Improvement of the higher-order tensor renormalization group method

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CBSM²
Challenge of Basic Science
– Exploring Extremes through
Multi-Physics and
Multi-Scale Simulations

CdmSi

Outline

- Introduction
  - Real-space renormalization based on TN
  - How to calculate a projector in HOTRG
- Calculation of higher-order moments by HOTRG
  - Renormalization of multi-impurity tensors
  - Finite-scaling analysis on q-state Potts model
- Entanglement filtering in HOTRG
  - HOTRG + Full Environment Truncation (FET)*
  - Benchmark on 2d Ising model*
- Summary

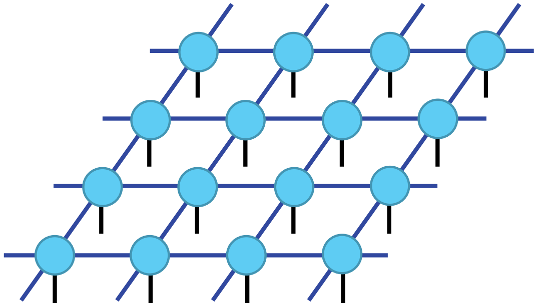
* Unpublished results are removed in this PDF.

Tensor network methods

- Hamiltonian mechanics
  - Wave function 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



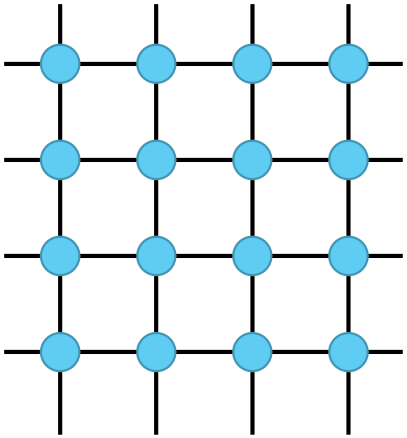
Approx. by tensor decomp.

- Lagrangian mechanics
  - Partition function (Action)

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

$O(d^N)$ terms

Representation by tensor decomp.

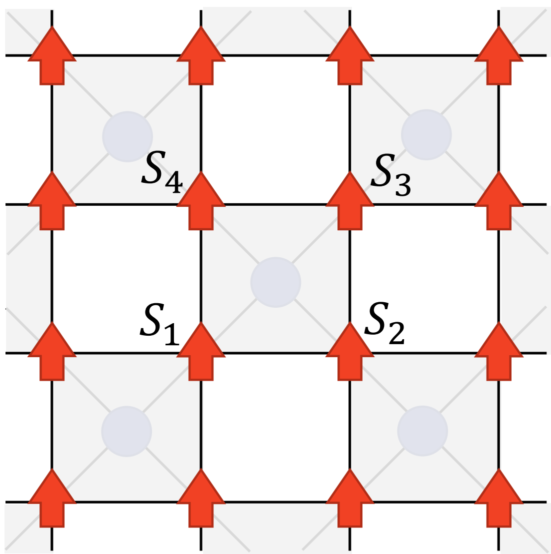


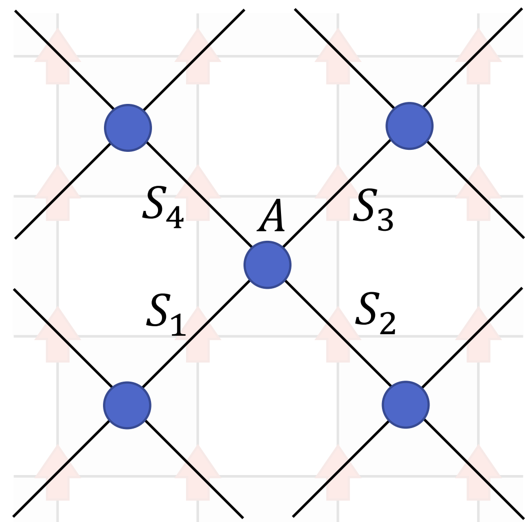
Tensor network representations reduce exponential computational cost to polynomial order.

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).

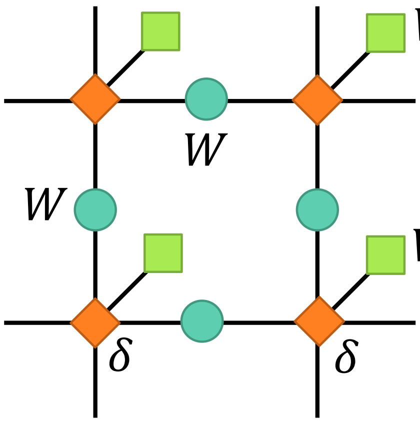
TN representation of the partition function

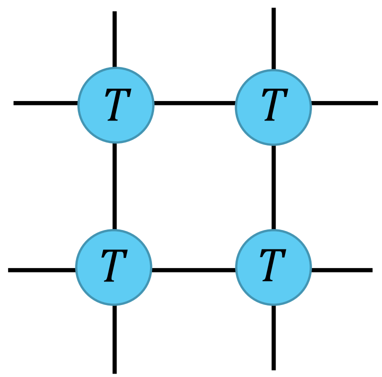
$$Z = \sum_{\{\sigma_i\}} \prod_{\langle ij \rangle} W_{\sigma_i \sigma_j} \prod_{i=1}^{N} V_{\sigma_i} = \mathrm{tTr} \prod_{i=1}^{N} T_{x_i y_i x'_i y'_i}$$

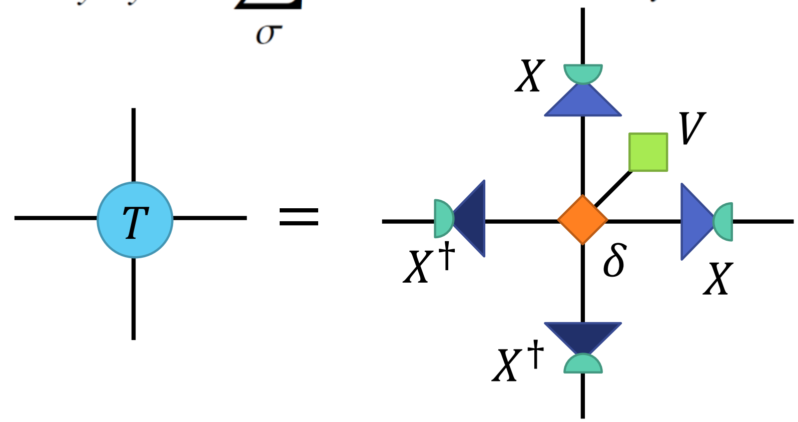
Sum over states

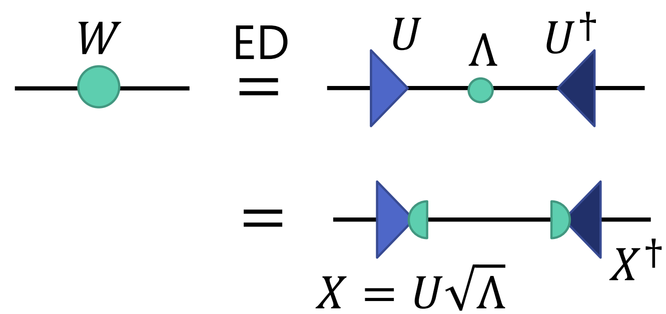
Tensor cont.

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









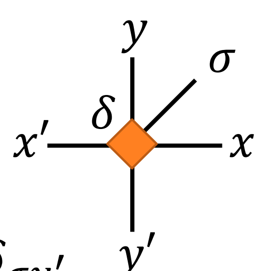
Local Boltzmann factors

$$W_{\sigma\sigma'} = e^{-\beta h_{\sigma\sigma'}}$$

$$V_{\sigma} = e^{-\beta h_{\sigma}}$$

Kronecker's delta

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



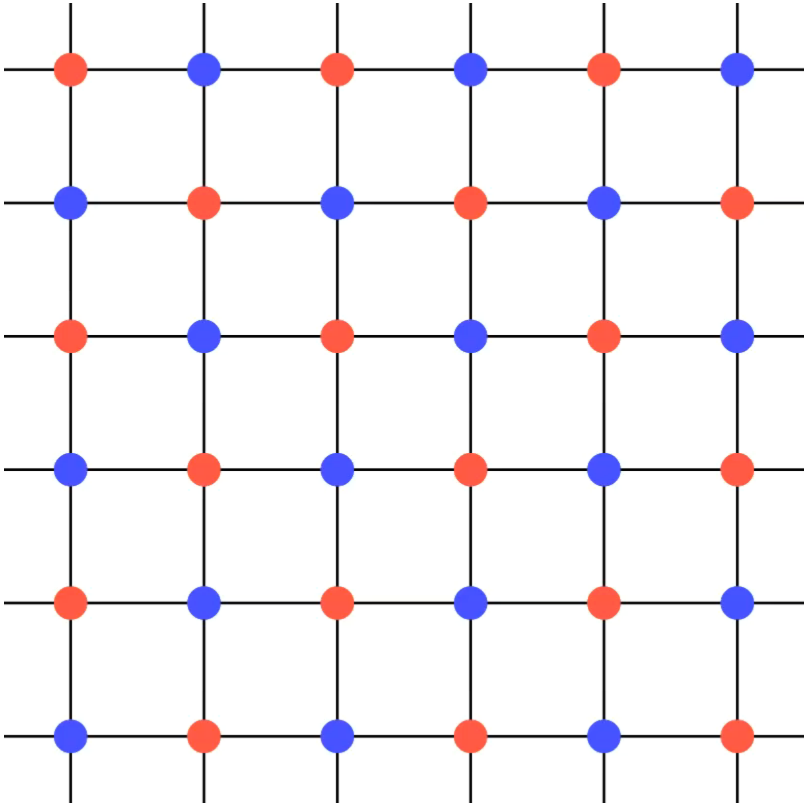
- Bond index is index of eigenvalue.
- Spin is already traced out.
- One tensor contains one spin.
- # of indices is $2d$.

Real-space renormalization group

○ TRG

Tensor Renormalization Group

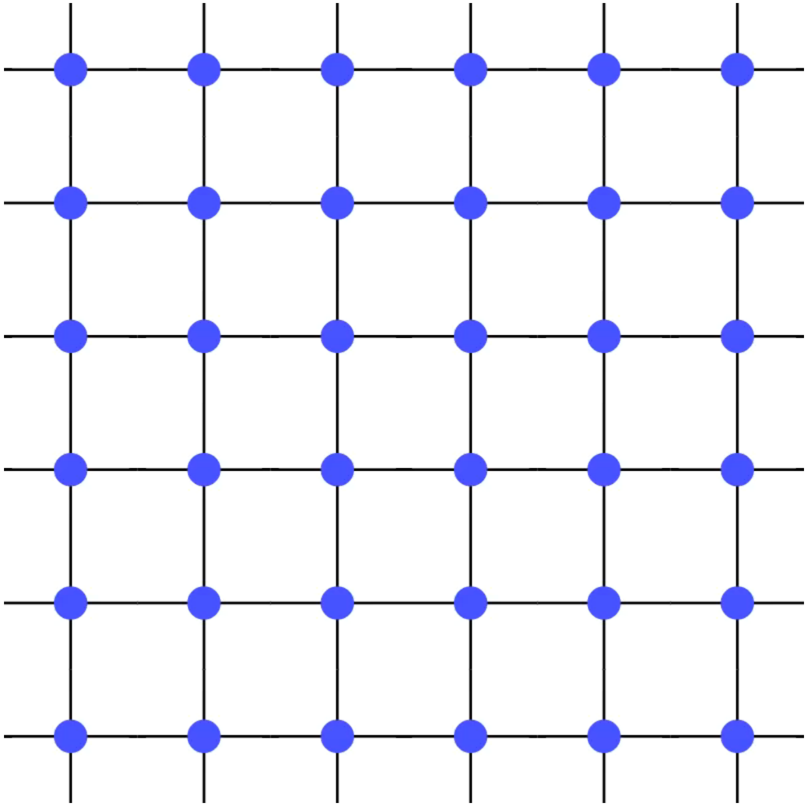
Levin, Nave (2007)



○ HOTRG

Higher-order Tensor Renormalization Group

Xie, et al. (2012)

