_B/2}} \sum_{\{m_{ij}\}} \prod_{i=1}^{N} \underbrace{\left[\delta^{(q)}_{\partial_i m,0} \left(\prod_{j\in\partial_i} \underline{\tilde{f}(m_{ij})^{1/2}}\right)\right]}_{T}$$

$$Z = q \sum_{\{n_{kl}\}} \prod_{k=1}^{N_D} \underbrace{\left[\delta^{(q)}_{\partial_k n,0} \prod_{l\in\partial_k} \underline{f(n_{kl})^{1/2}}\right]}_{T_D}$$

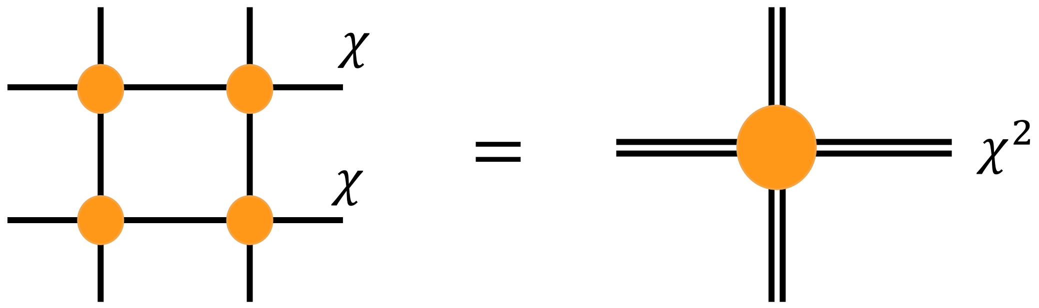
K. Homma, SM, N. Kawashima, arXiv:2403.17309

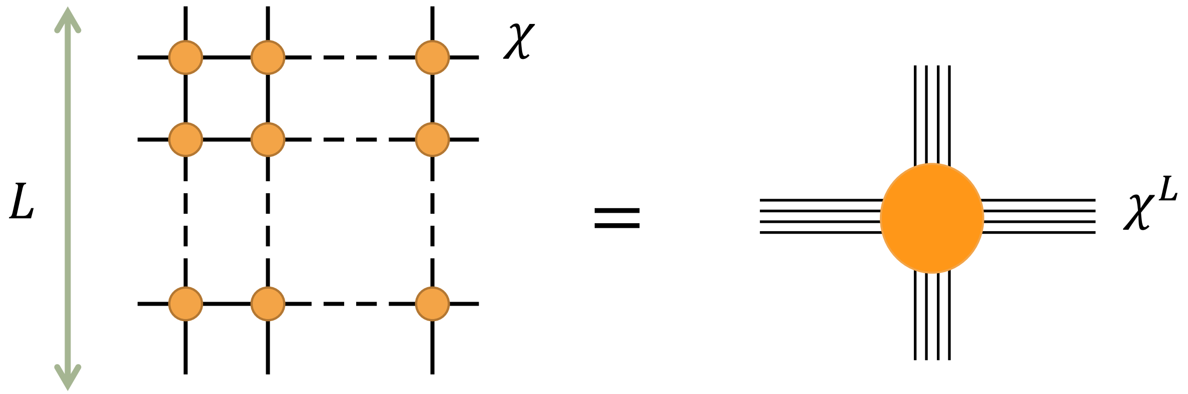
TN approach for 2D models

1. TN representations of partition function
2. Contraction of TN
3. Evaluation of physical quantities

Necessity of information compression

- Exact contraction still requires exponential cost.





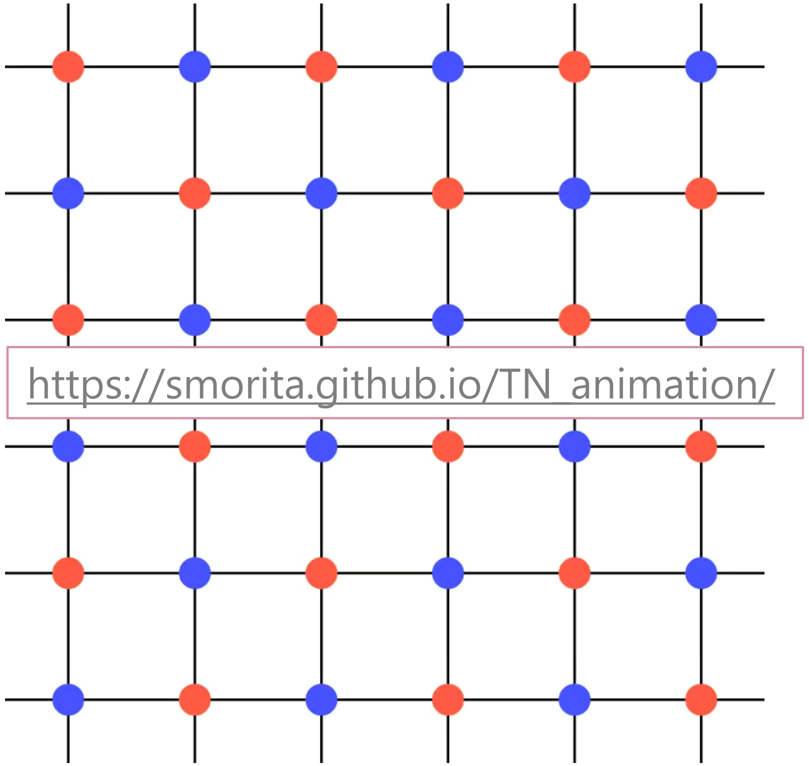
$$Z=\sum_{\{\sigma_i\}}\prod_{ij}e^{K\sigma_i\sigma_j}=\mathrm{tTr}\left(\bigotimes_{x=1}^{N}A\right)\quad\simeq ?$$

Sum over states Tensor contraction

Real-space renormalization approach

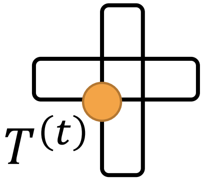
- TRG (Tensor Renormalization Group)

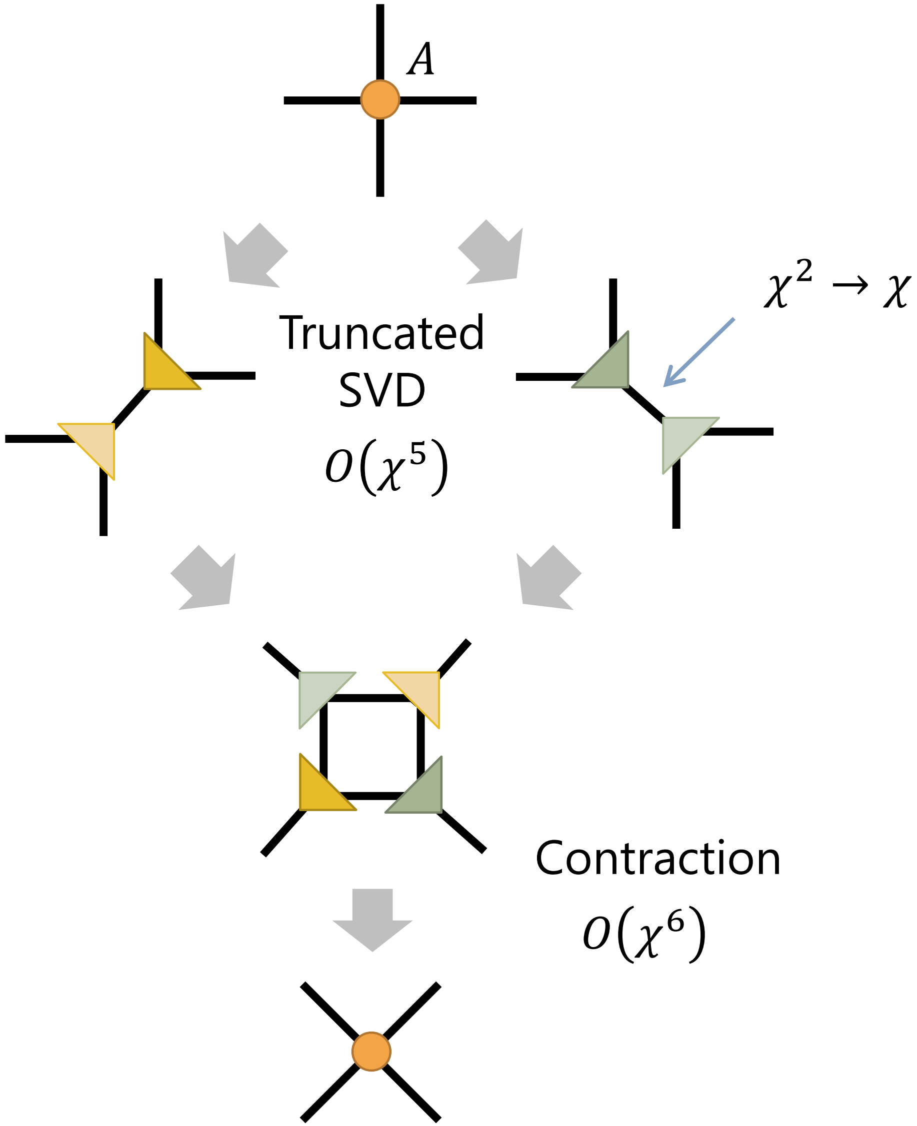
  Levin, Nave, Phys. Rev. Lett. **99**, 120601 (2007)