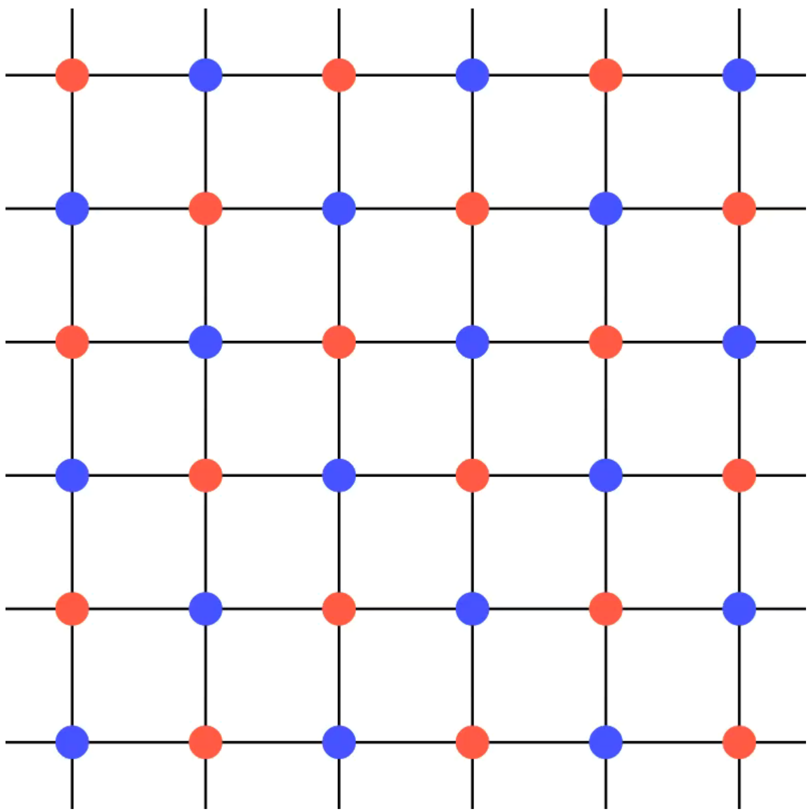


https://github.com/smorita/TN_animation

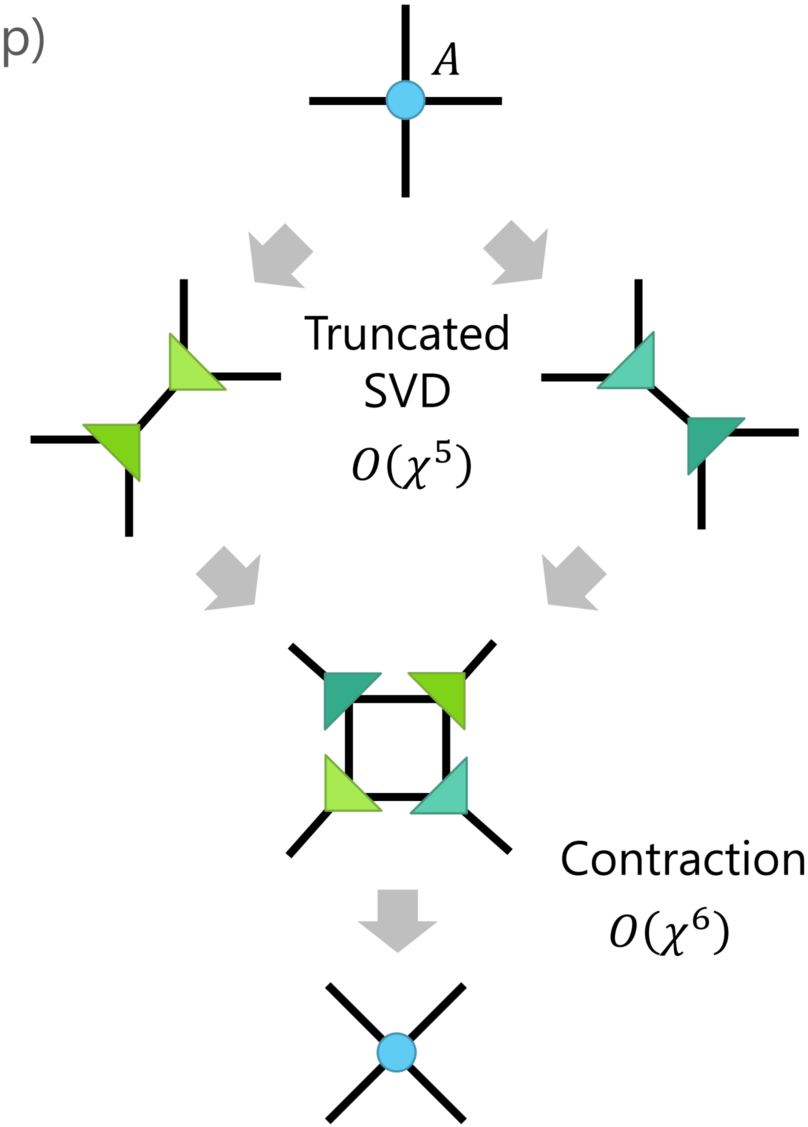
Real-space renormalization

- TRG (Tensor Renormalization Group)

  Levin, Nave (2007)

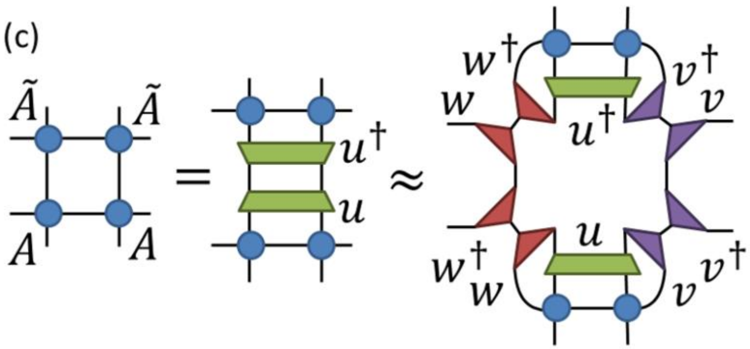


Decomposition & Contraction

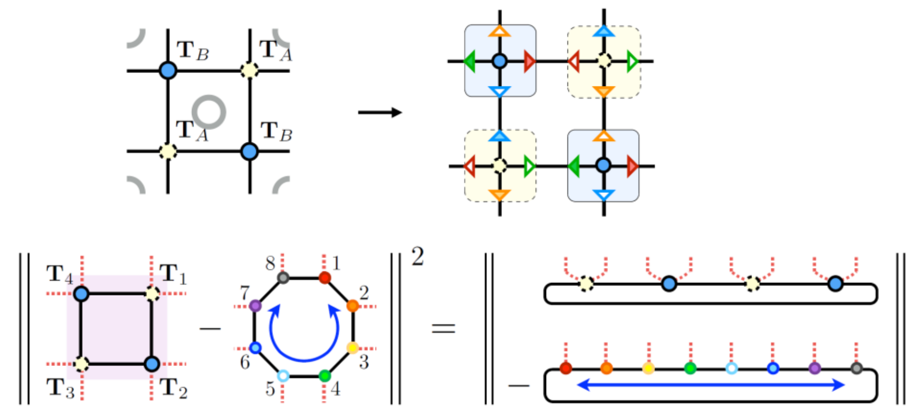


TRG-base methods

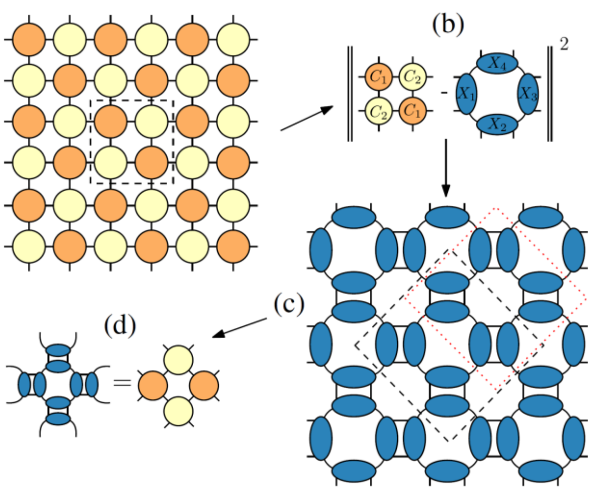
○ TNR (Tensor Network Renormalization) Evenbly, Vidal (2015)



○ Loop-TNR Yang, Gu, Wen (2017)



○ TNR+ Bal, et al. (2017)



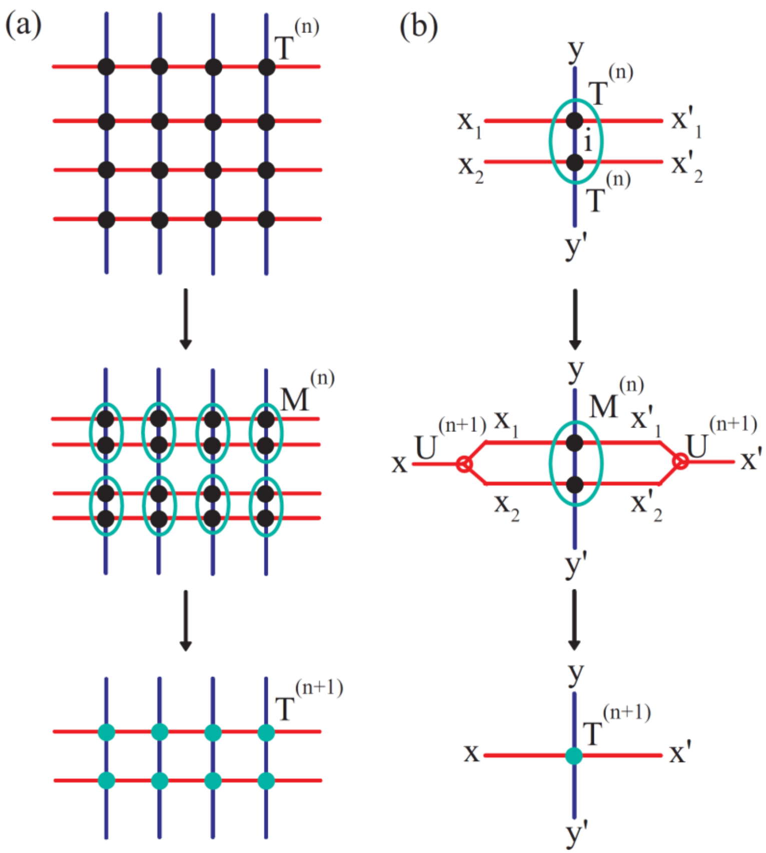
○ $O(\chi^5)$ algorithms

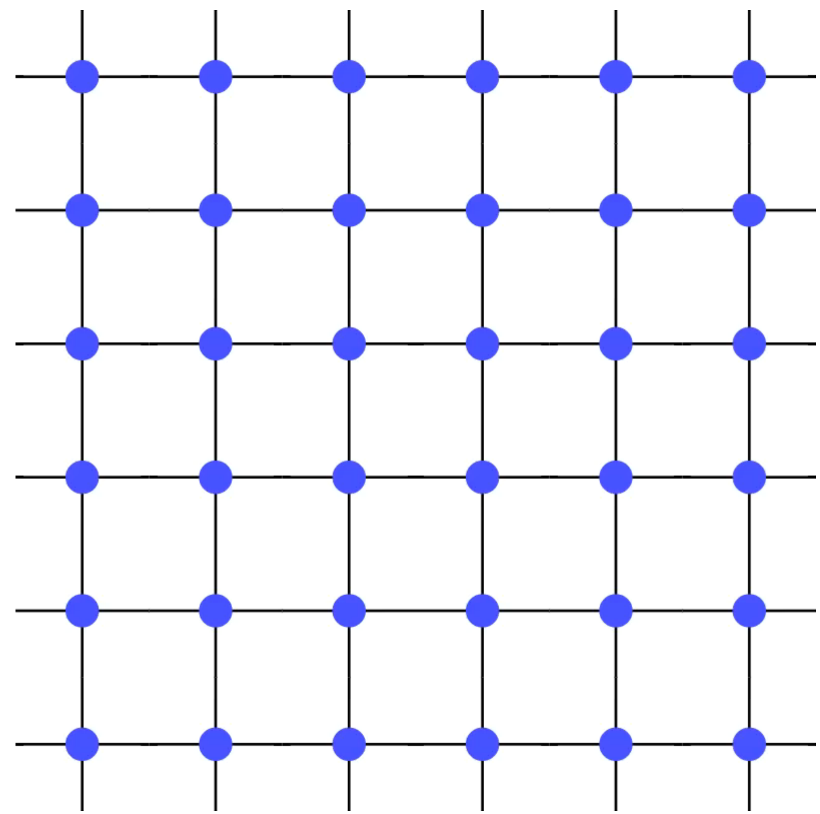
- TRG + Randomized SVD
  SM, Igarashi, Zhao, Kawashima (2018)
- Projectively Truncated TRG
  Nakamura, Oba, Takeda (2019)

Only for 2-d systems

HOTRG

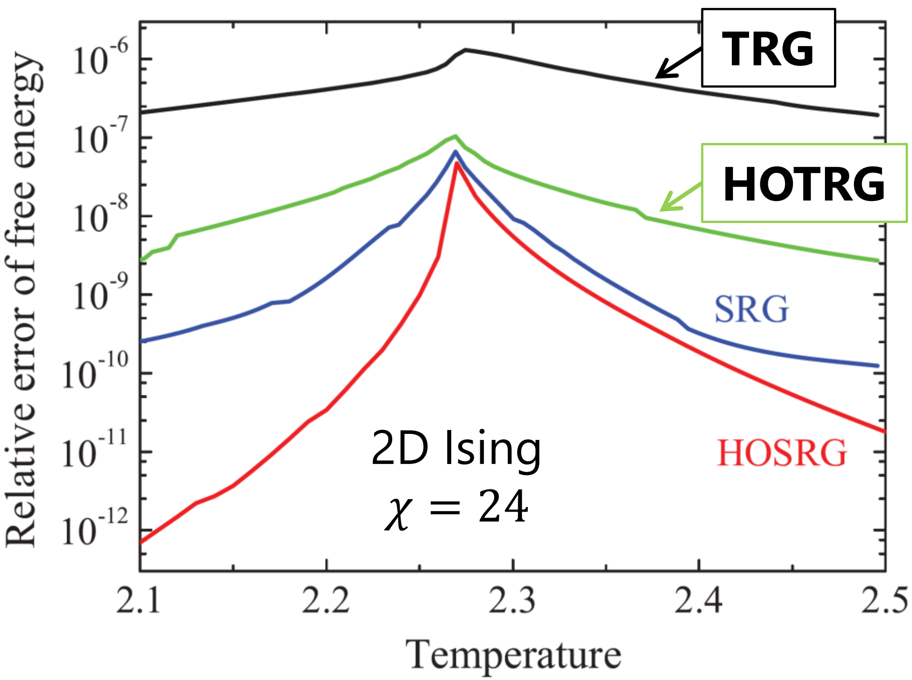
- Higher-order Tensor Renormalization Group
  Xie, et al. (2012)





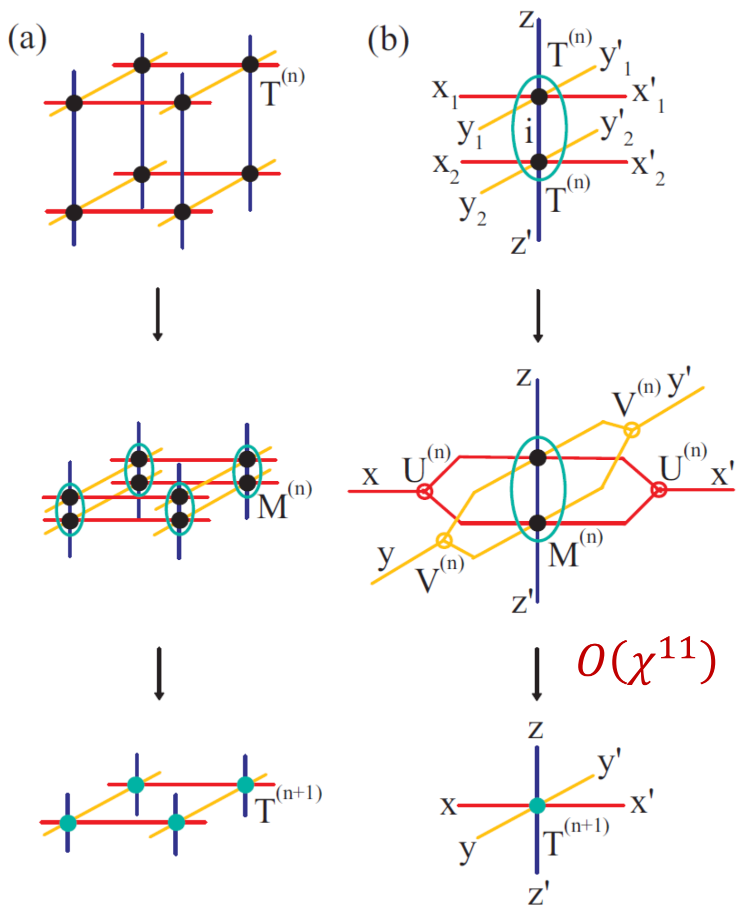
Advantage of HOTRG

- Accuracy



- Conservation of lattice structure
- No tensor decomposition

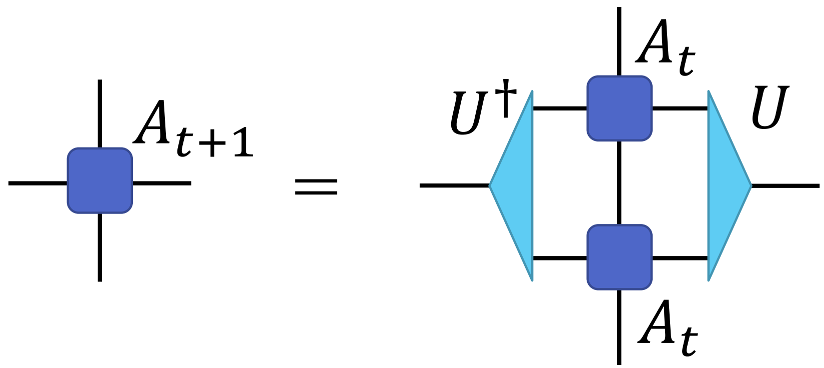
- Higher-dimensional systems



✓ 3-state Potts model on cubic lattice
Wang, et al., (2014) [arXiv:1405.1179]

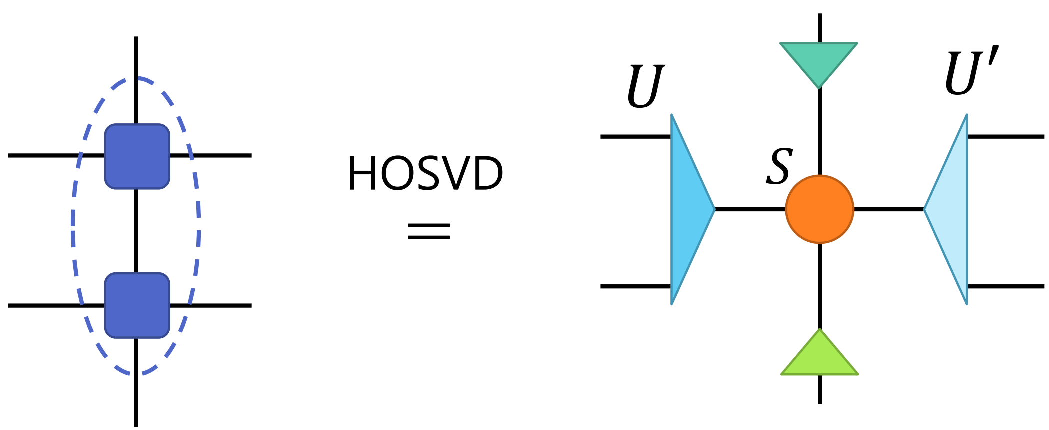
Key parts of HOTRG

- Renormalization



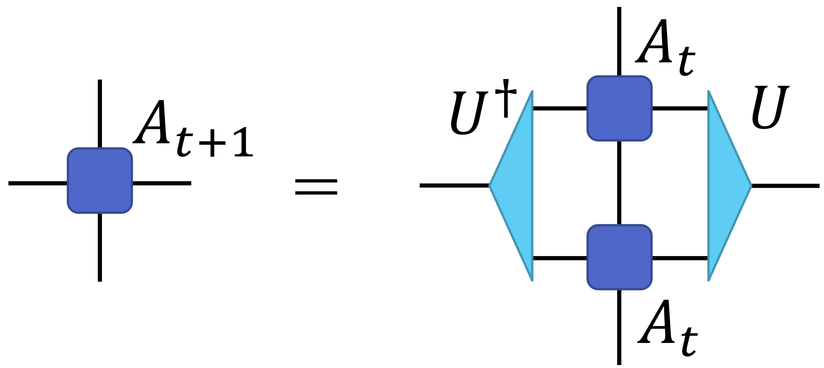
CPU cost: $O(\chi^7)$
Memory: $O(\chi^4)$

- HOSVD (Higher-Order Singular Value Decomposition)
  - truncated Tucker decomposition



Key parts of HOTRG

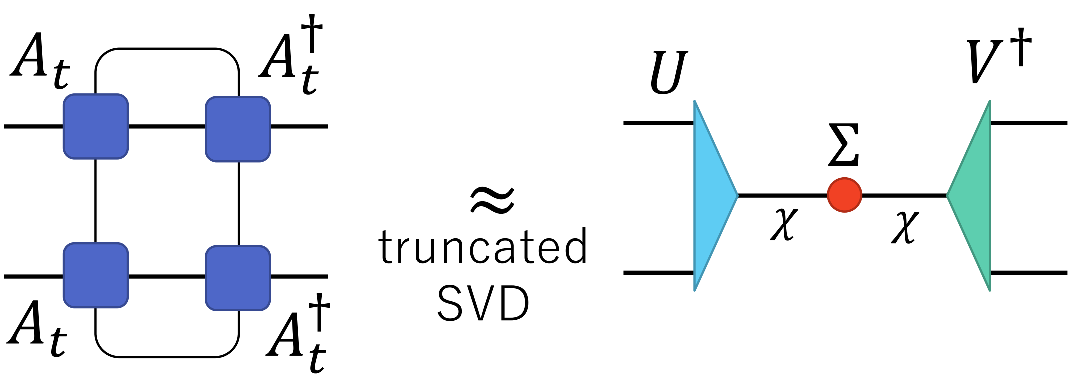
○ Renormalization



CPU cost: $O(\chi^7)$
Memory: $O(\chi^4)$

○ HOSVD (Higher-Order Singular Value Decomposition)

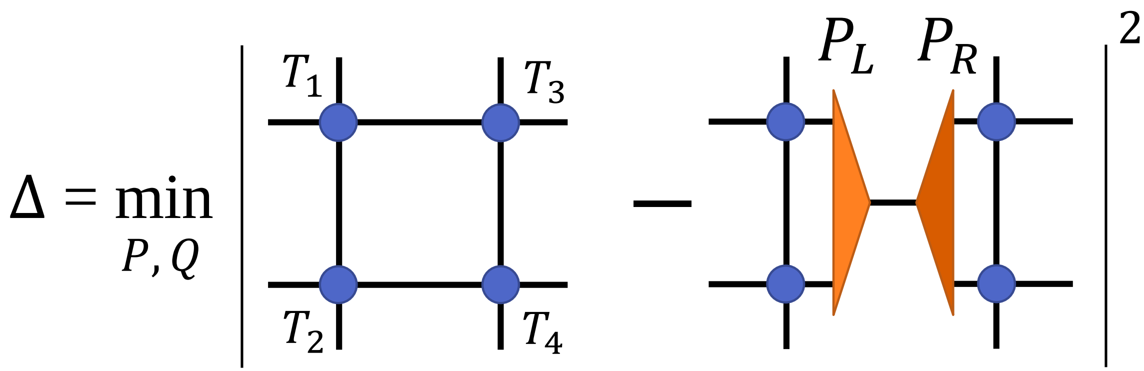
➢ truncated Tucker decomposition



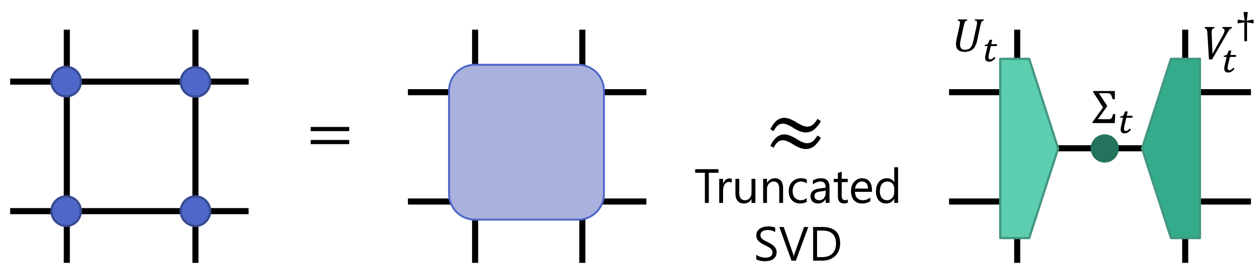
CPU cost: $O(\chi^6)$

Optimal Projector for 2x2 Cluster

○ Problem



Lower bound

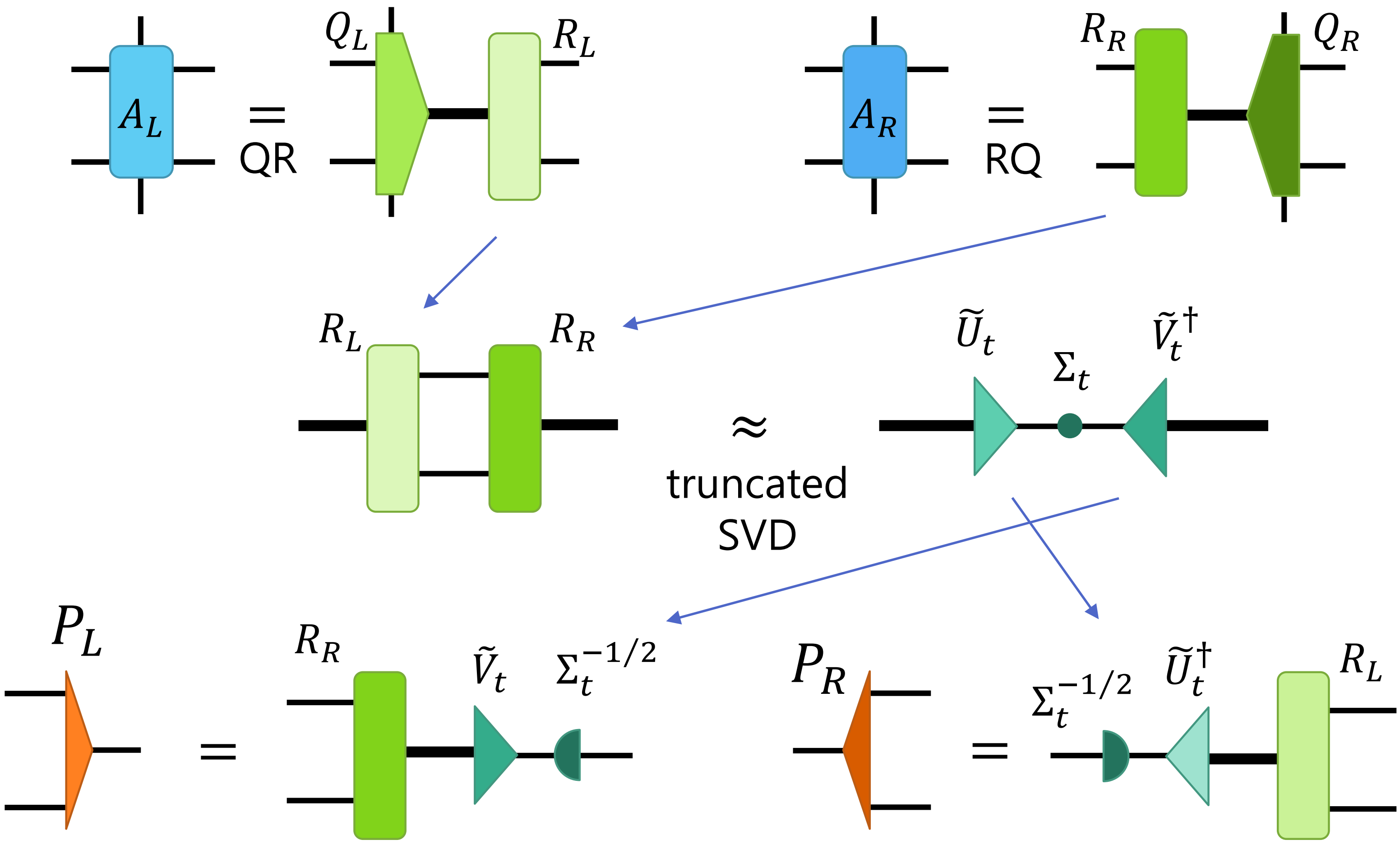


$$\Delta \geq \sum_{i>\chi} \sigma_i^2$$

How do we obtain P_L and P_R satisfying the follow conditions?