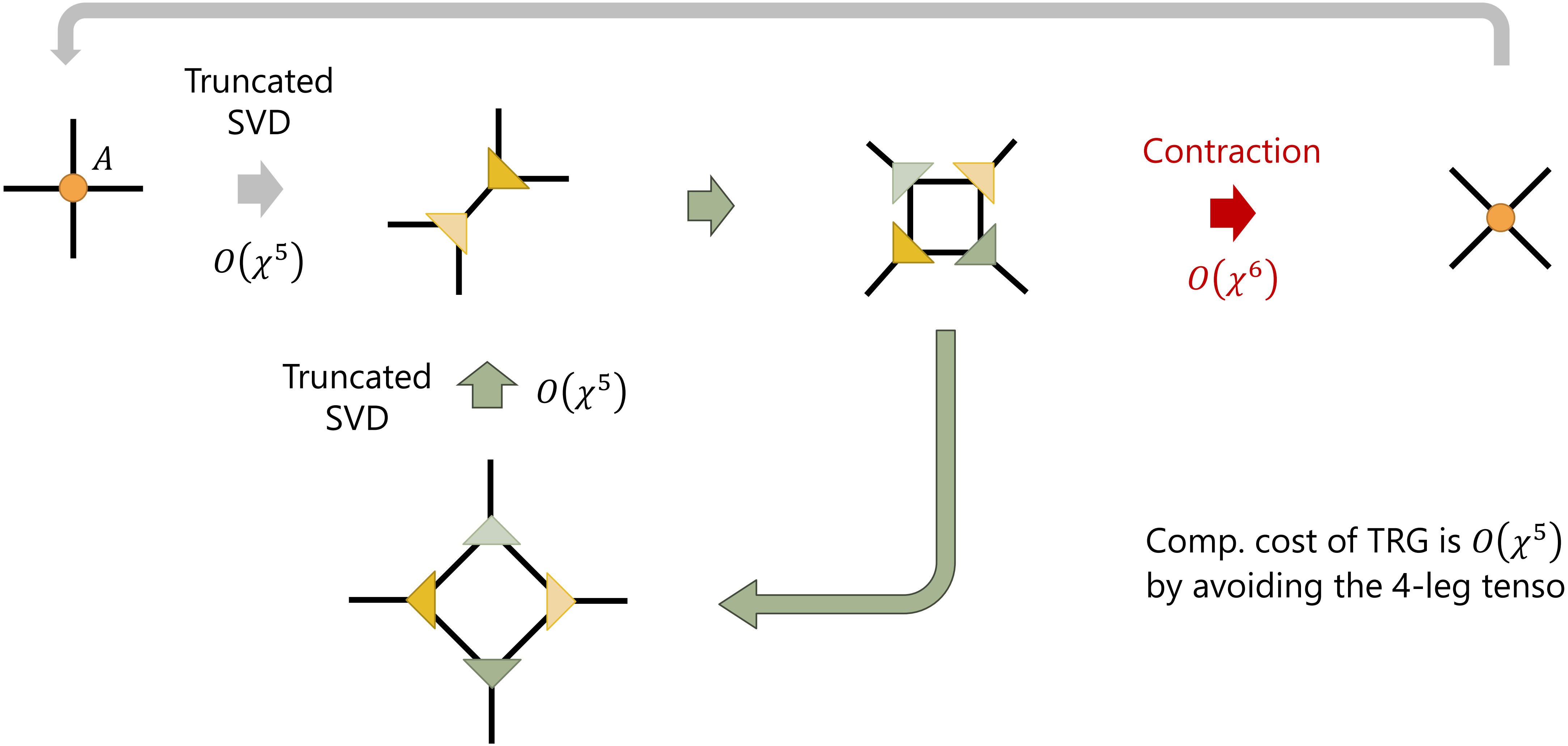
https://smorita.github.io/TN_animation/

$$Z_N \simeq \mathrm{Tr}\, T^{(t)} = \sum_{i,j} T^{(t)}_{ijij} =$$





Reduction of computational cost for TRG



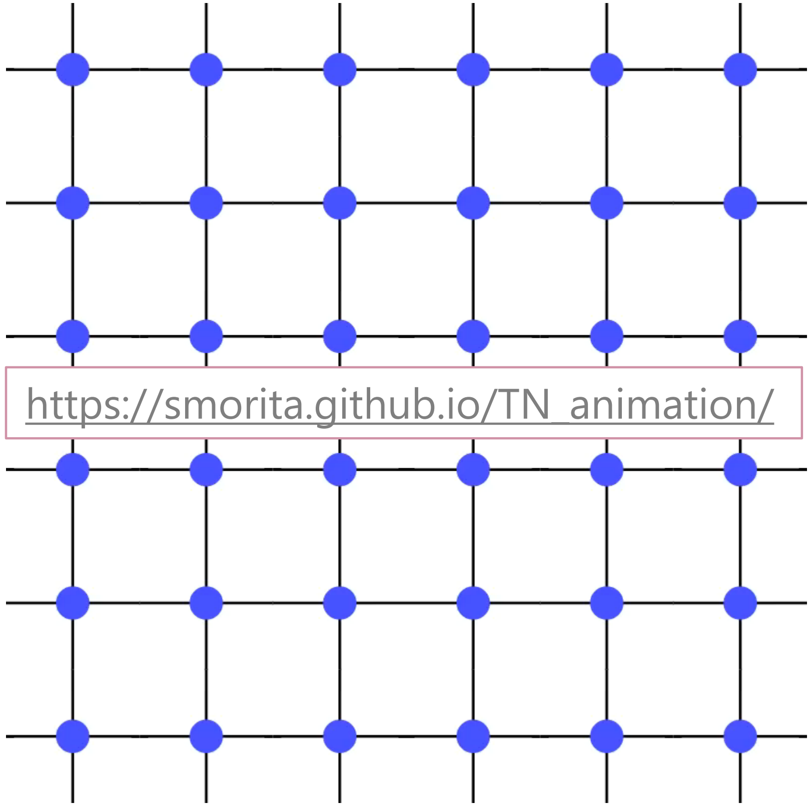
Comp. cost of TRG is $O(\chi^5)$
by avoiding the 4-leg tensors.

TRG with randomized SVD SM, Igarashi, Zhao, Kawashima, PRE **97**, 033310 (2018)

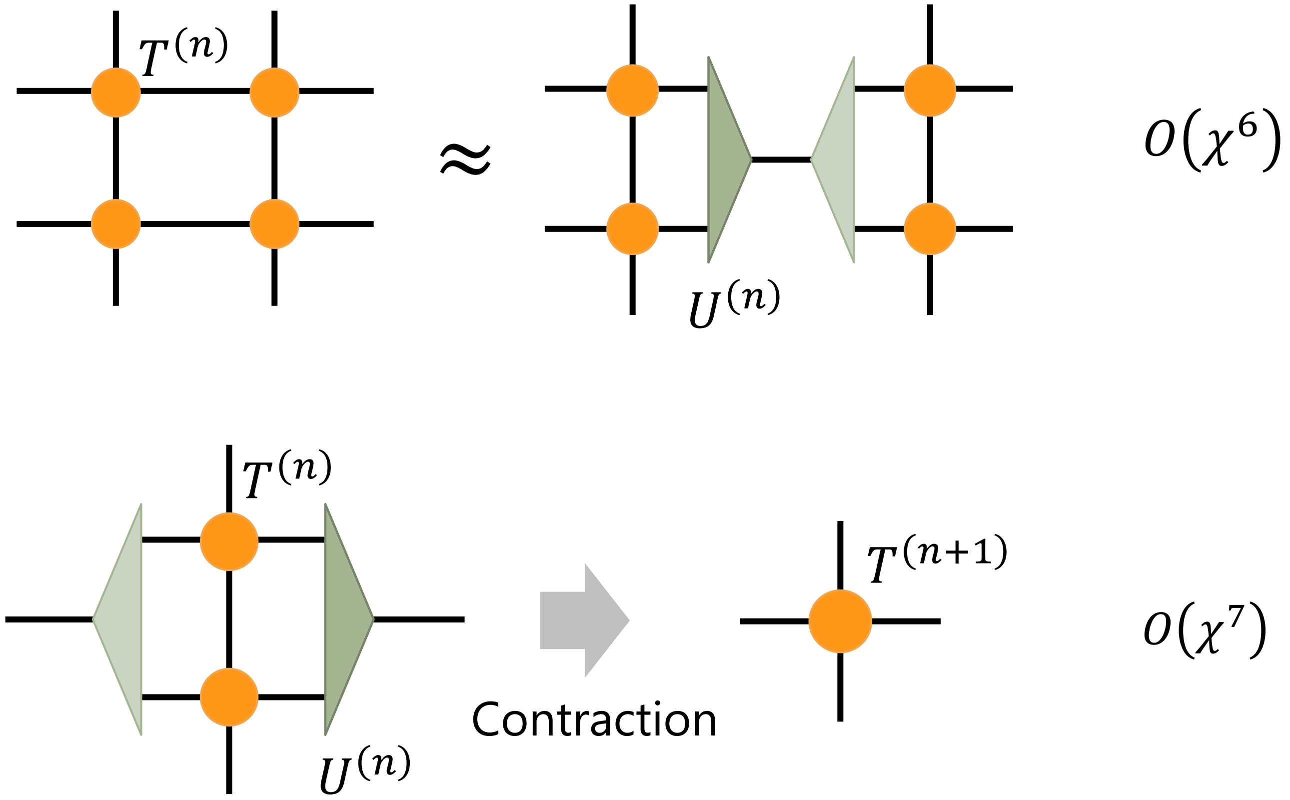
Real-space renormalization approach

- HOTRG (Higher-order Tensor Renormalization Group)

  Xie, et al., PRB **86**, 045139 (2012)



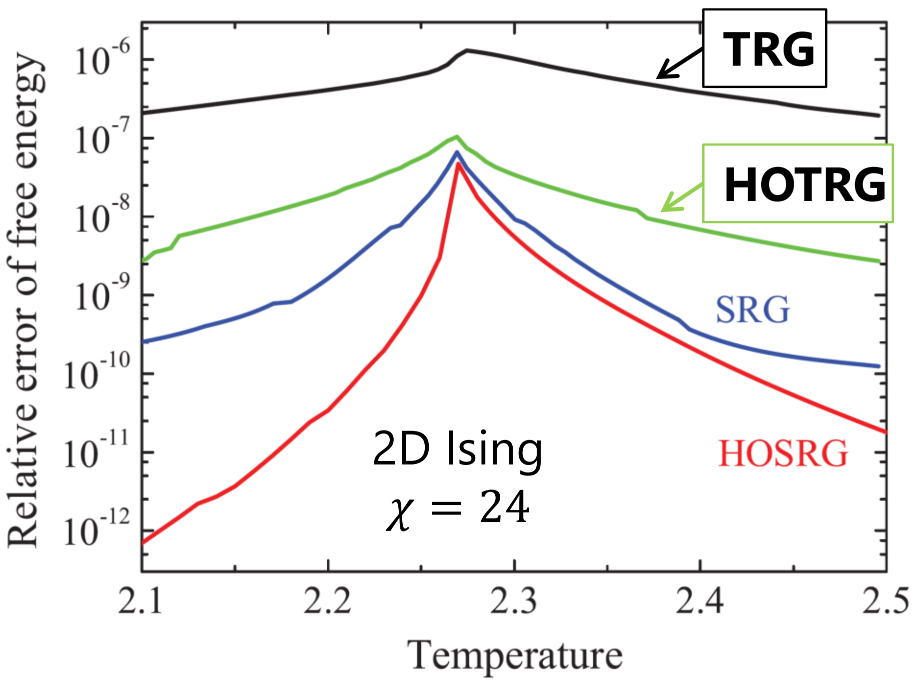
https://smorita.github.io/TN_animation/



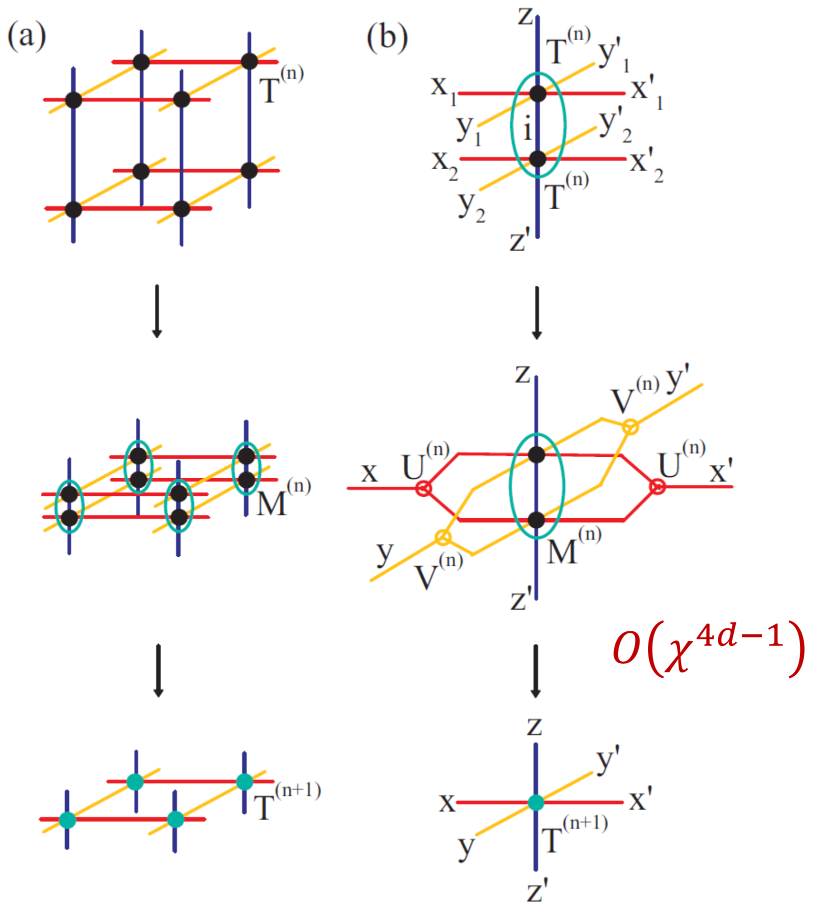
Construction of oblique projectors Iino, SM, Kawashima: Phys. Rev. B **100**, 035449 (2019)