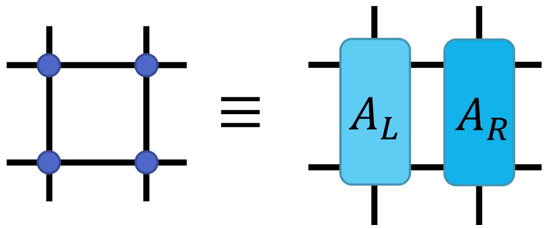
Algorithm based on QR decomposition

Wang, Verstraete, arXiv:1110.4362, Corboz, Rice, Troyer, PRL **113**, 046402 (2014)



$(P_L P_R)$ is an "oblique" projector

Derivation of "Oblique" Projector



$$A_L A_R = U\,\Sigma\,V^\dagger \approx U_t\,\Sigma_t\,V_t^\dagger$$

SVD truncation

$$A_L = Q_L R_L \qquad A_R = R_R Q_R$$

QR decomp. RQ decomp.

$$R_L R_R = \tilde{U}\,\Sigma\,\tilde{V}^\dagger = \tilde{U}_t\,\Sigma_t\,\tilde{V}_t^\dagger$$

SVD truncation

Comparing two SVDs, we obtain

$$U_t = Q_L \tilde{U}_t \qquad V_t^\dagger = \tilde{V}_t^\dagger Q_R$$

$$\tilde{U}_t^\dagger = U_t^\dagger Q_L \qquad \tilde{V}_t = Q_R V_t$$

$$A_L P_L = U_t \sqrt{\Sigma_t} \quad \times \sqrt{\Sigma} V^\dagger V \Sigma_t^{-1/2}$$

$$= U \Sigma V^\dagger\, V_t \Sigma_t^{-1/2}$$

$$= (A_L A_R) V_t \Sigma_t^{-1/2}$$

$$= A_L (R_R Q_R) V_t \Sigma_t^{-1/2}$$

$$= A_L\, \underbrace{R_R \tilde{V}_t \Sigma_t^{-1/2}}_{P_L}$$

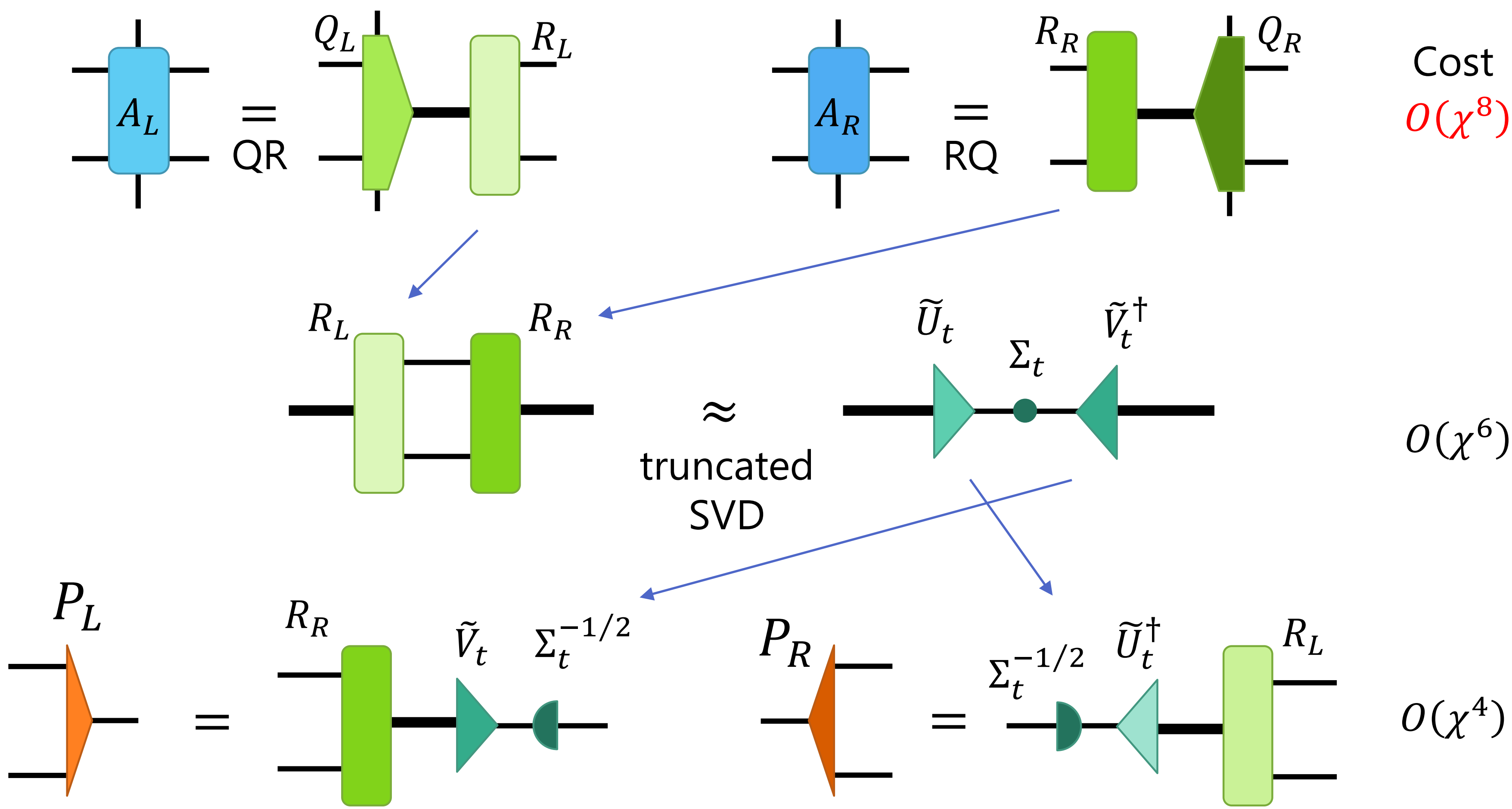
In the same way, we obtain

$$P_R = \Sigma_t^{-1/2} \tilde{U}_t^\dagger R_L$$

We can easily prove $P_L P_R = (P_L P_R)^2$.

Computational Cost

Wang, Verstraete, arXiv:1110.4362, Corboz, Rice, Troyer, PRL **113**, 046402 (2014)



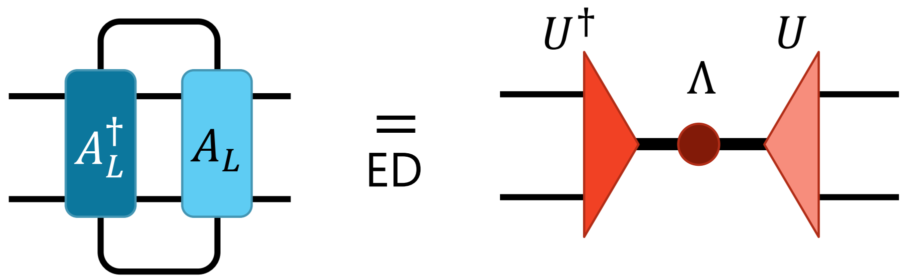
For HOTRG, $O(\chi^8)$ cost is unacceptable.

We can avoid the QR decomp by using ED because Q_L and Q_R is unnecessary.

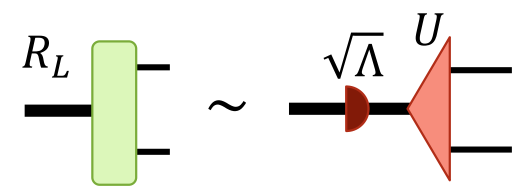
Modified Algorithm for “Oblique” Projector

cf. Iino, SM, Kawashima, arXiv:1905.02351, to be published in PRB

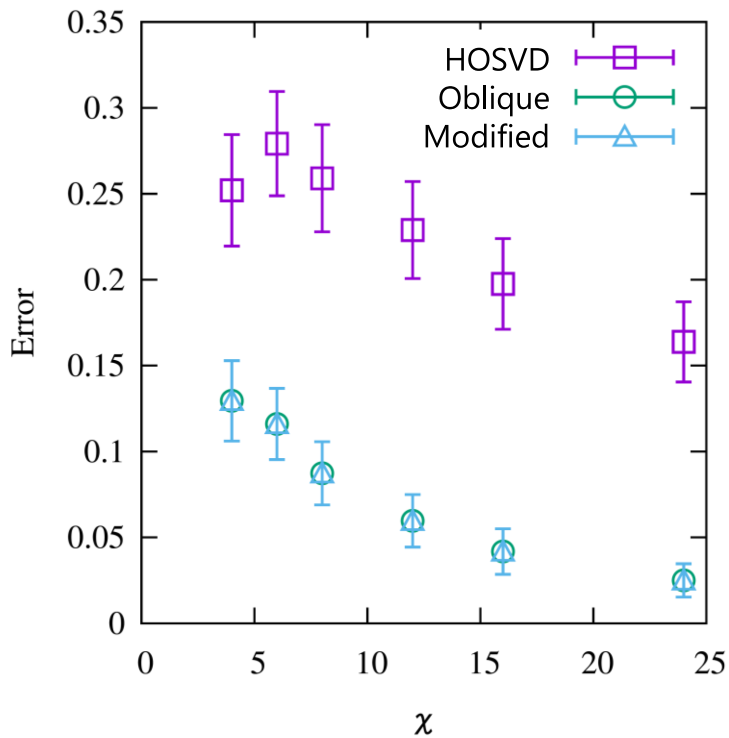
Cost
$O(\chi^8)$

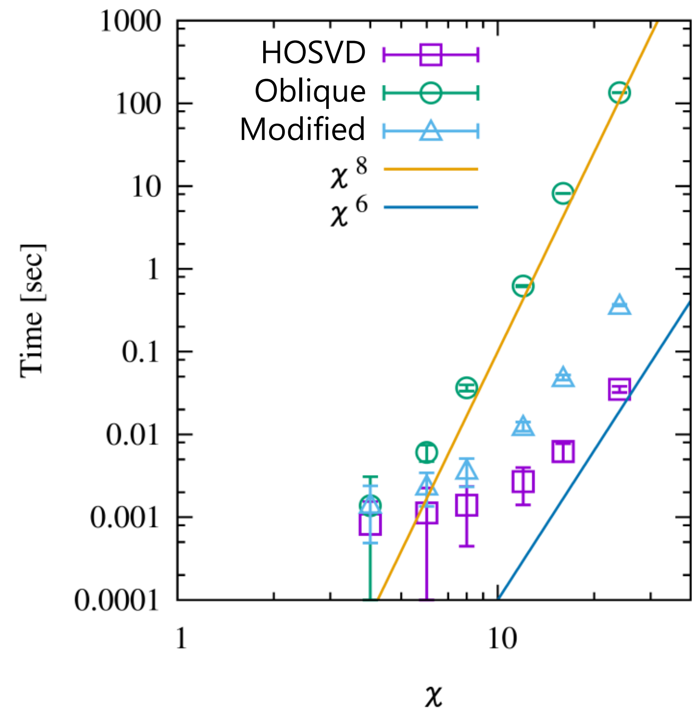


Use $\sqrt{\Lambda}\,U$ instead of R_L



➢ Benchmark on random tensors



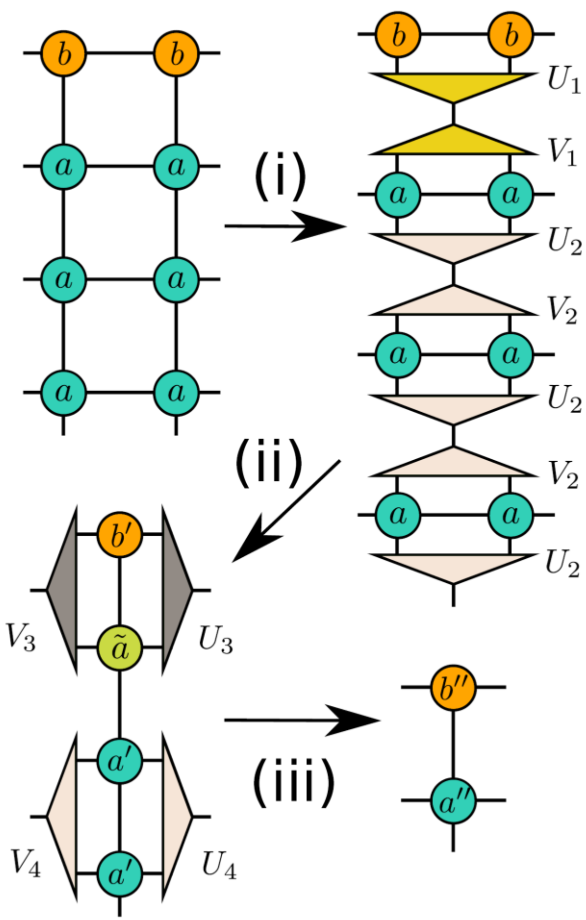


Boundary Tensor Renormalization Group

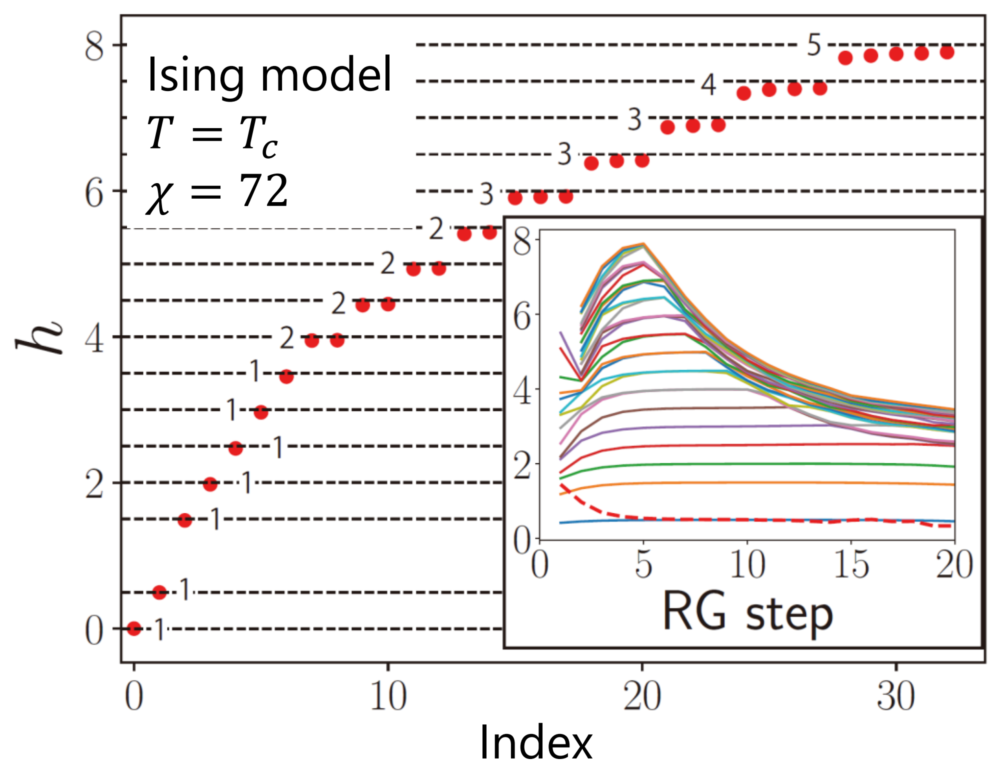
Iino, SM, Kawashima, arXiv:1905.02351, to be published in PRB

Iino's talk
July 22, 15:30-

○ HOTRG with open boundaries



Scaling dimension of boundary CFT



$$Z_{\text{free,free}} = \chi_0 + \chi_{\frac{1}{2}}$$

1^{st} Part:
Higher-order moments by Higher-order Tensor Renormalization Group

Binder ratio

K. Binder: Z. Phys. B **43**, 119 (1981)

$$U_4 \equiv \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2}$$

Magnetization

$$m = \frac{1}{N} \sum_i S_i$$

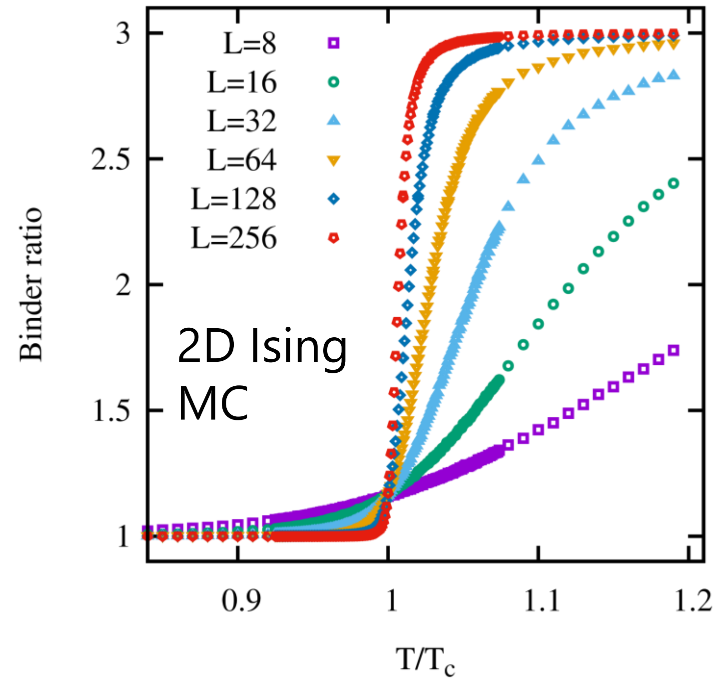
$$\lim_{T \to 0} U_4 = 1 \qquad \lim_{T \to \infty} U_4 = 3$$

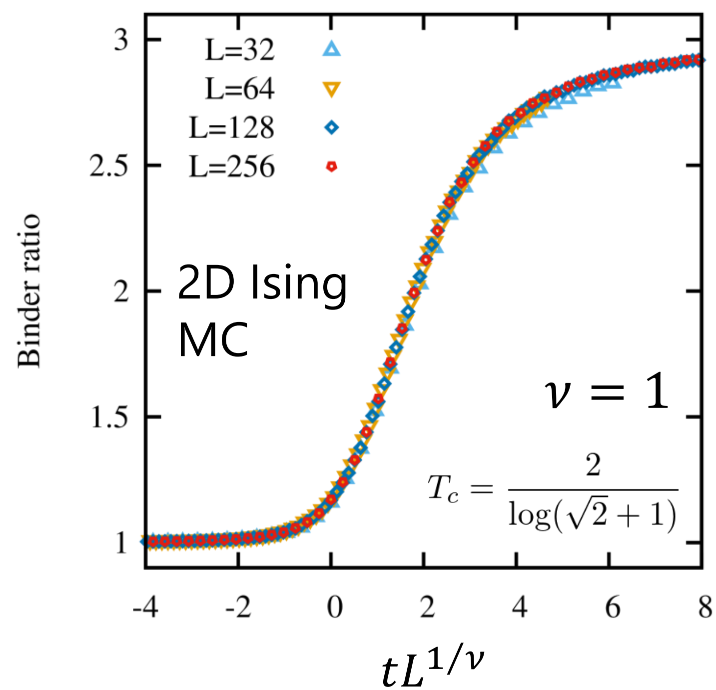
(Ising model)

- ✓ Dimensionless quantity
- ✓ Step function in $N \to \infty$
- ✓ Crossing point → T_c

Finite-size scaling analysis

$$U_4(t, L) = \Psi(t L^{1/\nu}) \qquad t \equiv \frac{T - T_c}{T_c}$$



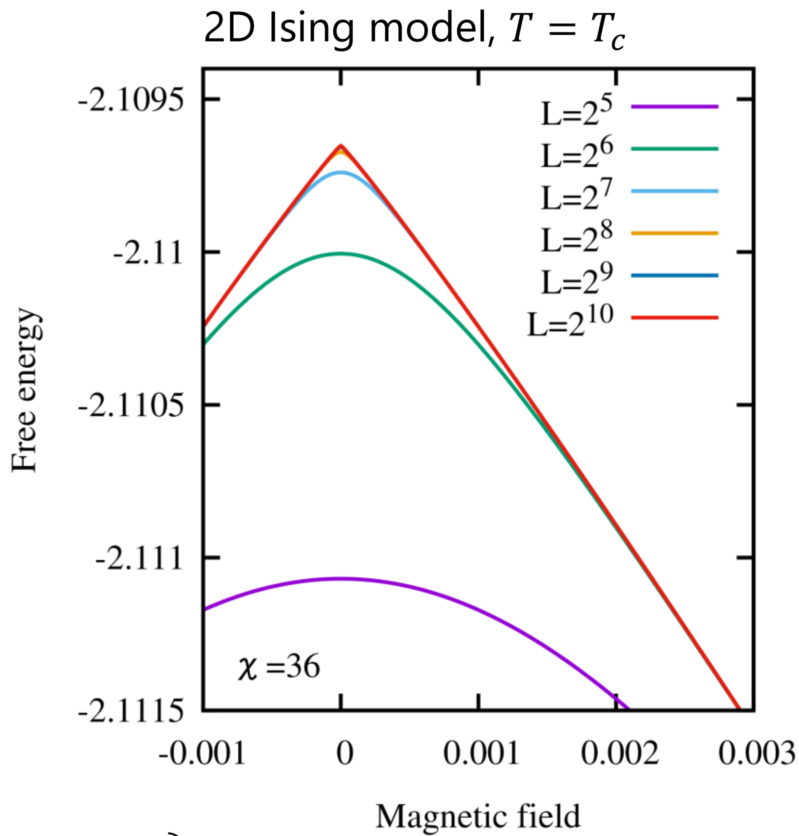


Order parameter $\langle m \rangle$

1. Derivative of free energy

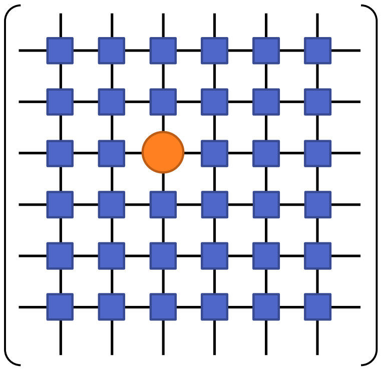
$$\langle m \rangle = -\frac{\partial f}{\partial h}$$

- Error from numerical differential approximation.
- External field breaks symmetry of tensor.



2. Impurity tensor

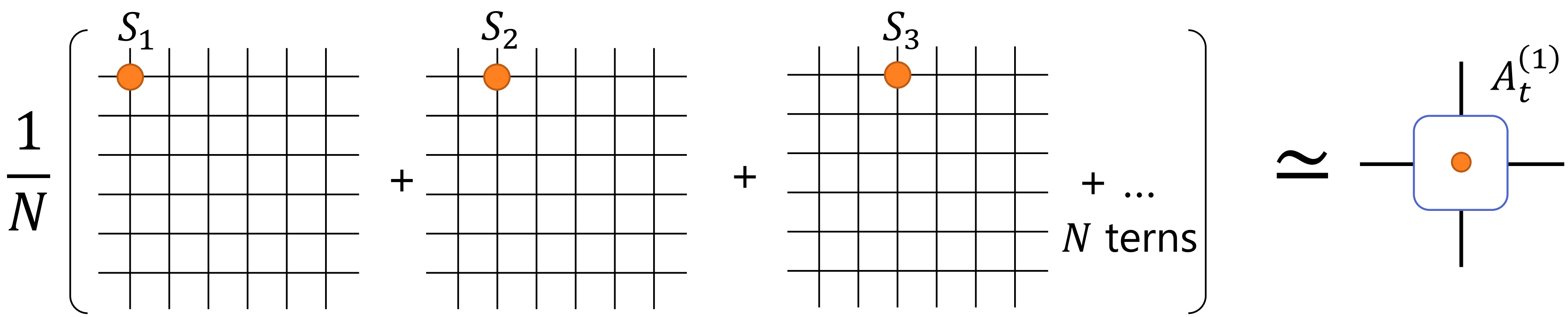
$$\mathrm{Tr}\, S_i\, e^{-\beta H} = \mathrm{tTr}$$



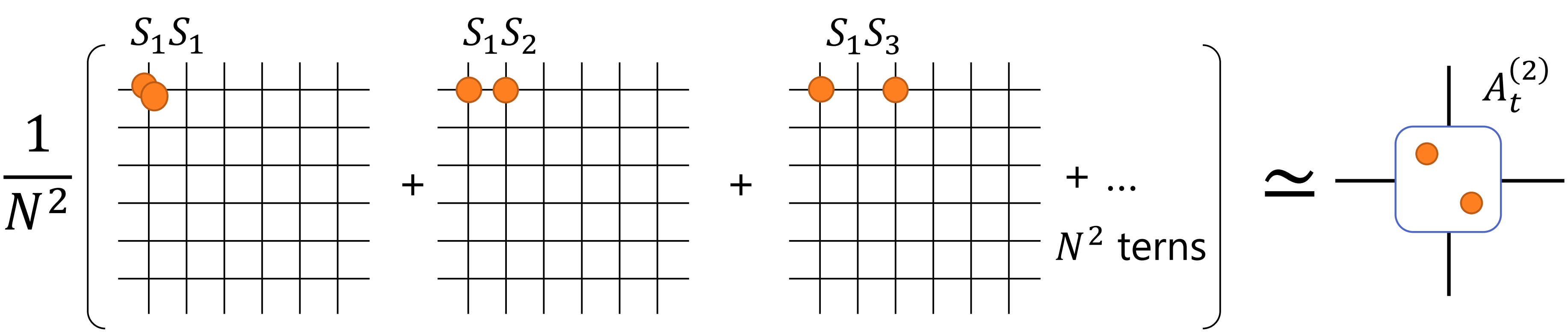
Multi-point correlations are necessary for high-order moments $\langle m^n \rangle$.