Advantage of HOTRG

➢ Accuracy



➢ Higher-dimensional systems



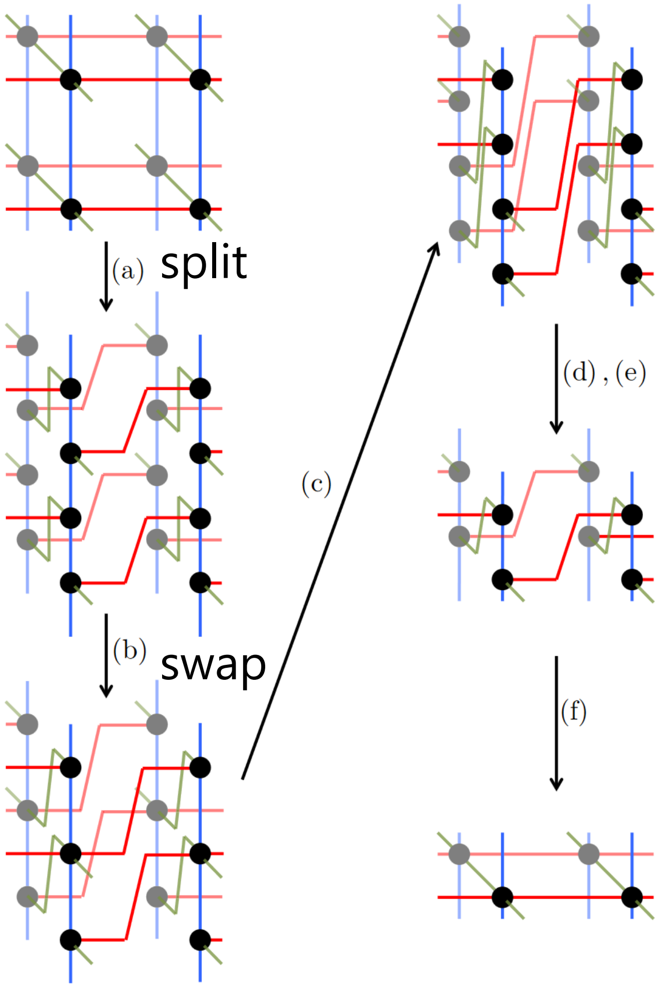
➢ Conservation of lattice structure

➢ No tensor decomposition

TRG variants for higher-dimensional systems

◻ Anisotropic TRG (ATRG)

Adachi, Okubo, Todo, PRB **102**, 054432 (2020)

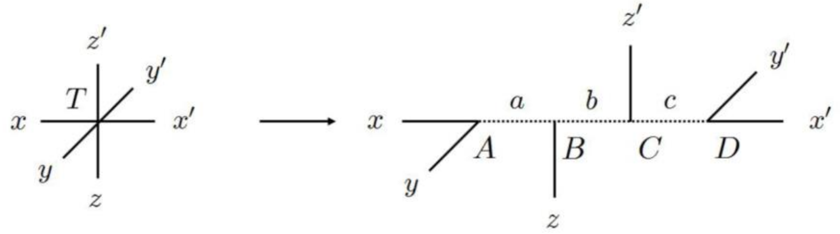


(d+1)-leg

$O(\chi^{2d+1})$

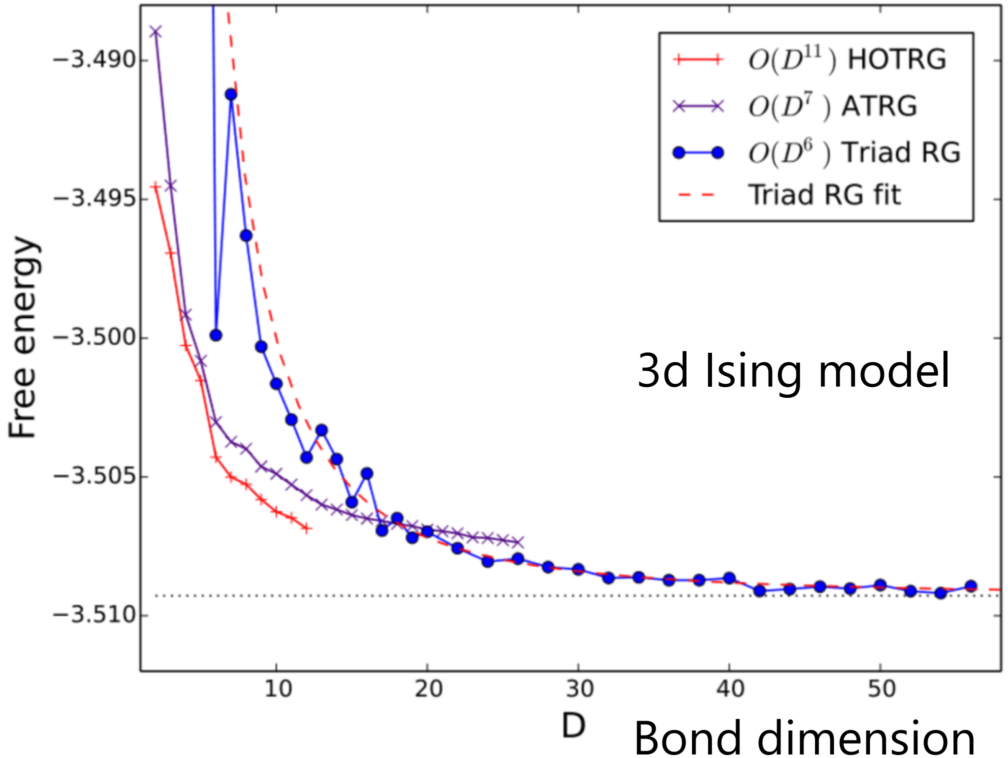
◻ Triad TRG

Kadoh, Nakayama, arXiv:1912.02414



triad = 3-leg

$O(\chi^{d+3})$

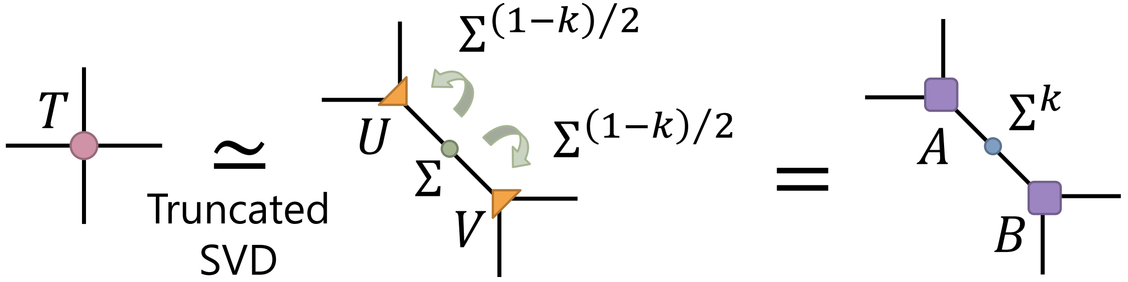


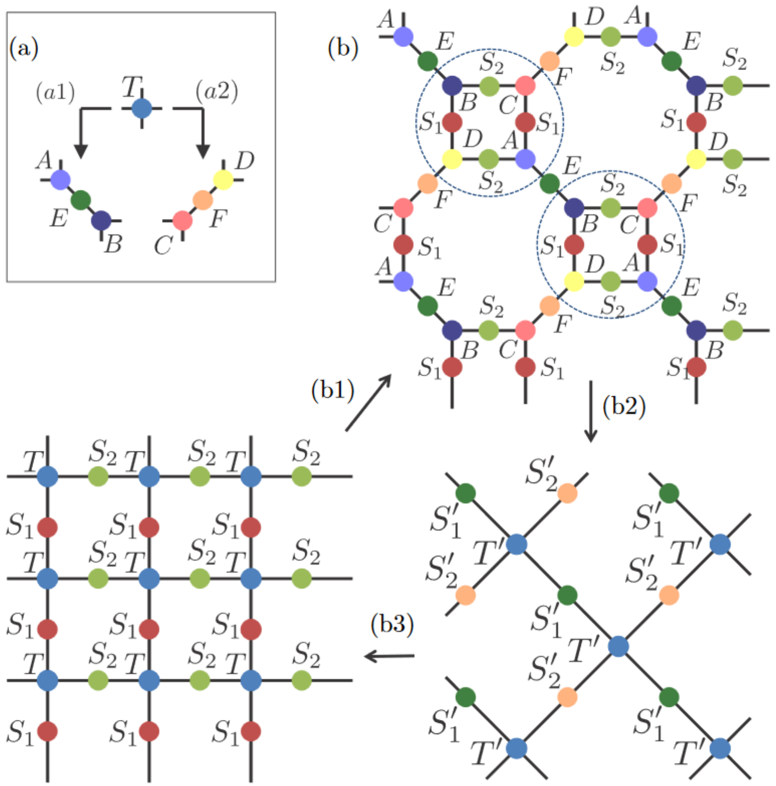
3d Ising model

Bond dimension

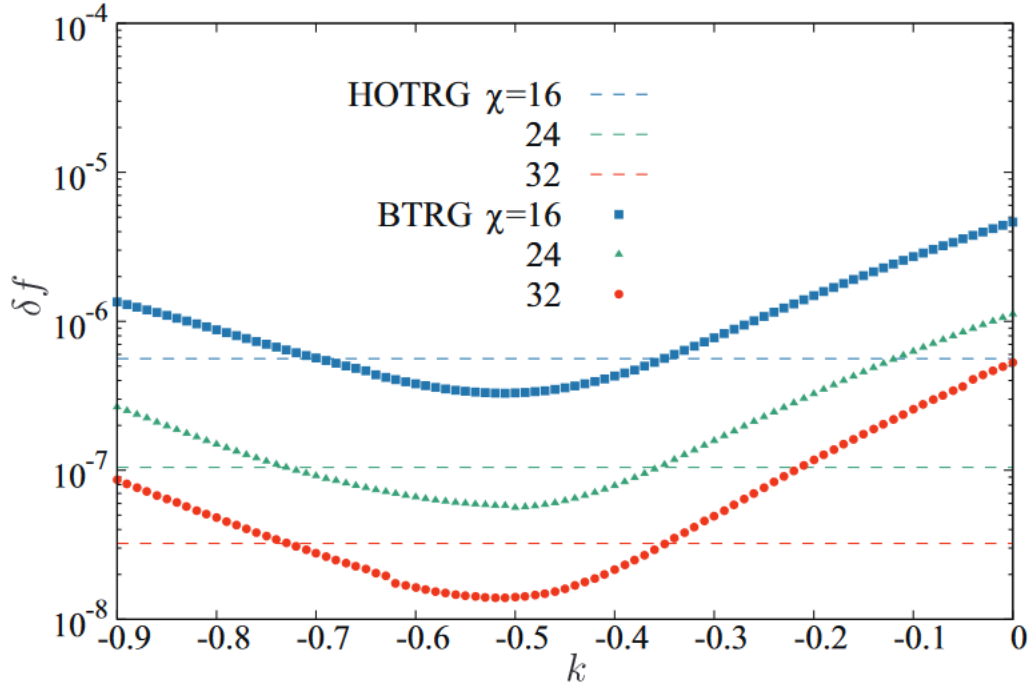
Bond-Weighted Tensor Renormalization Group (BWTRG)

Adachi, Okubo, Todo, PRB **105**, L060402 (2022)





- **Hyperparameter k**
  - $k = 0$: original TRG (no bond-weight)
  - $k = -1/2$: Expected optimal value

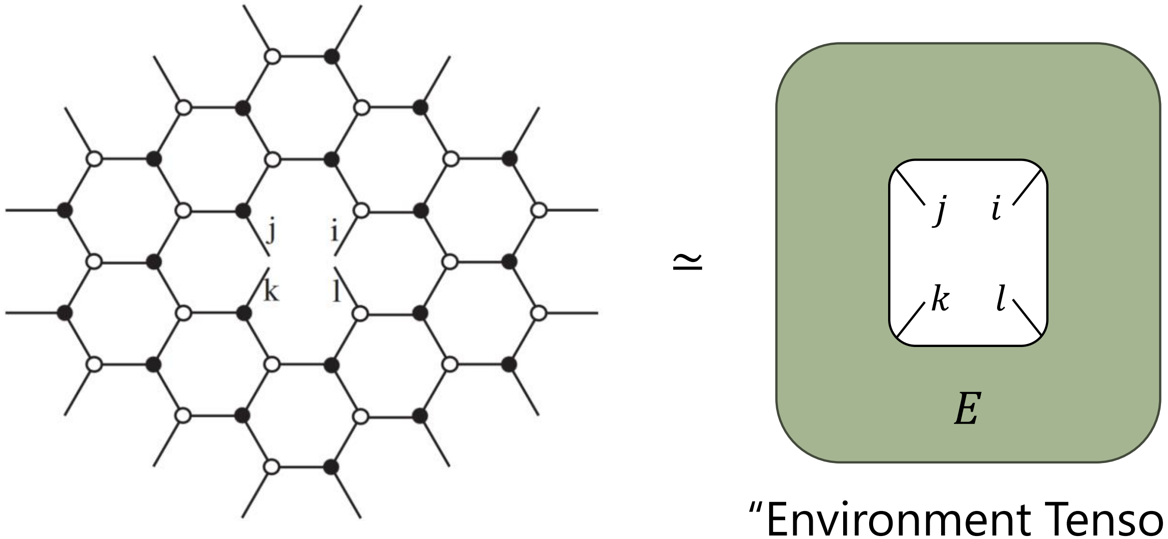


- ✓ Its computational cost is the same order as TRG $O(\chi^5)$
- ✓ It is **more accurate** than TRG and HOTRG.