Multipoint correlation functions

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

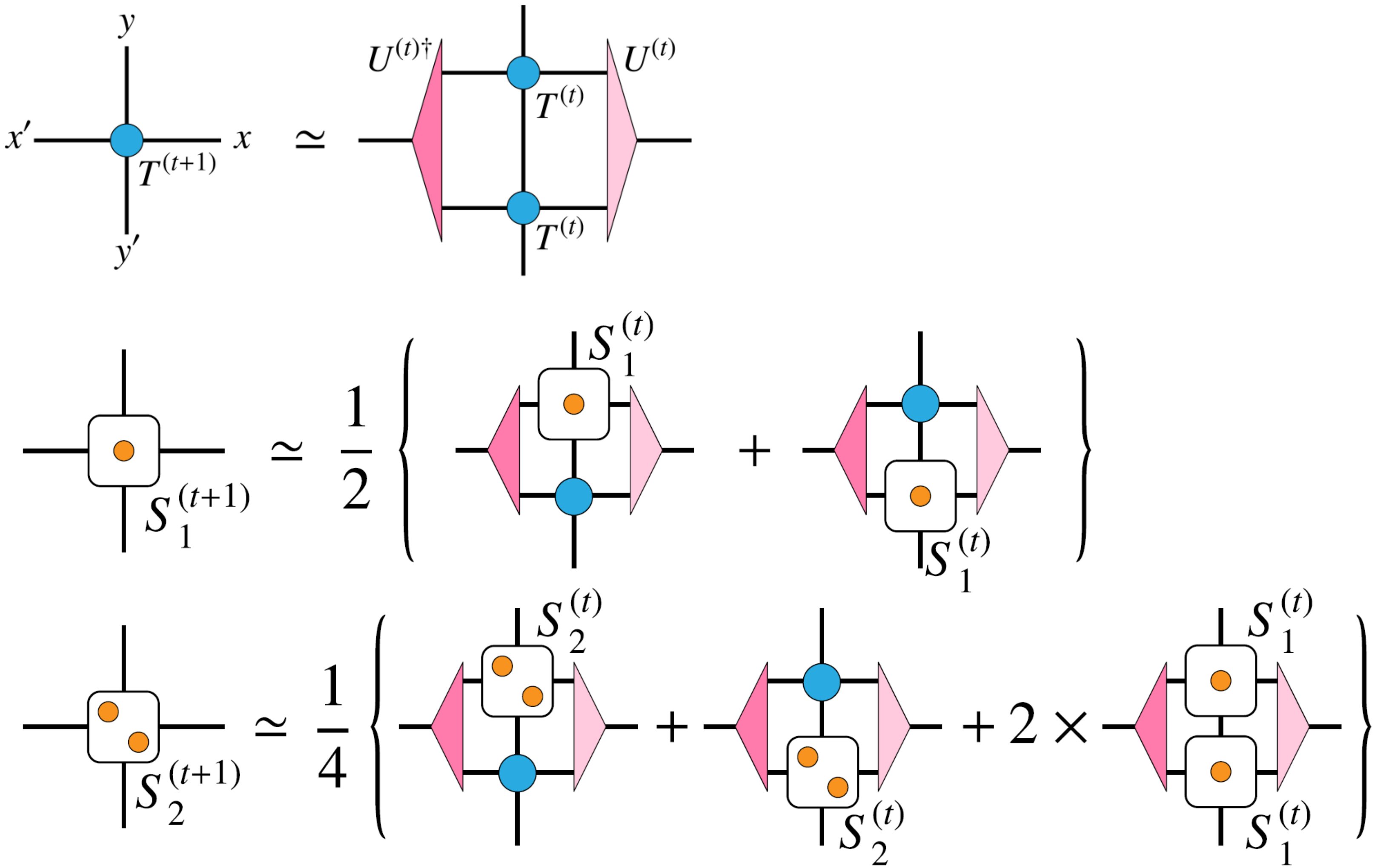


- 2nd-order moment $\left\langle \frac{1}{N^2}\sum_{i,j} S_i S_j \right\rangle$

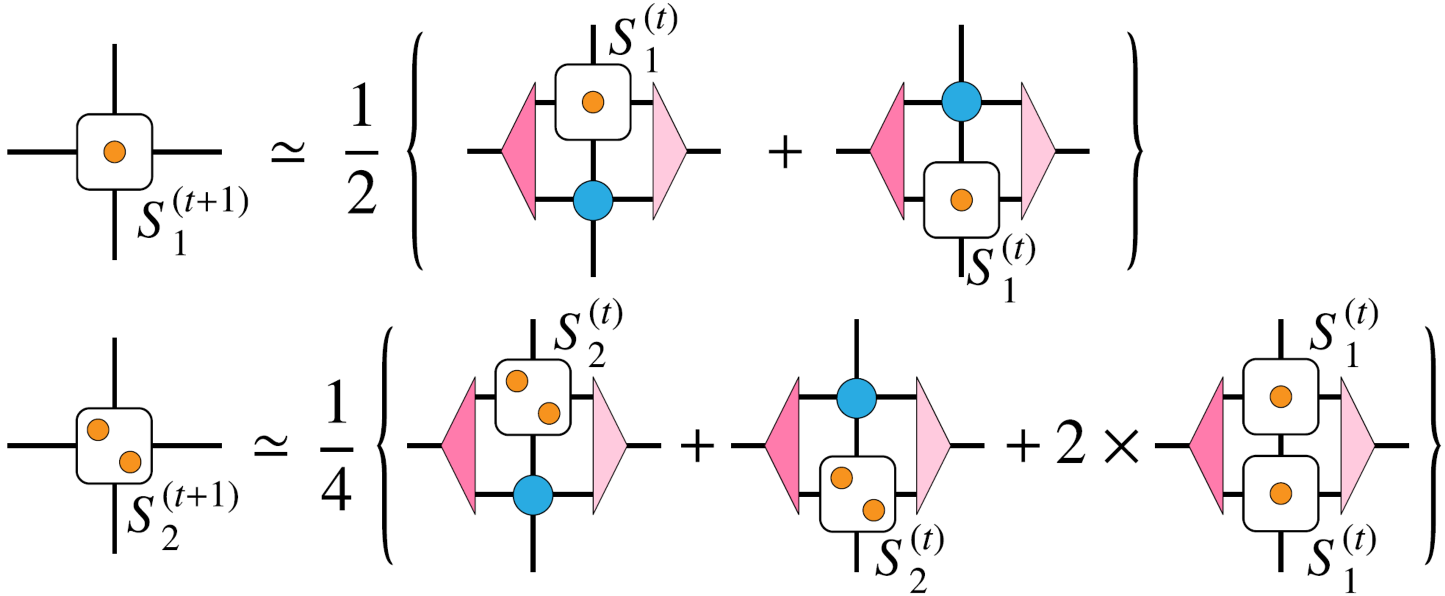


We calculate the renormalized tensor of the summation of multipoint correlation functions by using HOTRG.

Renormalization of multi-impurity tensors



Renormalization of multi-impurity tensors



$$S_3 \leftarrow \frac{1}{8}(S_3T + 3S_2S_1 + 3S_1S_2 + TS_3)$$

$$S_4 \leftarrow \frac{1}{16}(S_4T + 4S_3S_1 + 6S_2S_2 + 4S_1S_3 + TS_4)$$

- Use the same isometry $U^{(t)}$ for the local tensor $T^{(t)}$
- Generalization for multiple kinds of impurities

2D q-state classical Potts model

$$H = -J \sum_{\langle ij \rangle} \delta_{\sigma_i,\sigma_j} - h \sum_i \delta_{\sigma_i,0}$$

$$(\sigma_i = 0, 1, \ldots, q-1)$$

We consider $h = 0$.

- Phase transition at $T_c = \dfrac{J}{\log(\sqrt{q}+1)}$
  - $q \leq 4$: 2nd-order
  - $q > 4$: 1st-order
  - Correlation length

q	4	5	6	7	8	9	10
ξ	∞	2512.2	158.9	48.1	23.9	14.9	10.6

Weakly 1st-order

TN representation

- Local tensor

$$T^{(0)}_{xyx'y'} = \frac{\sqrt{\lambda_x \lambda_y \lambda_{x'} \lambda_{y'}}}{q} \delta^{[q]}_{x+y,x'+y'}$$

Z_q symmetry

$x + y - x' - y' \equiv 0 \bmod q$

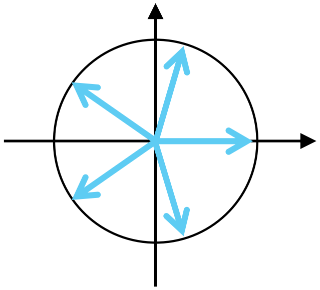
$$\lambda_x = e^K - 1 + q\delta_{x,0}$$

Eigen value of local Boltzmann factor $W_{\sigma,\sigma'} = e^{K\delta_{\sigma,\sigma'}}$

- Order parameter
  - Complex magnetization

$$m = \frac{1}{N} \sum_{i=1}^{N} \exp\left[i \frac{2\pi}{q} S_i \right]$$

$$U_4 \equiv \frac{\langle |m|^4 \rangle}{\langle |m|^2 \rangle^2}$$



  - Impurity tensor for $m^k m^{*k'}$

$$S^{(0)}_{k,k';xyx'y'} = \frac{\sqrt{\lambda_x \lambda_y \lambda_{x'} \lambda_{y'}}}{q} \delta^{[q]}_{x+y+k,x'+y'+k'}$$

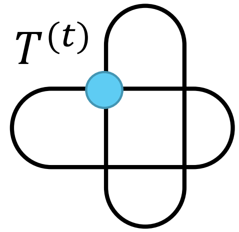
Covariant with spin rotation (charge $k - k'$)

$x + y - x' - y' \equiv k - k' \bmod q$

Magnetization

$$\langle |m|^2 \rangle_N \simeq \frac{\mathrm{Tr}\ S^{(t)}_{1,1}}{\mathrm{Tr}\ T^{(t)}}$$

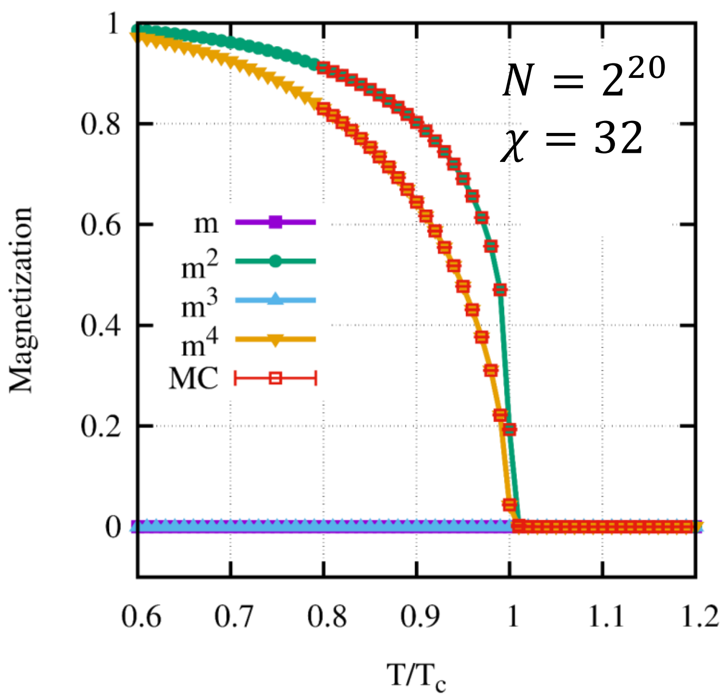
$$\mathrm{Tr}\ T^{(t)} = \sum_{x,y} T^{(t)}_{xyxy}$$