Further improvements of TRG

Global optimization using environment

- Second Renormalization Group (SRG)
  Xie, et al., PRL **103**, 160601 (2009)

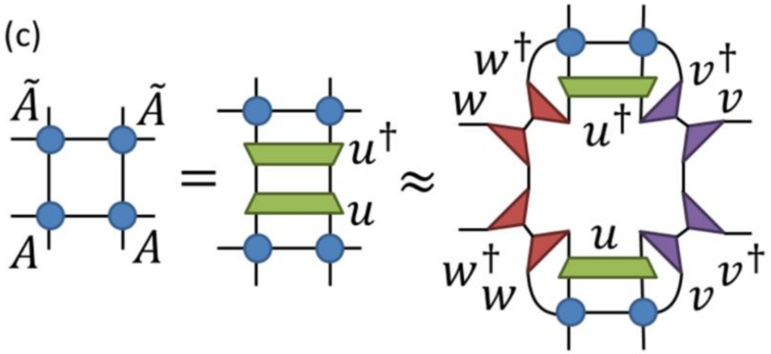


"Environment Tensor"

- HOSRG Xie, et al. PRB (2012)
- CTM-TRG SM, Kawashima, PRB (2021)
- Triad-SRG Kadoh, Oba, Takeda, JHEP (2022)

Entanglement filtering

- Tensor Network Renormalization (TNR)
  Evenbly, Vidal, PRL **115**, 180405 (2015)



"Disentangler" u removes short-range entanglement in a loop

- Loop TNR Yang, Gu, Wen, PRL (2017)
- Graph-Independent Local Truncation (GILT)
  Hauru, et al., PRB (2018)
- Entanglement branching Harada, PRB (2018)
- Nuclear-norm regularization
  Homma, Okubo, Kawashima, Phys. Rev. Research (2024)

TN approach for 2D models

1. TN representations of partition function
2. Contraction of TN
3. Evaluation of physical quantities

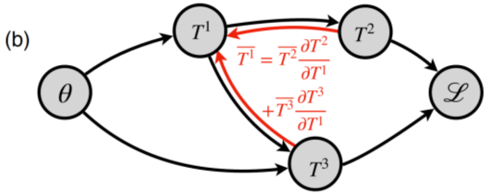
Evaluation of physical quantities

1. Derivative of free energy

magnetization $\langle m \rangle = -\dfrac{\partial f}{\partial h}$

$$\frac{\partial f}{\partial h} \simeq \frac{f(h+\delta h) - f(h)}{\delta h}$$

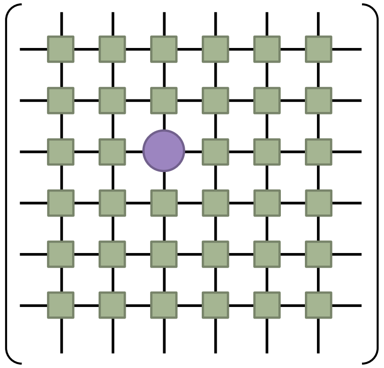
- Numerical differentiation
- Automatic differentiation (AD)
  Liao, et al, PRX (2019)



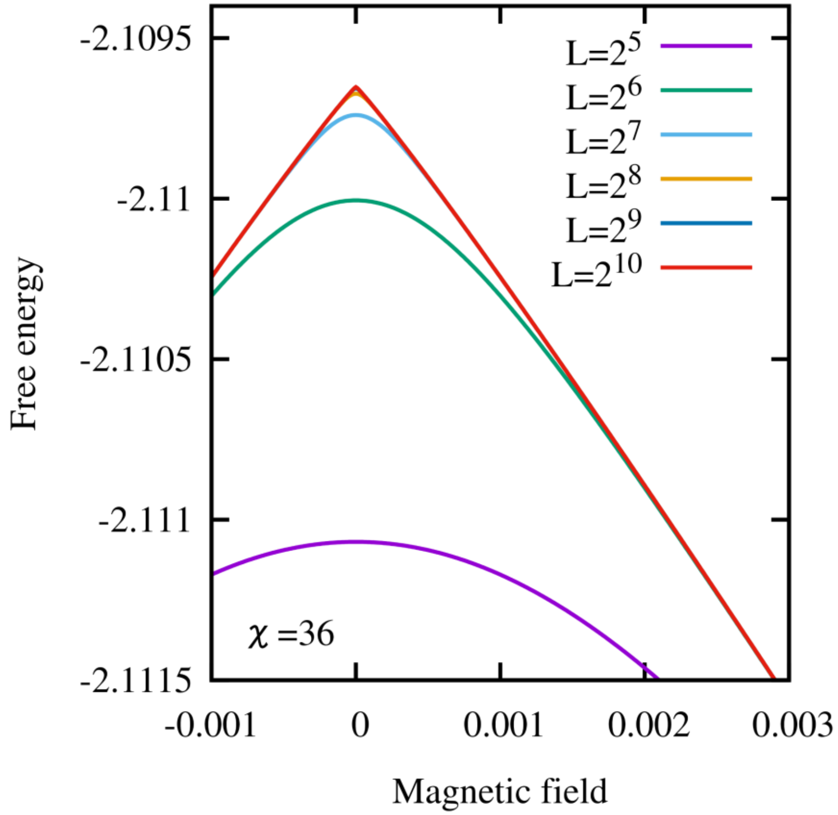
"Reverse-mode AD"

2. Impurity method

$$\mathrm{Tr}\, S_i\, e^{-\beta H} = \mathrm{tTr}$$



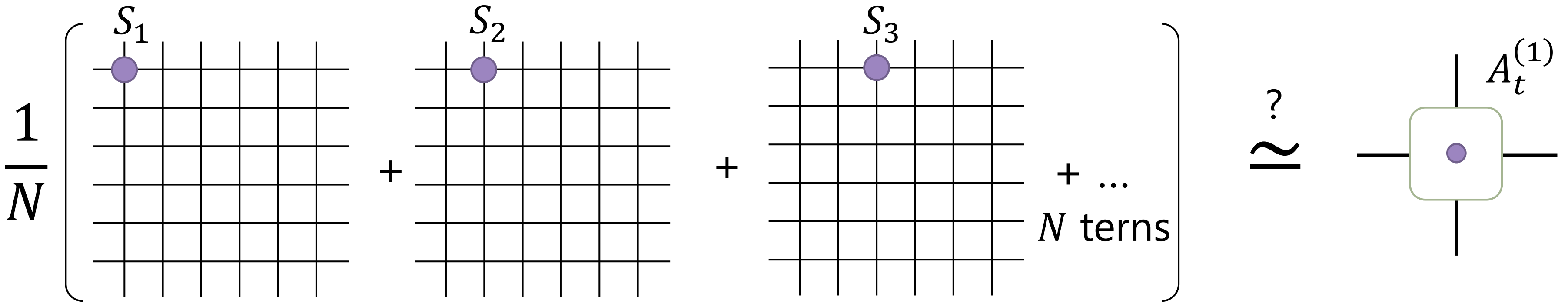
2D Ising model, $T = T_c$



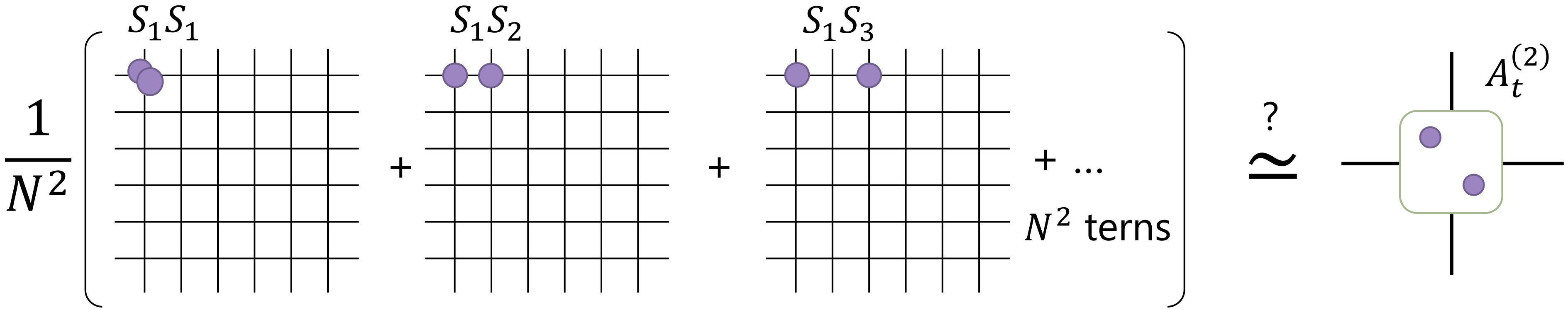
Multi-point correlations are necessary for high-order moments $\langle m^n \rangle$.

Multipoint correlation functions

- 1^{st}-order moment $\left\langle \frac{1}{N}\sum_{i=1}^{N} S_i \right\rangle$ "average of the local operators"



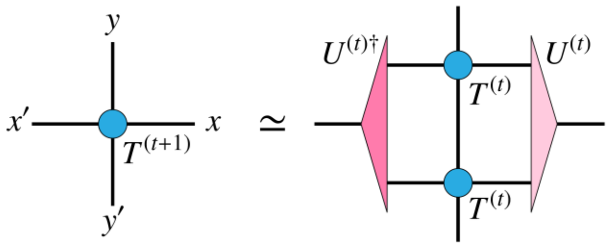
- 2^{nd}-order moment $\left\langle \frac{1}{N^2}\sum_{i,j} S_i S_j \right\rangle$ "average of all possible 2-point correlation functions"



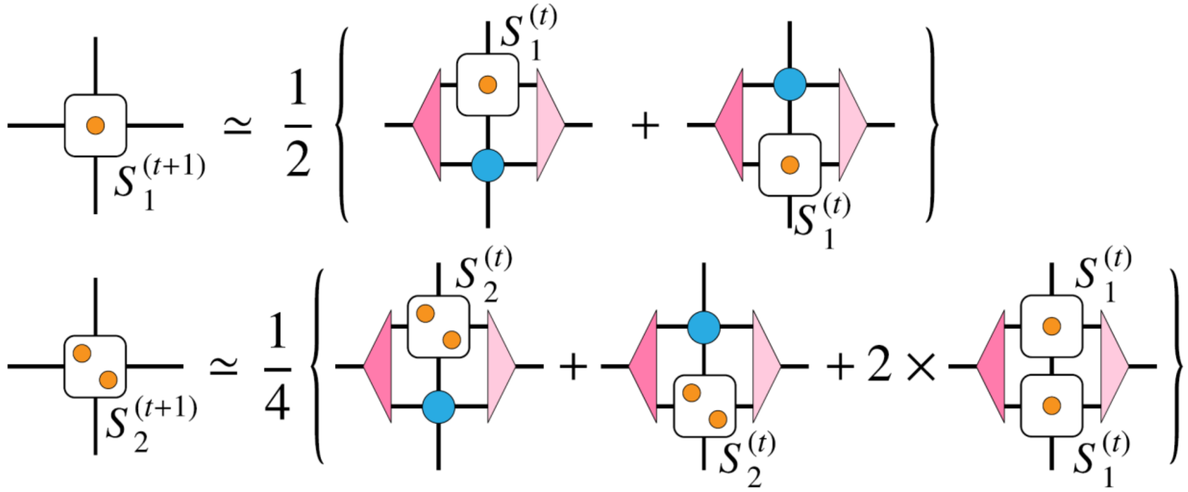
We calculate the renormalized tensor of the summation of multipoint correlation functions