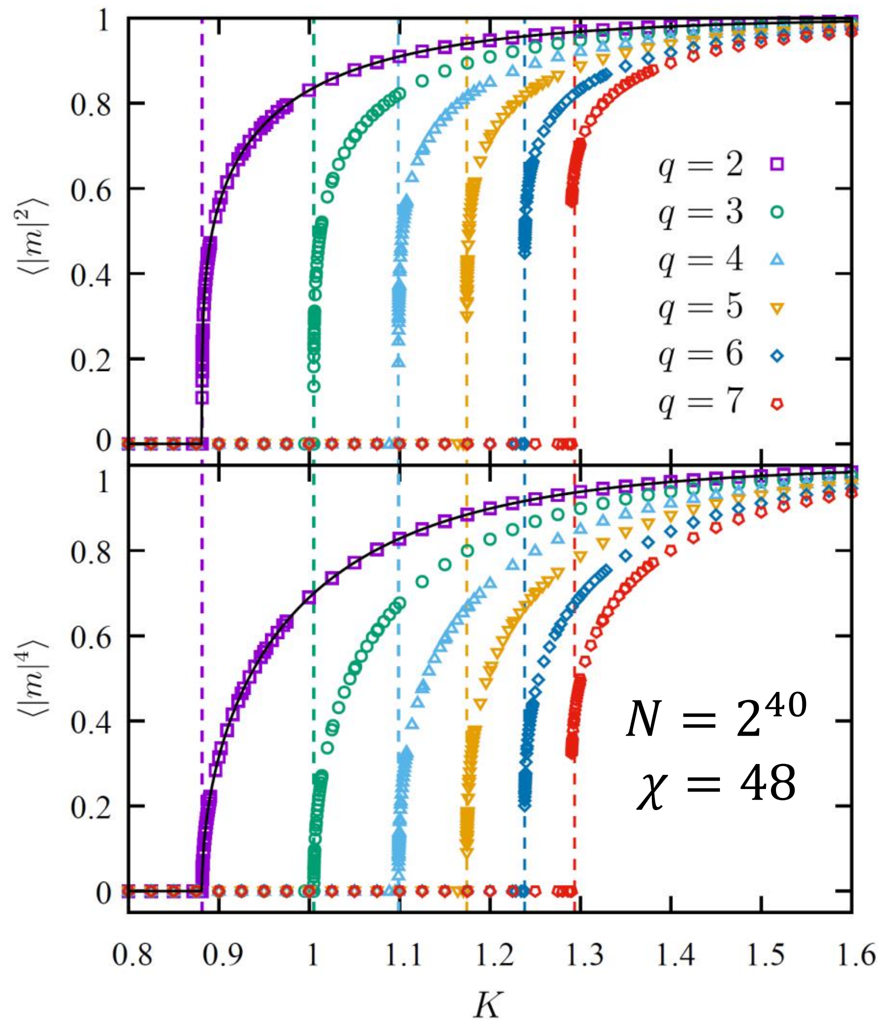
Periodic BC

$N = 2^t$

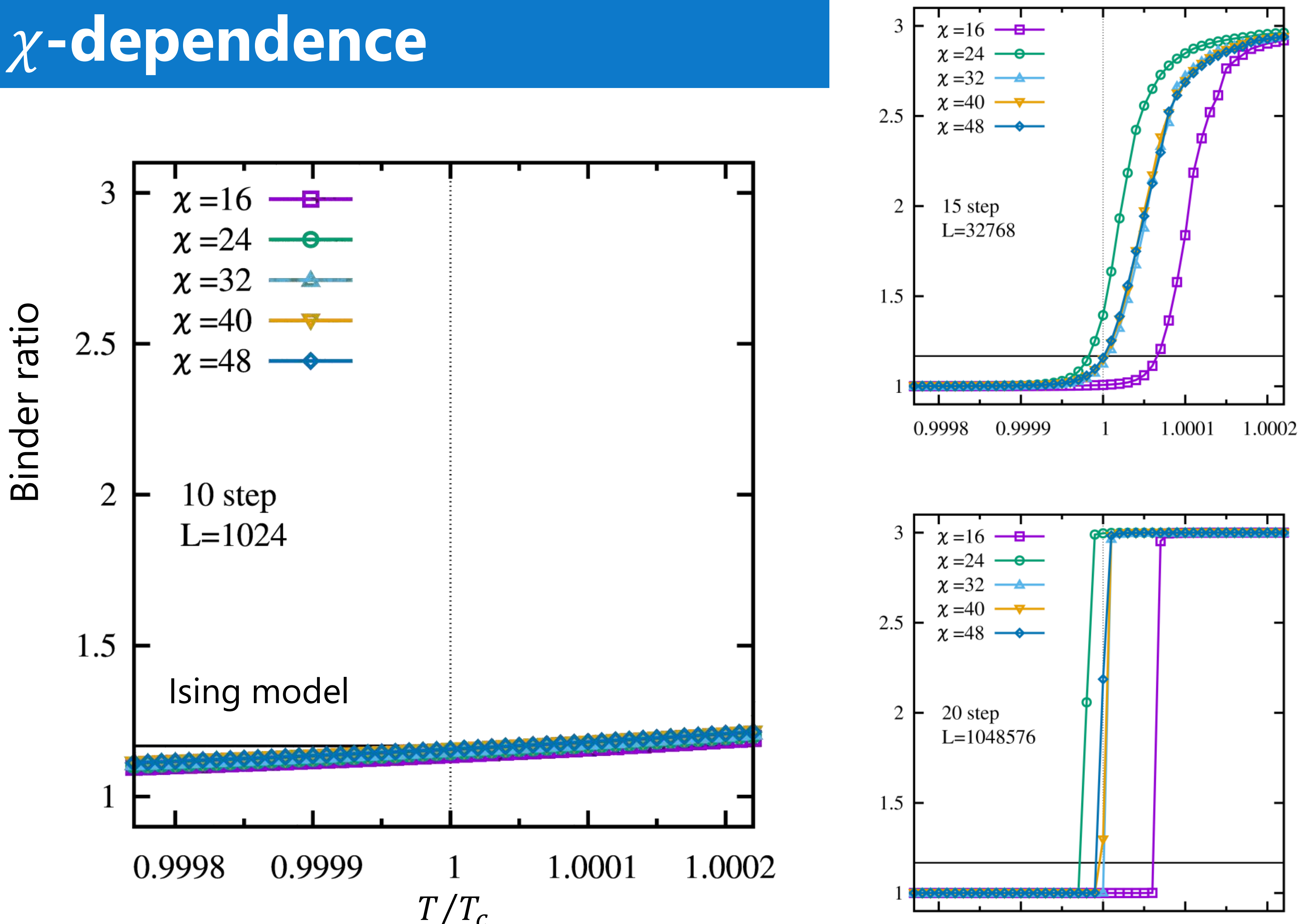
- Ising model ($q = 2$)



- q-state Potts model

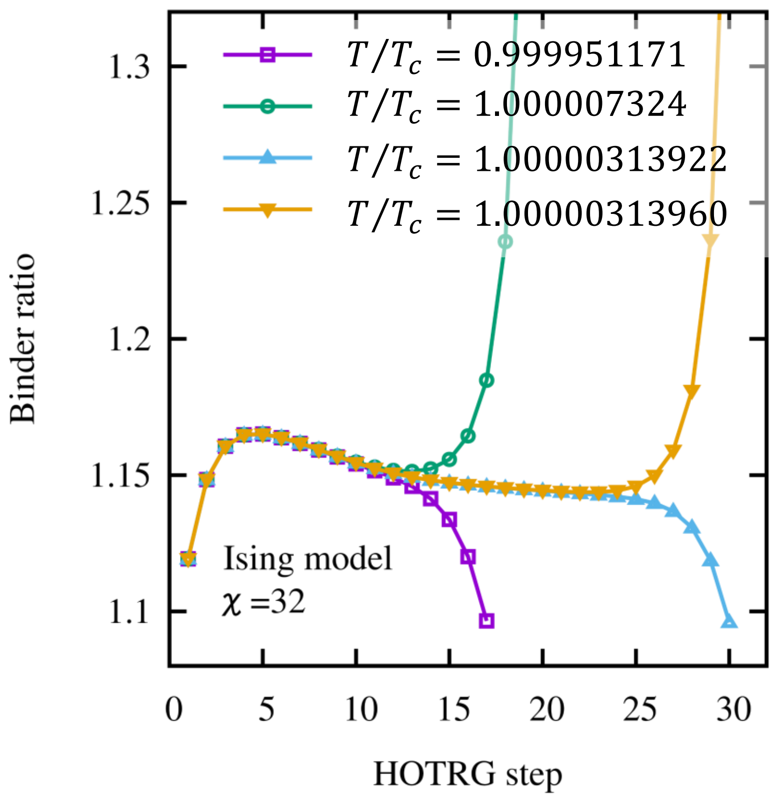


χ-dependence

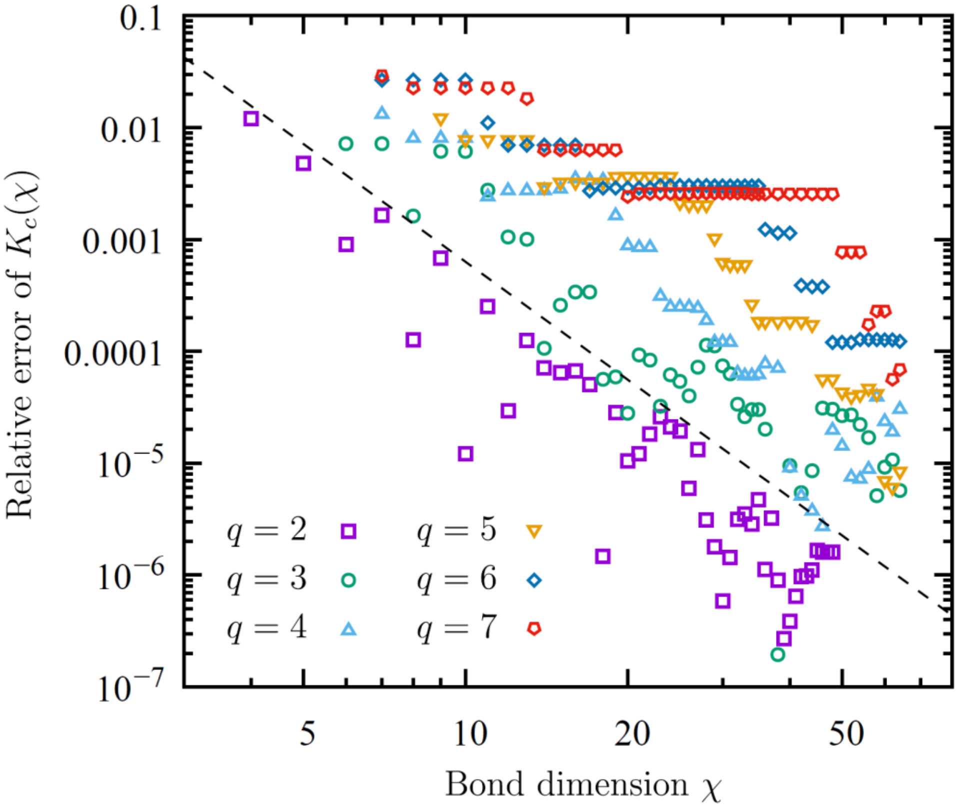


Transition temperature

Bisection search



χ-dependence

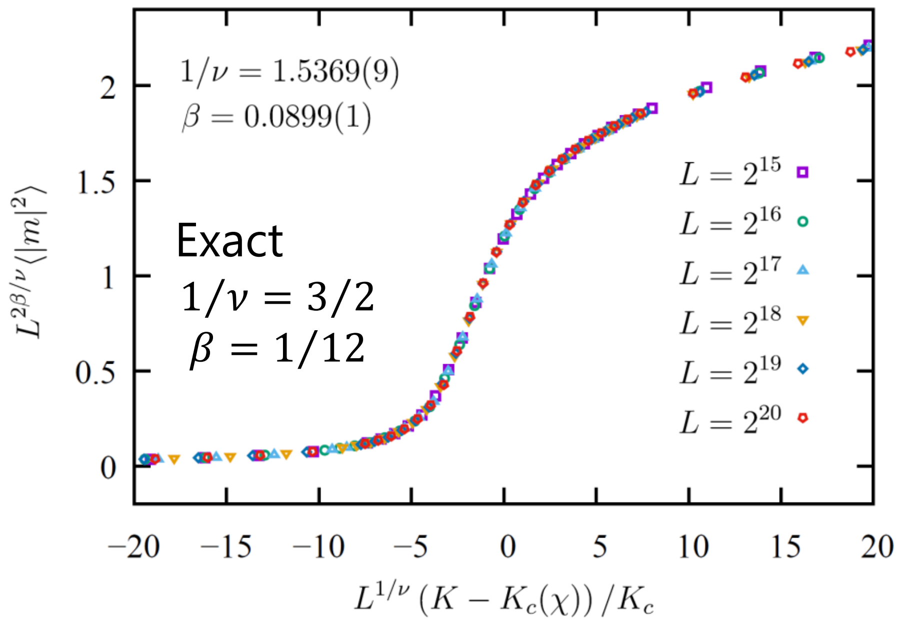


- Estimated values converge to the exact value with oscillation
- Relative error seems to decay in proportion to $\chi^{-3.5}$

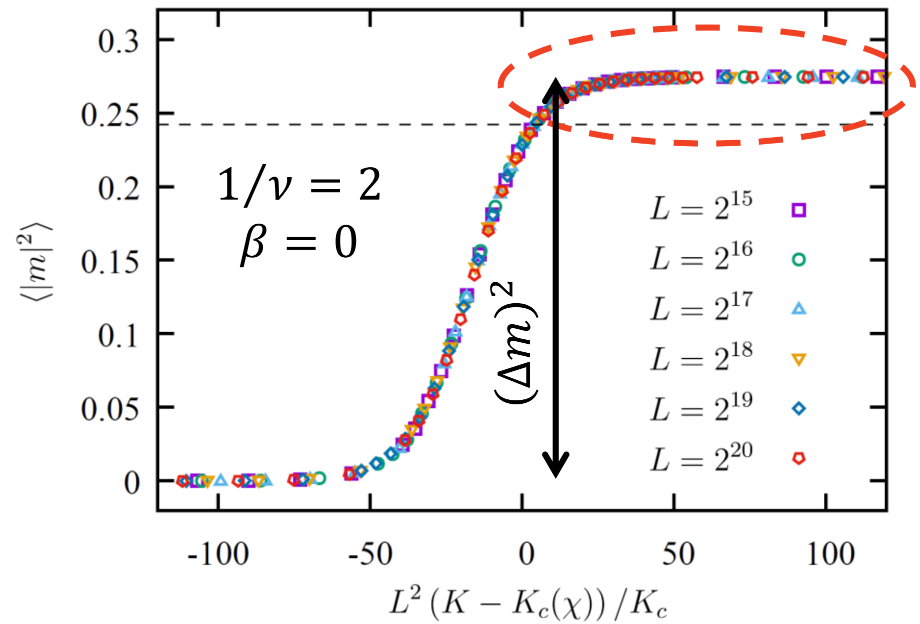
Finite-size scaling analysis

$$\langle |m|^2 \rangle \sim L^{-2\beta/\nu} g(L^{1/\nu}\delta) \qquad \delta \equiv (K - K_c(\chi))/K_c$$

4-state Potts model



5-state Potts model

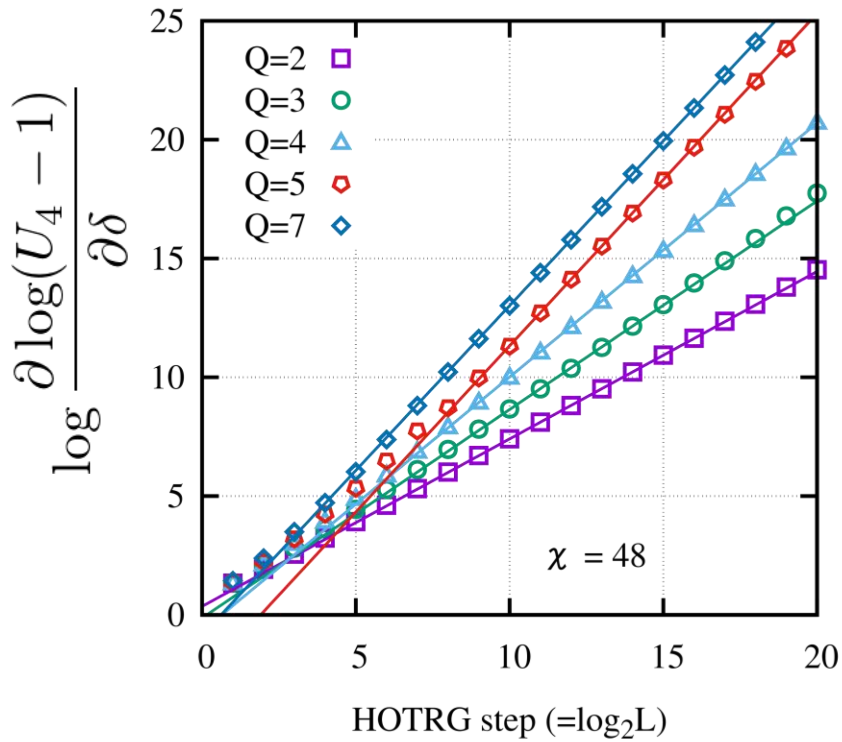


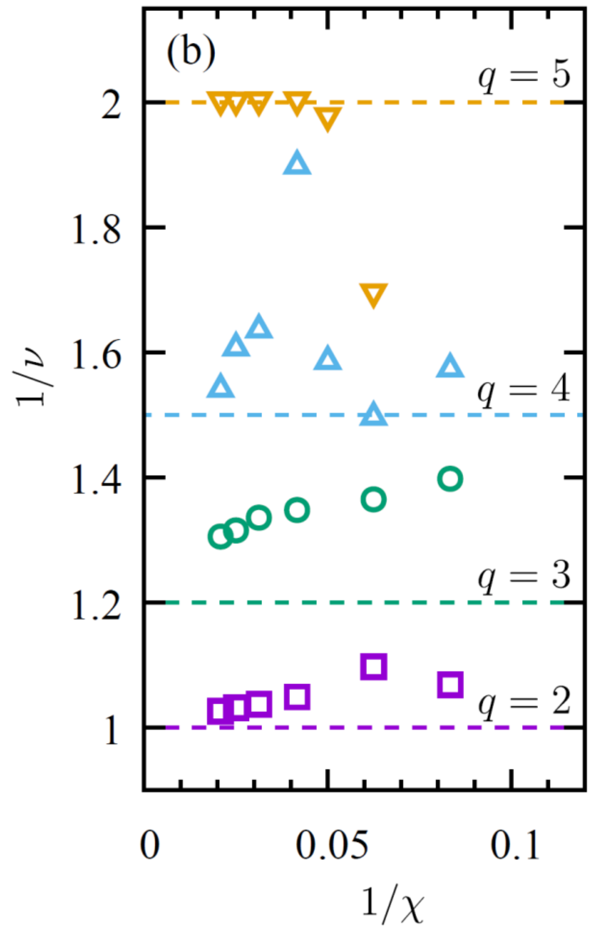
- ✓ Fitting by Bayesian scaling (Harada, 2011)
- ✓ Effect of logarithmic correction is small

- ✓ No fitting
- ✓ Plateau indicate the 1st-order phase transition.