Renormalization of multi-impurity tensors in HOTRG

SM, Kawashima, Comput. Phys. Comm **236**, 65 (2019)

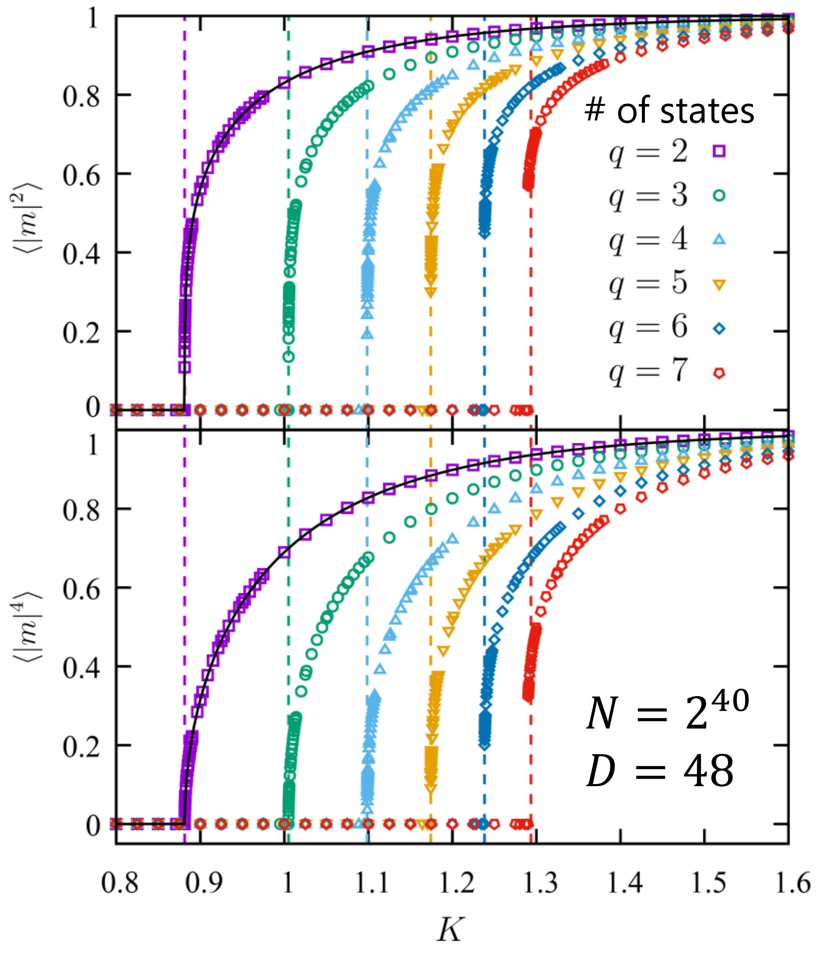


- Recursion formula of multi-impurity tensors



Use the same projector

Magnetization of Potts model

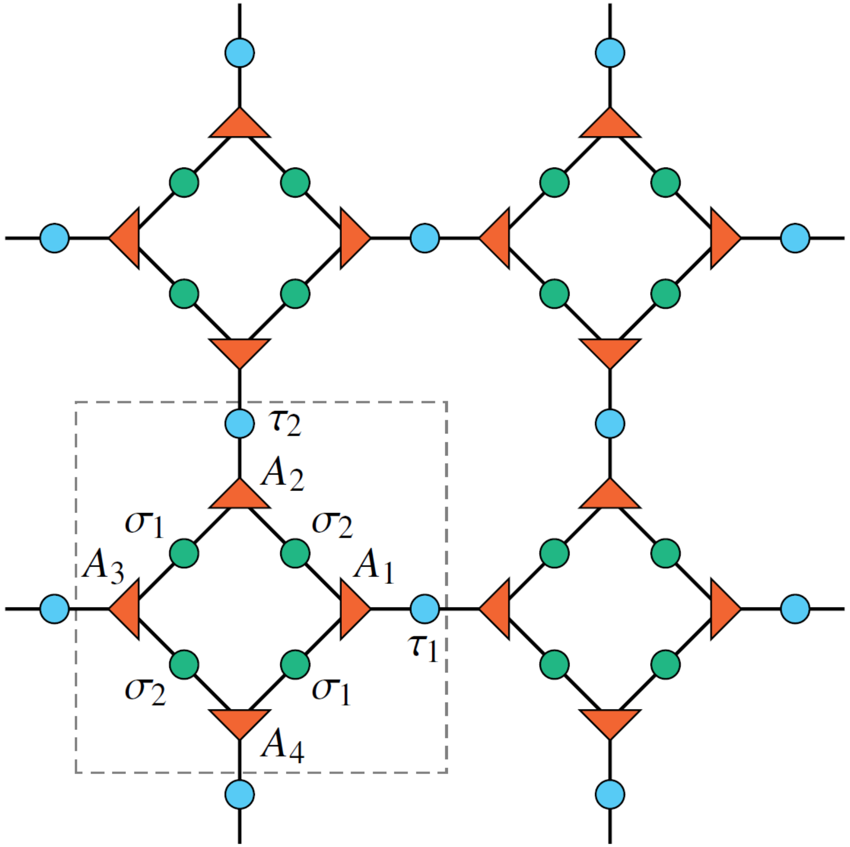


Would this approach be possible in BWTRG?

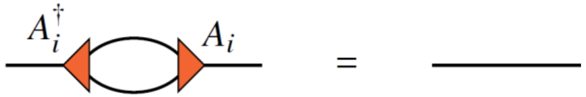
Multi-impurity method for Bond-Weighted TRG

SM, Kawashima, arXiv:2411.13998

BWTRG on a triad network

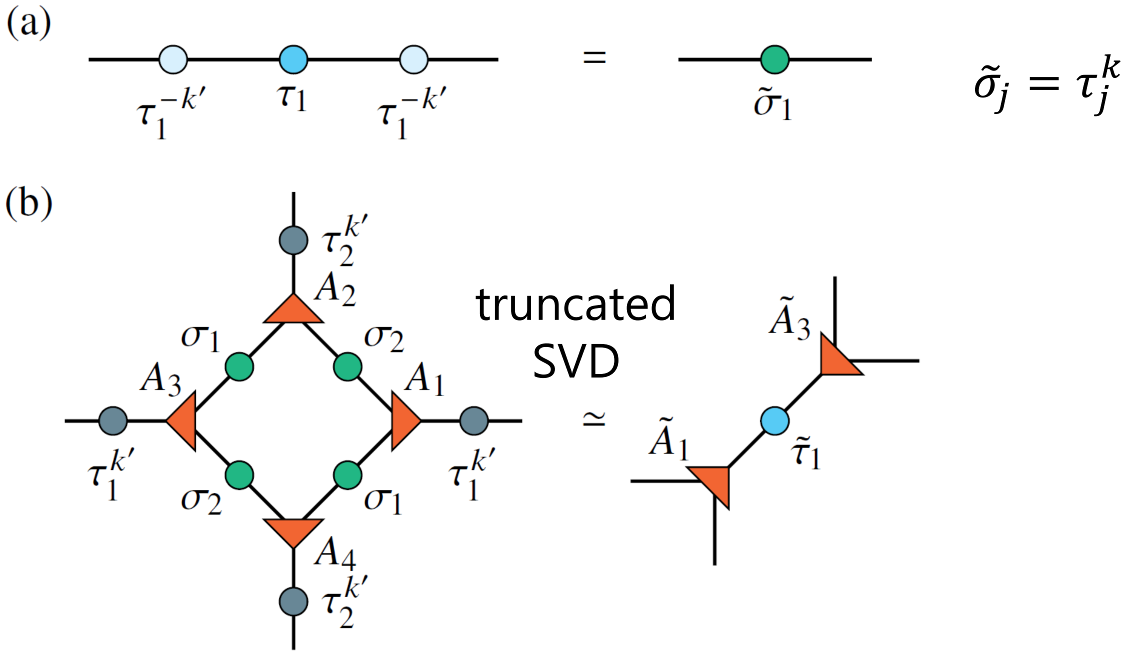


τ_i : "outer" bond-weight (diagonal)
σ_i : "inner" bond-weight (diagonal)
A_i : isometry

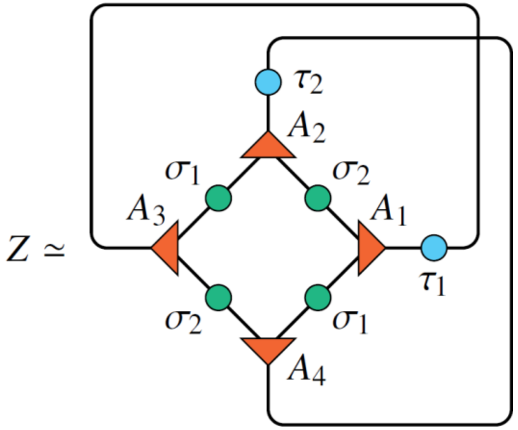


$$k' \equiv \frac{1-k}{2}$$

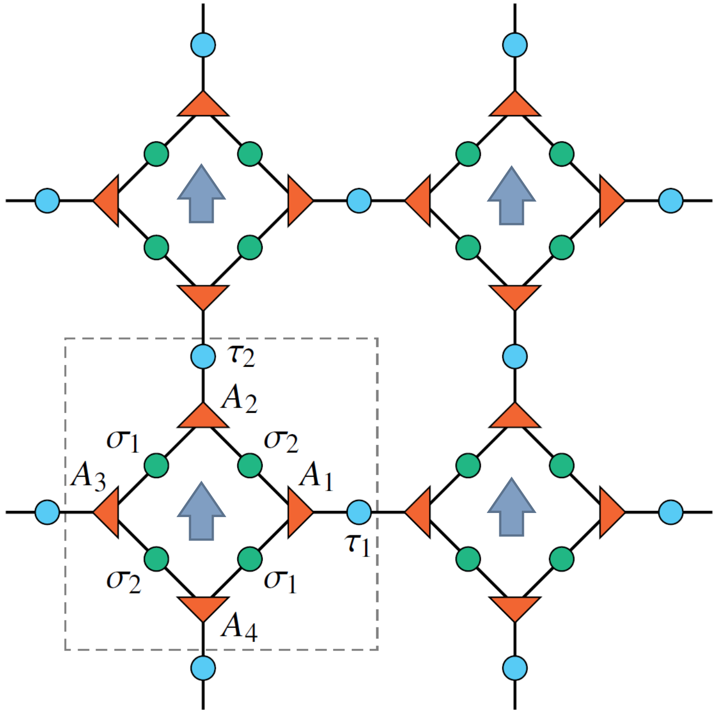
- Update rule



- Partition function



Initial tensors of Ising model w/o magnetic field



$$\tau_i = \begin{pmatrix} e^{K} & e^{-K} \\ e^{-K} & e^{K} \end{pmatrix}$$

$$\sigma_i = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\left(A_j\right)_{abc} = \delta_{ab}\delta_{bc}$$

TN with $\mathbb{Z}_2$ symmetry

$$\tau_i = \begin{pmatrix} 2\cosh K & 0 \\ 0 & 2\sinh K \end{pmatrix}$$

$$\sigma_i = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\left(A_j\right)_{abc} = \begin{cases} 1/\sqrt{2} & (a+b+c = \text{even}) \\ 0 & \end{cases}$$

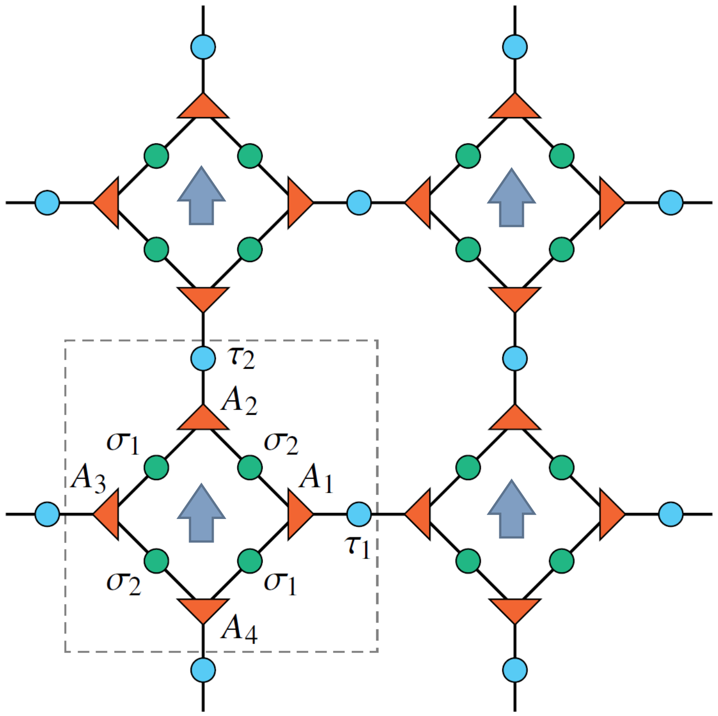
- Ising spins locate at the center of plaquette
- τ_j corresponds to $e^{KS_iS_j}$
- σ_j, A_j carry spin info

Gauge transformation

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

Initial impurity tensors

Local physical quantities are expressed by replacing bond-weights



- Magnetization $$m = \frac{1}{N}\sum_{x=1}^{N} S_x$$

$$S_i \Rightarrow S[m] = U^\dagger \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} U = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

"inner" impurity matrix

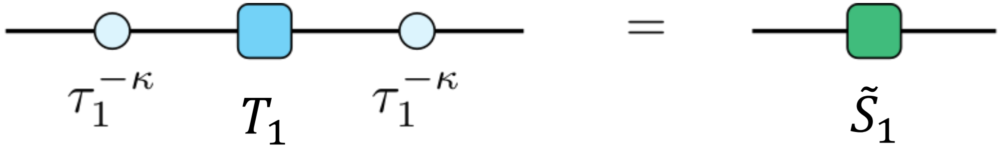
- Energy $$e = -\frac{J}{N}\sum_{\langle xy \rangle} S_x S_y$$

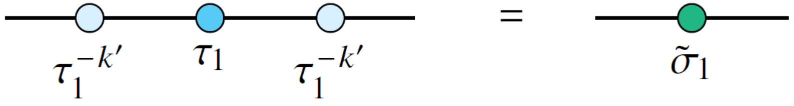
$$-S_i S_j e^{K S_i S_j} \Rightarrow T[e] = \begin{pmatrix} -2\sinh K & 0 \\ 0 & -2\cosh K \end{pmatrix}$$

"outer" impurity matrix

Update rule for impurity tensors

◻ From T to S

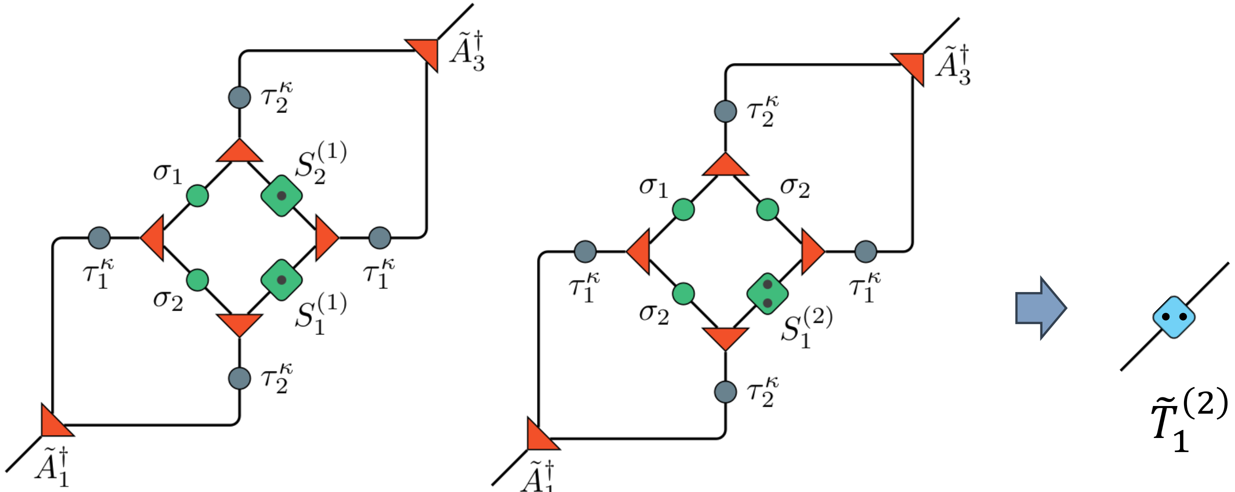




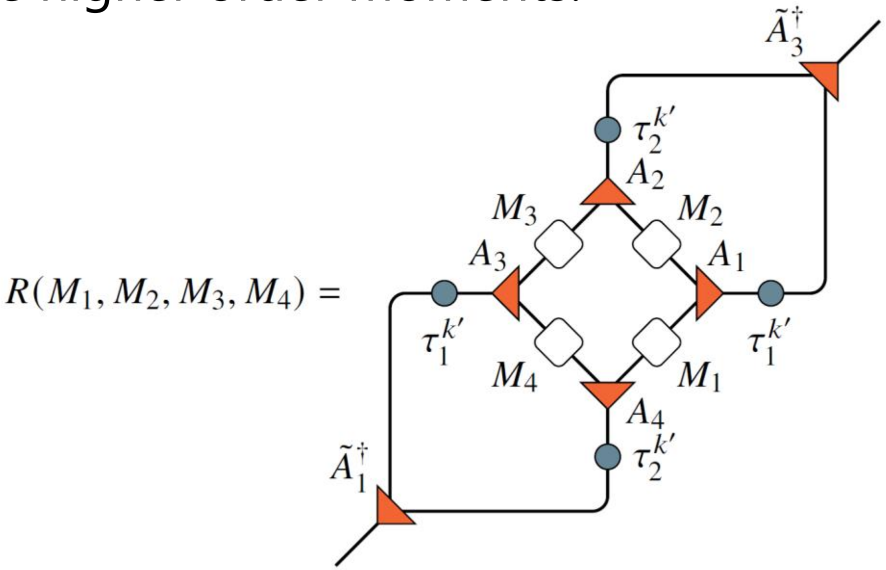
The number of impurities does not change.

◻ From S to T

- ➢ The sum over the possible patterns is necessary to compute the higher order moments.
  - ✓ For the 2nd moment, we need 6+4 patterns.



(6 patterns) (4 patterns)

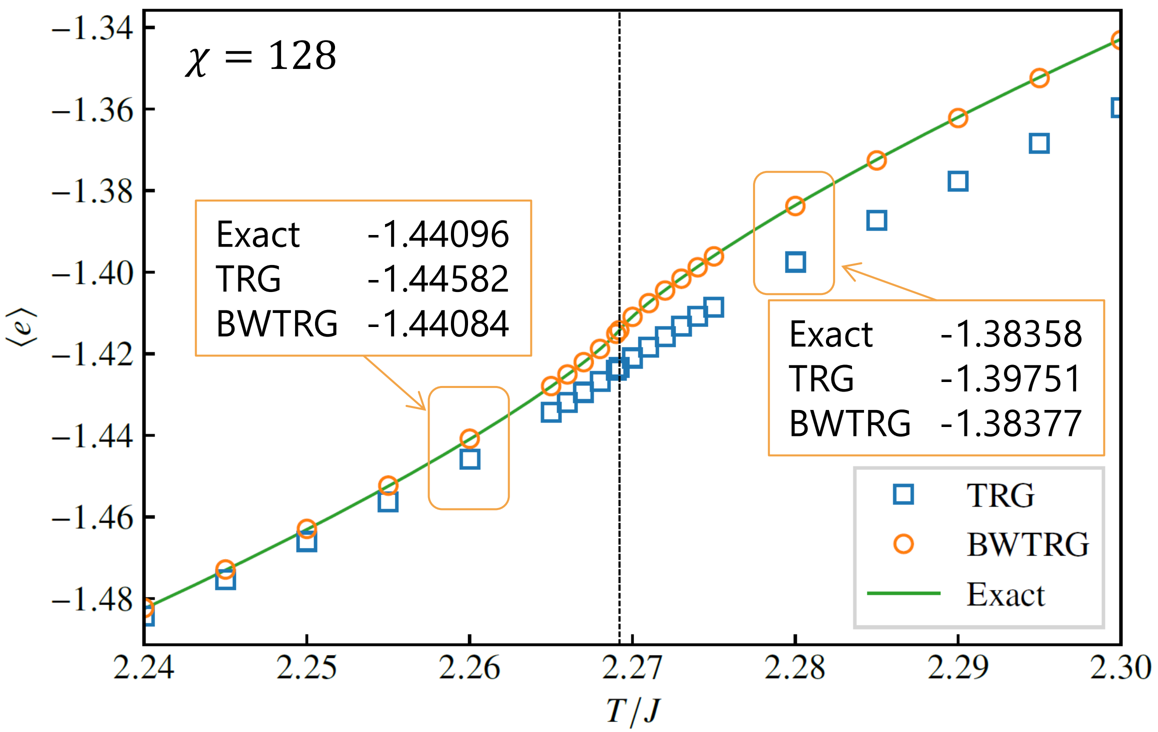


$R(\sigma_1, \sigma_2, \sigma_1, \sigma_2) = \tilde{\tau}_1$

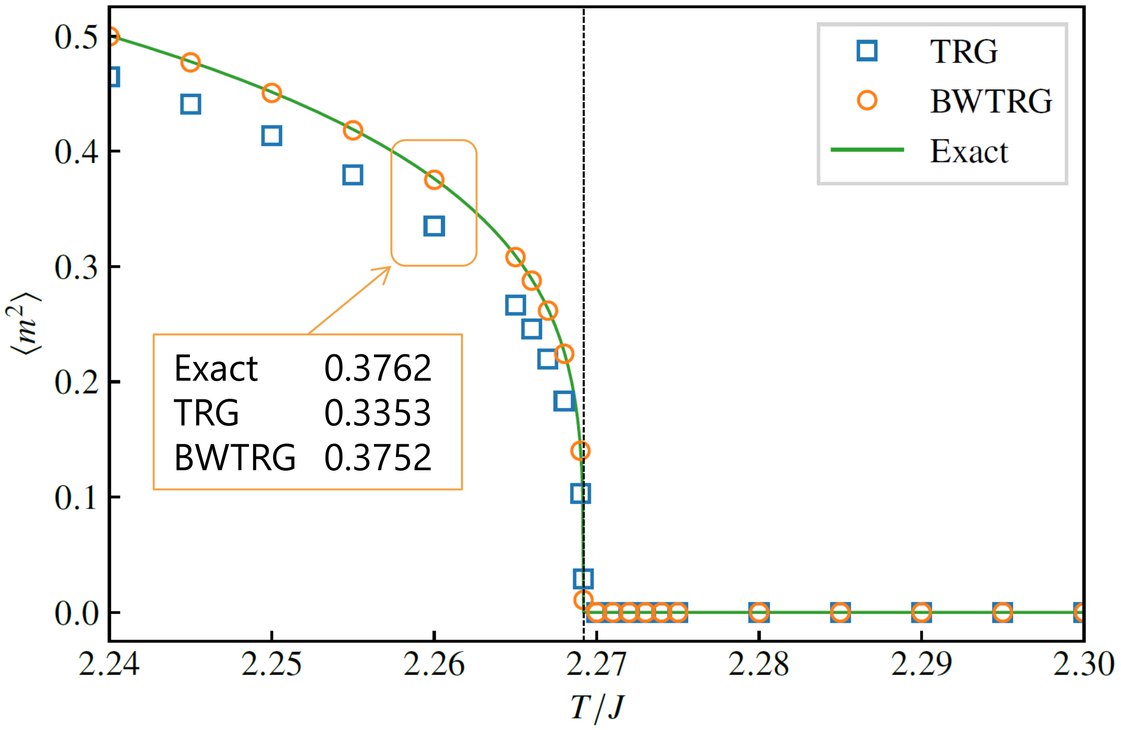
Results: the 2D Ising model

- Physical quantities in the thermodynamic limit

Energy $\langle e \rangle$



Order parameter $\langle m^2 \rangle$



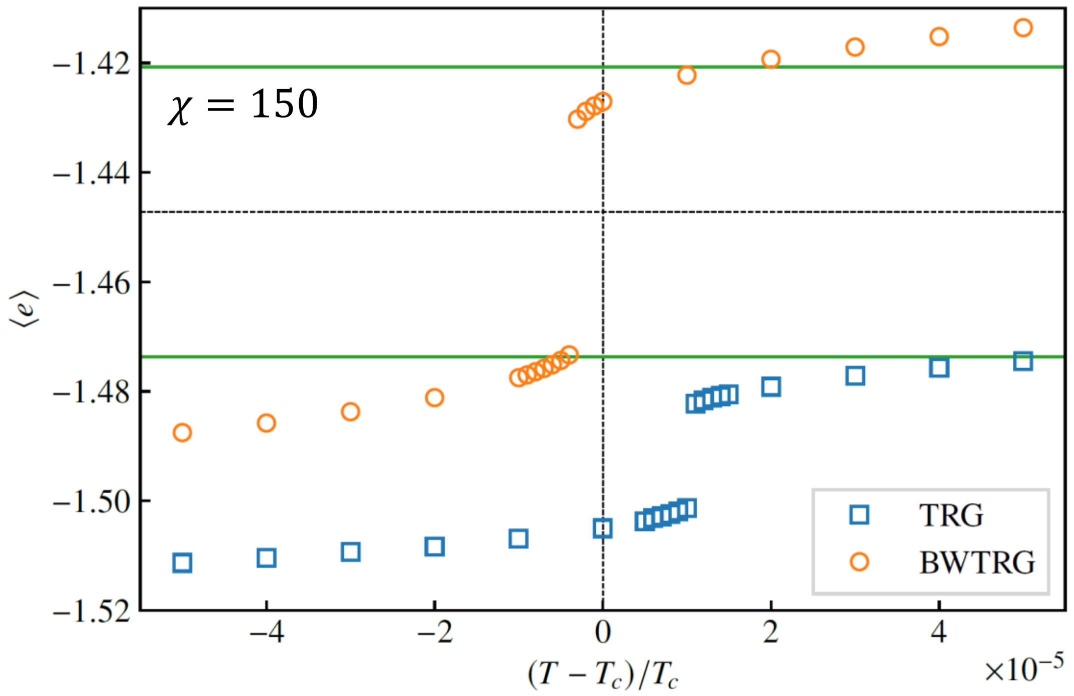
- The relative error for BWTRG is smaller than 2.5% of the relative error for TRG.
- Both BWTRG and TRG have the same computational cost scaled as $O(\chi^5)$.

Results: the 5-state Potts model

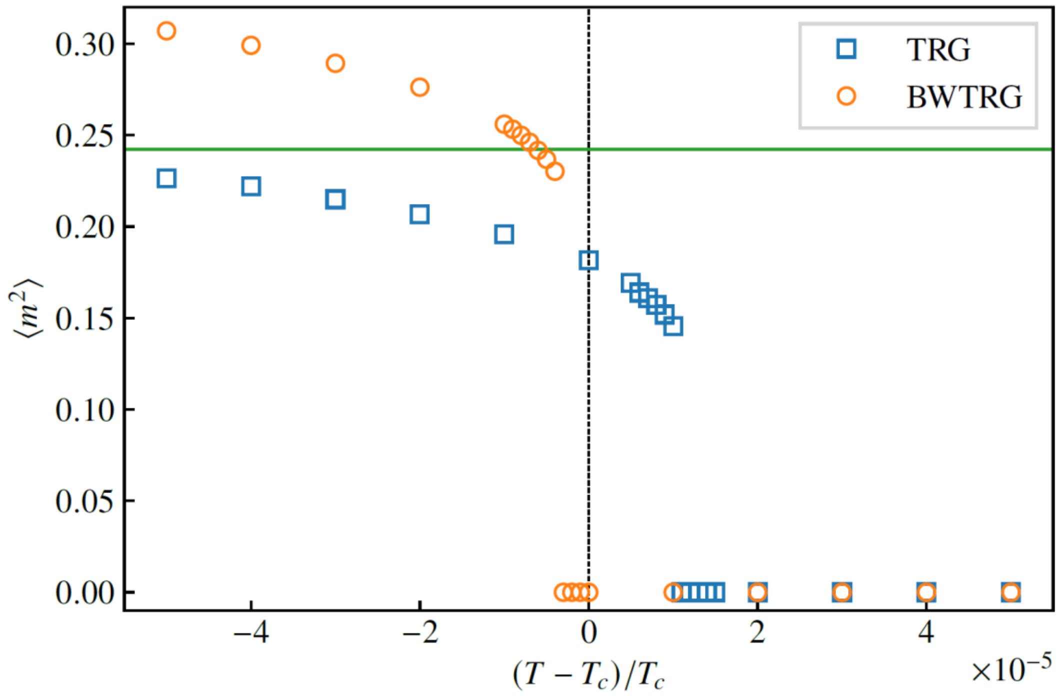
$$H = -J \sum_{\langle ij \rangle} \delta_{S_i, S_j}$$

◻ Weakly first-order phase transition

Energy $\langle e \rangle$



Order parameter $\langle |m|^2 \rangle$



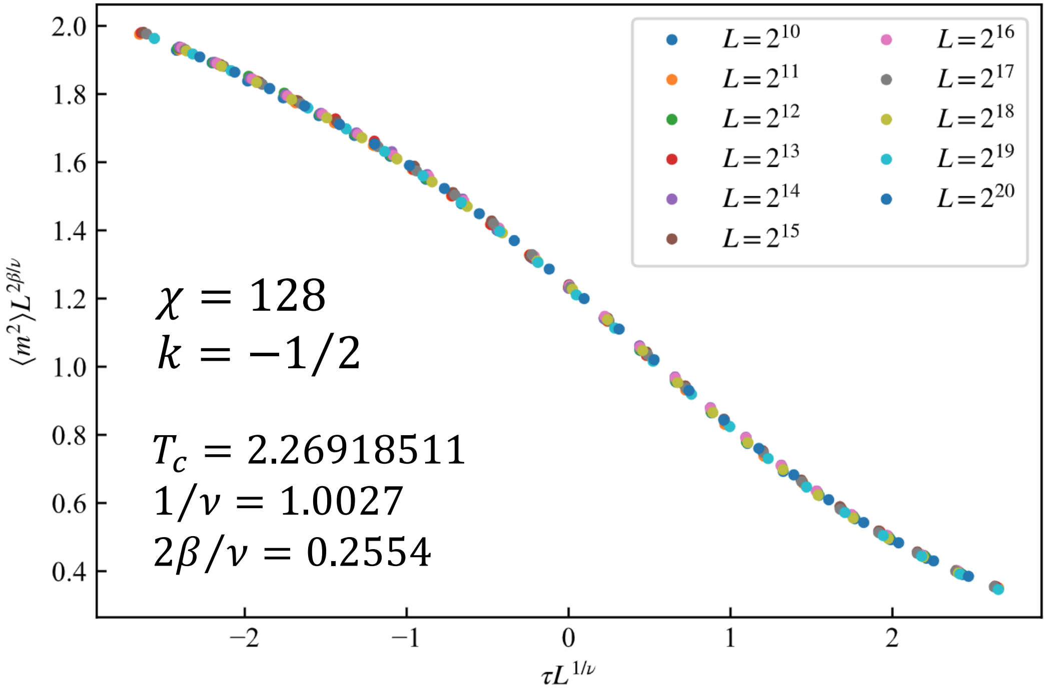
➢ The proposed method can directly and more accurately observe jumps in physical quantities, even in the weakly first-order phase transition.

Exact results: Baxter, J. Phys. C: Solid State Phys. **6**, L445 (1973)
Baxter, J. Phys. A: Math. Gen. **15**, 3329 (1982)

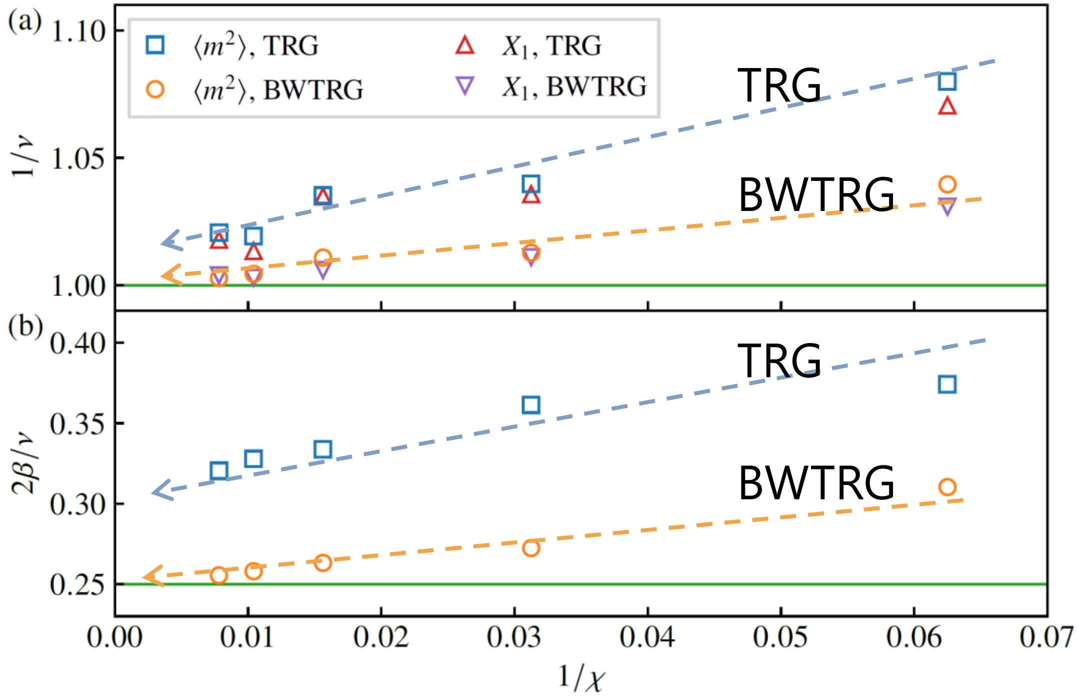
Finite-size scaling analysis in the 2D Ising model

- Finite-size scaling plot of m^2

$$L^{2\beta/\nu}\langle m^2\rangle \simeq f(L^{1/\nu}\tau) \qquad \tau = (T - T_c)/T_c$$



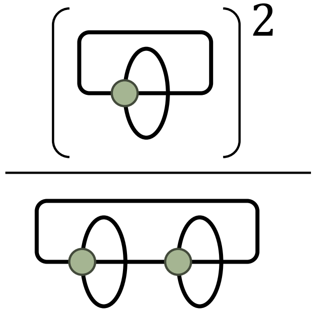
Critical exponents

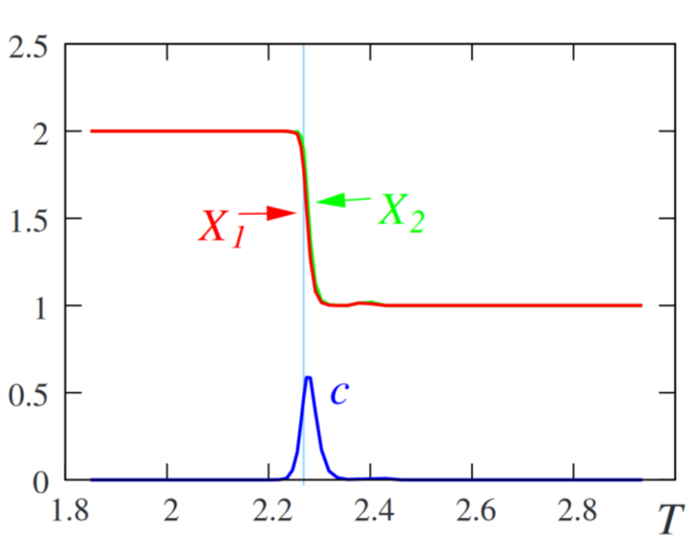


- FSS analysis of BWTRG slightly overestimates the critical exponents, $1/\nu$ and β/ν.
- Relative error in the estimated T_c is about 10^{-8} in BWTRG and 10^{-6} in TRG at $\chi = 128$.

Dimensionless quantity X_1 Gu, Wen, PRB (2009)

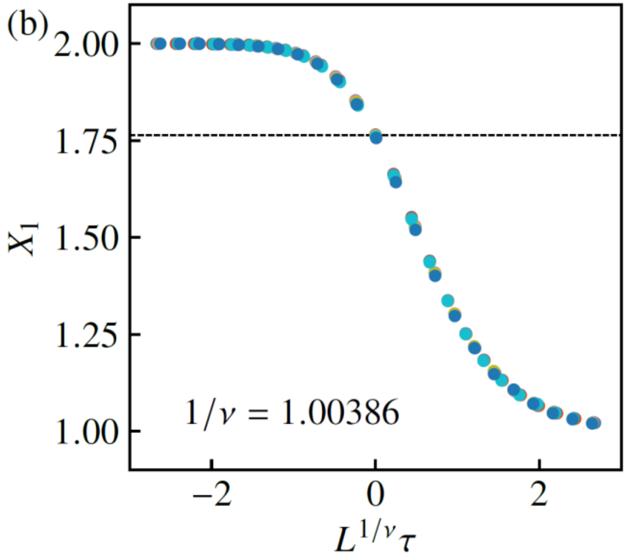
$$X_1 = \frac{\left(\sum_{ru} B_{ruru}\right)^2}{\sum_{ruld} B_{rulu} B_{ldrd}} =$$





It visualized structure of fixed-point tensors

- Finite-size scaling form $X_1 = g(L^{1/\nu}\tau)$



$L = 2^{10} \sim 2^{20}$
$\chi = 128$

- Universal value at criticality

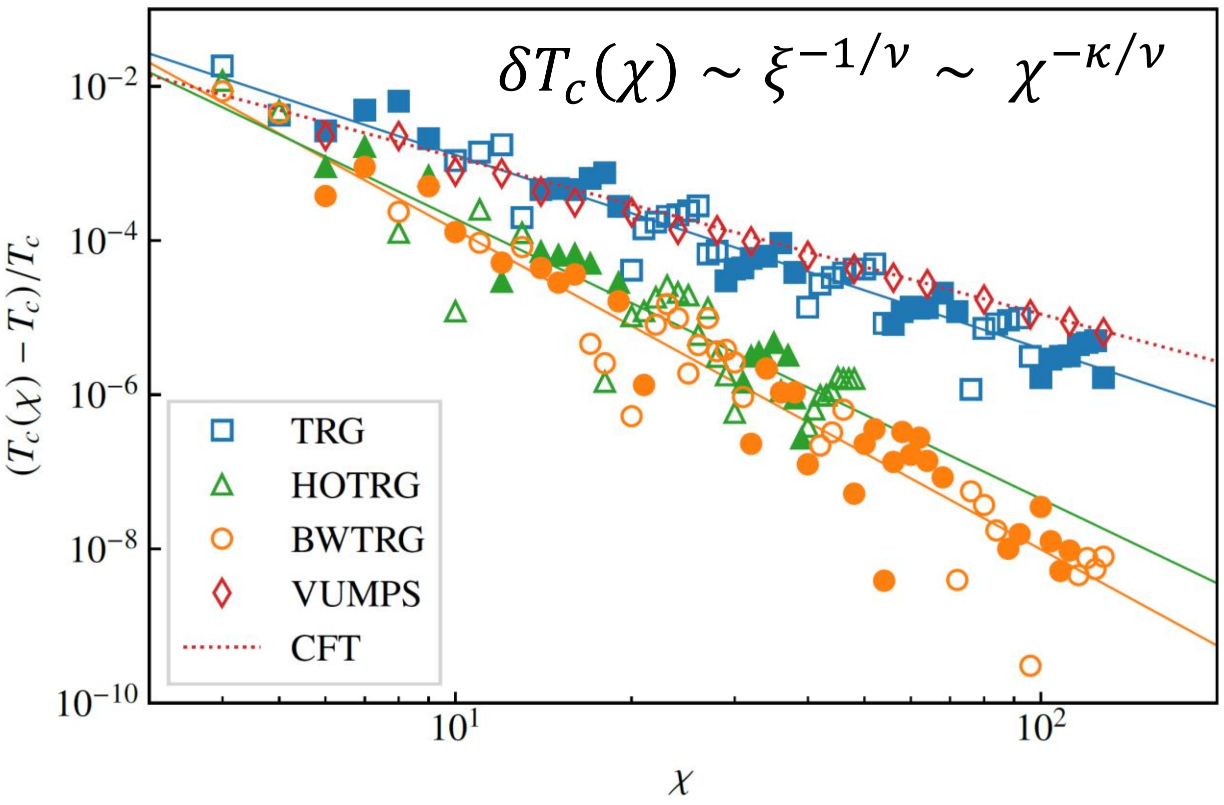
From modular invariant partition function in CFT

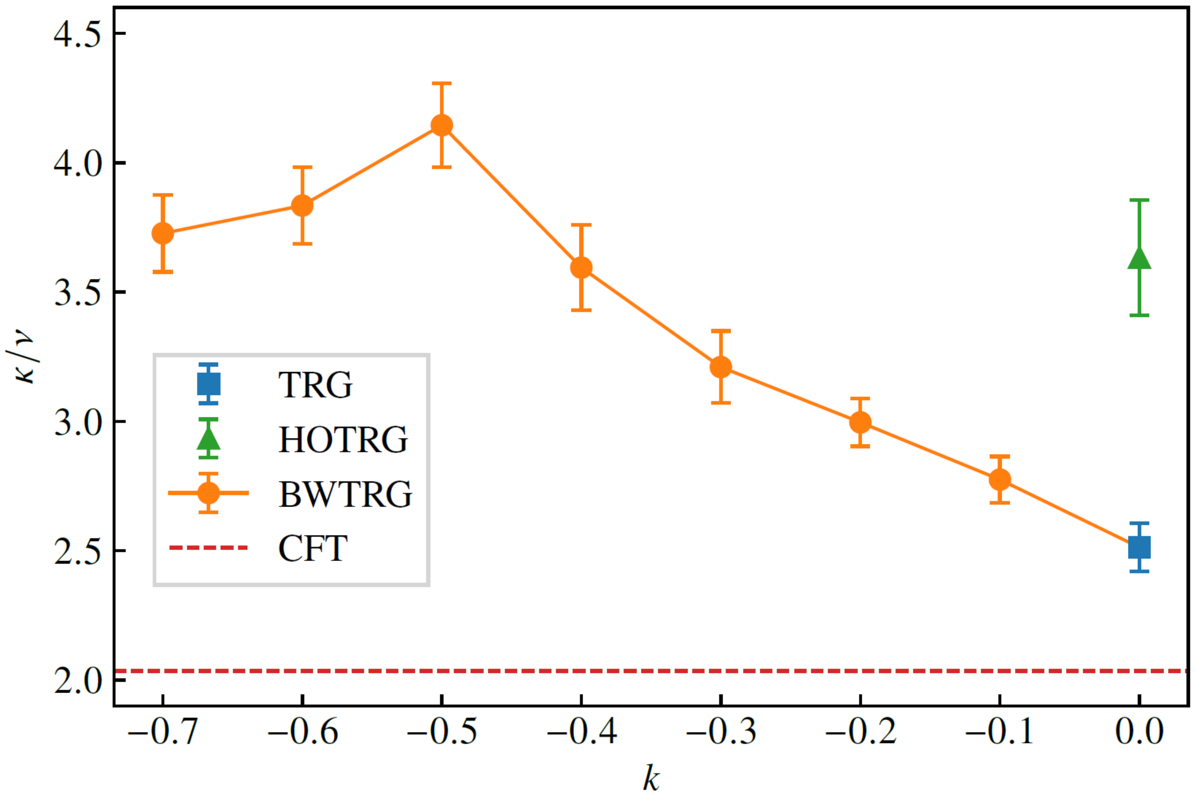
$$X_1 = \frac{\left(\sum_\alpha e^{-2\pi x_\alpha}\right)^2}{\sum_\alpha e^{-4\pi x_\alpha}}$$

x_α : scaling dimension

$X_1 = 1.7635955$ for Ising universality class

χ-dependence of relative error in T_c





- BWTRG with $k = -1/2$ has the largest exponent κ/ν.
- Even considering computational cost, BWTRG is more efficient.

$$\kappa_{\mathrm{CFT}} = \frac{6}{c\left(\sqrt{12/c} + 1\right)}$$

Pollmann, et al., PRL (2009)

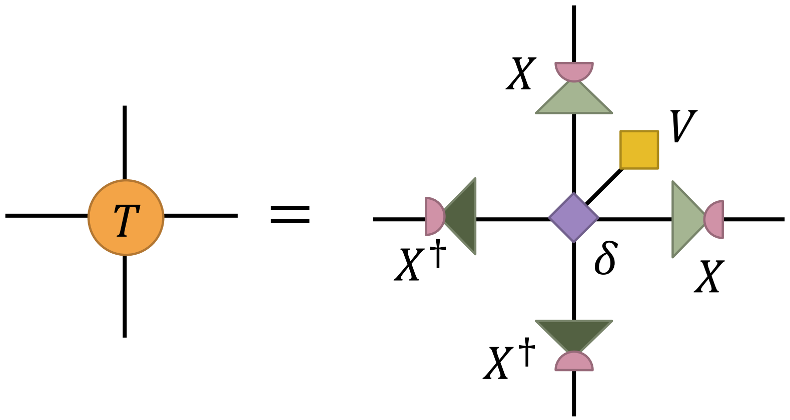
BWTRG: $\delta T_c \sim t^{-\kappa/5\nu} \sim t^{-0.80}$

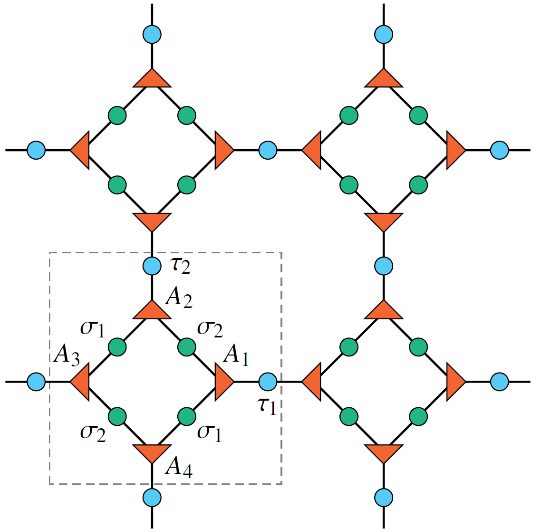
MPS approach: $\delta T_c \sim t^{-\kappa/3\nu} \sim t^{-0.68}$ (assuming $t \sim \chi^3$)

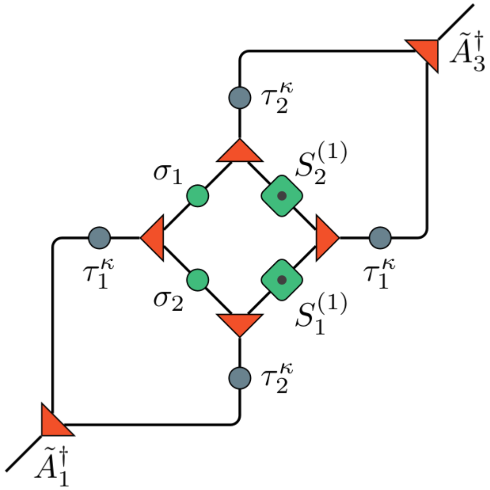
Summary

◻ TN approach to statistical physics

- ➢ TN representations of the partition function
- ➢ Approximation of TN contraction
  - ✓ Real-space renormalization group approach
- ➢ Evaluation of physical quantities
  - ✓ Multi-impurity method for HOTRG and BWTRG
    SM, Kawashima, arXiv:2411.13998







◻ Further issues

- ➢ Application to more interesting models
- ➢ Generalization to higher dimensional systems
- ➢ Improvement of BWTRG