Slope of Binder ratio

$$\log\left|\frac{\partial U_4}{\partial \delta}\right|_{\delta=0} = a + \frac{1}{\nu}\log L + \cdots$$

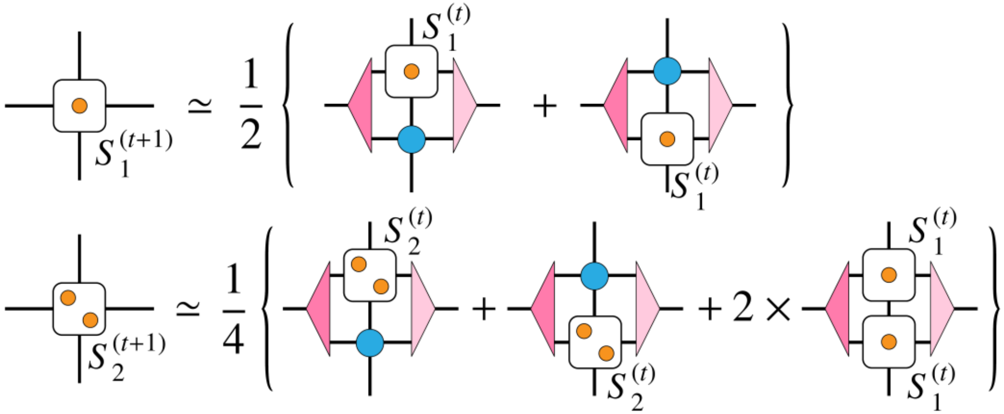




q	2	3	4	5	7
Exact	1	6/5	3/2	2	2
Slope	1.026(2)	1.305(10)	1.544(1)	2.006(2)	2.0001(5)

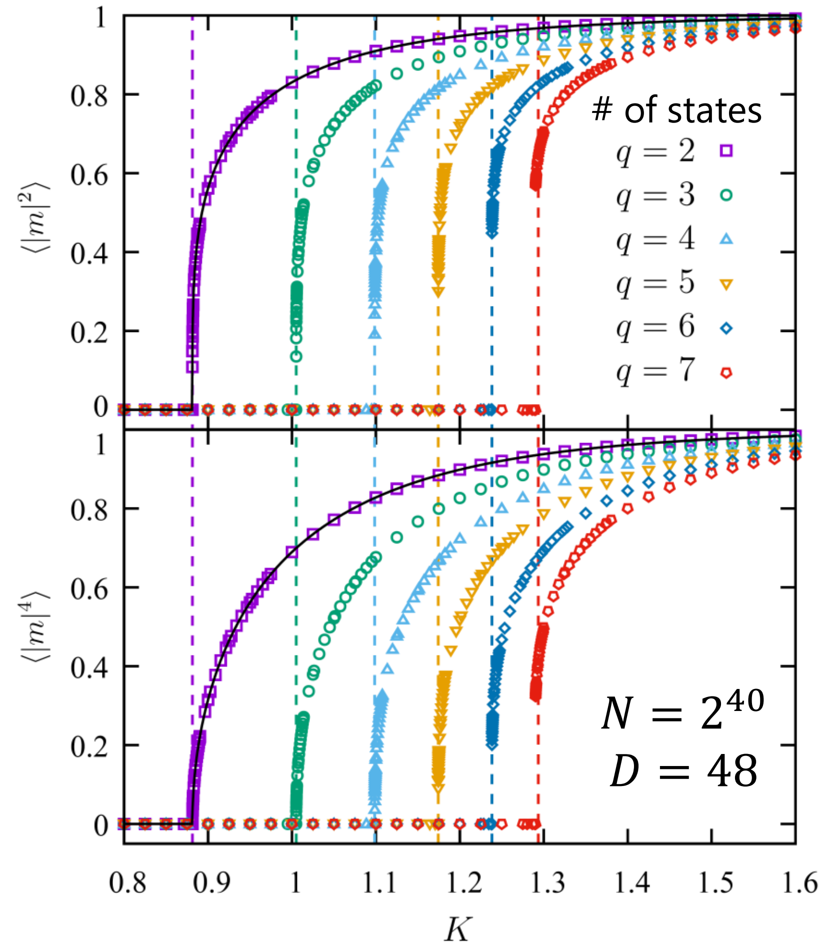
Summary of the 1st part

○ Renormalization of tensors with multiple impurities



- ✓ Beyond the system size which the Monte-Carlo method can treat.
- ✓ Finite-size scaling analysis of the magnetization and the Binder ratio.
- ✓ Distinguish weakly first-order and continuous phase transitions

Magnetization of Potts model



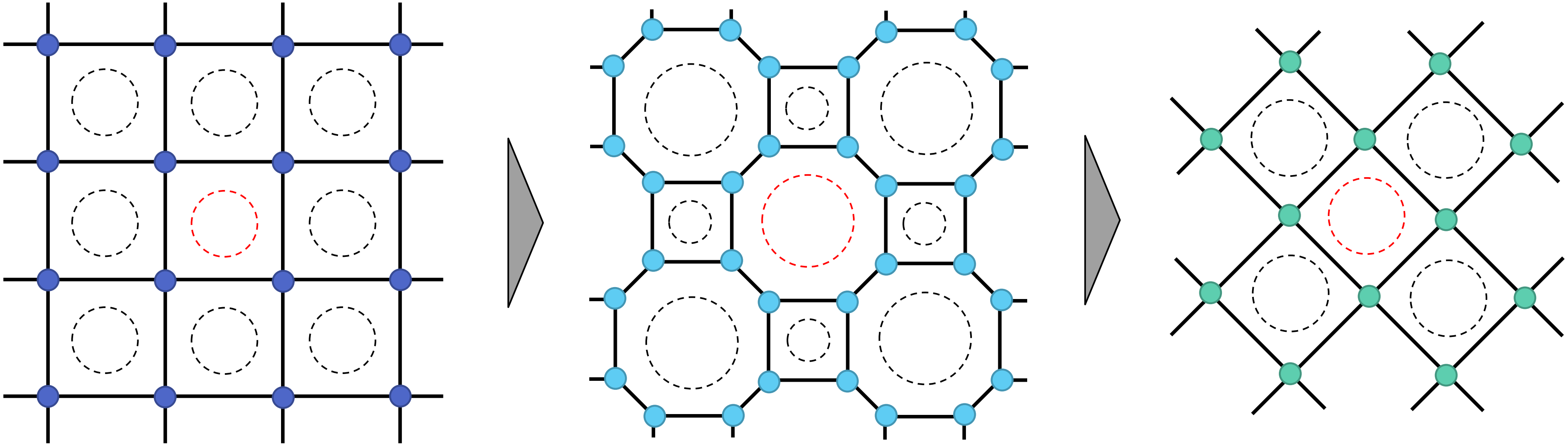
SM and N. Kawashima, Comput. Phys. Comm **236**, 65 (2019)

2^{nd} Part:

HOTRG with entanglement filtering

Unpublished results are removed in this part.

Internal Correlations

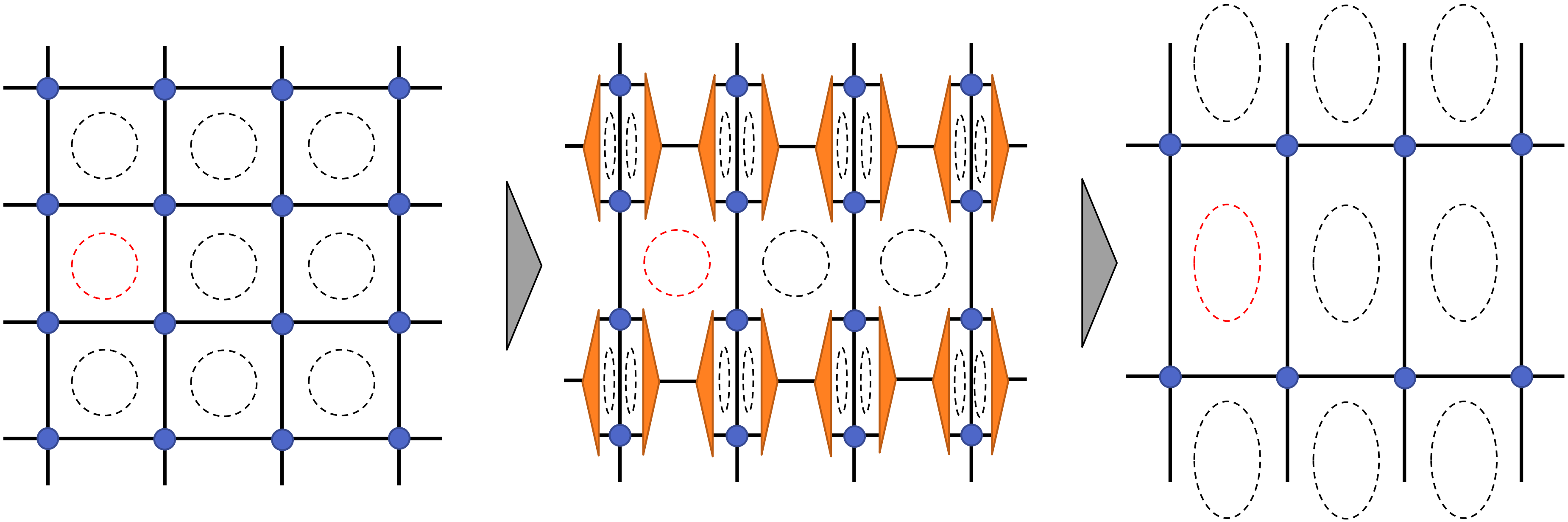


- Irrelevant correlations with $O(1)$ length scale
- Converge to a fictitious fixed-point tensor
    - Corner Double Line structure

We need to remove internal correlations within a loop.

"Entanglement Filtering"

Internal Correlations



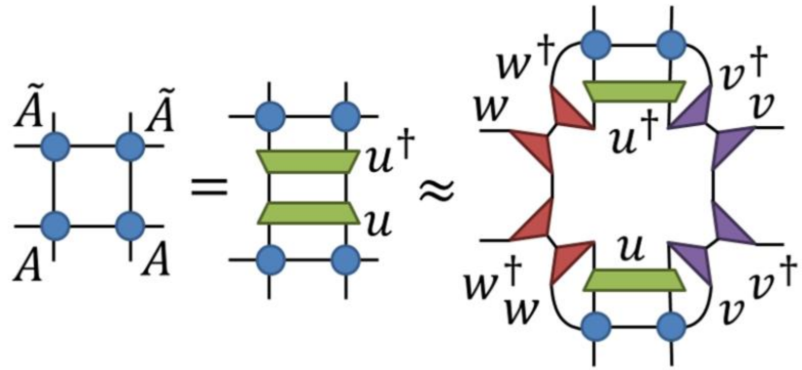
- Irrelevant correlations with $O(1)$ length scale
- Converge to a fictitious fixed-point tensor
  - Corner Double Line structure   Gu, Wen (2009)

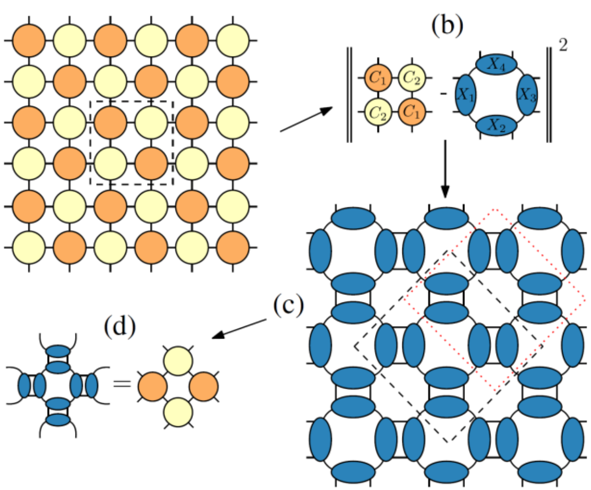
We need to remove internal correlations within a loop.

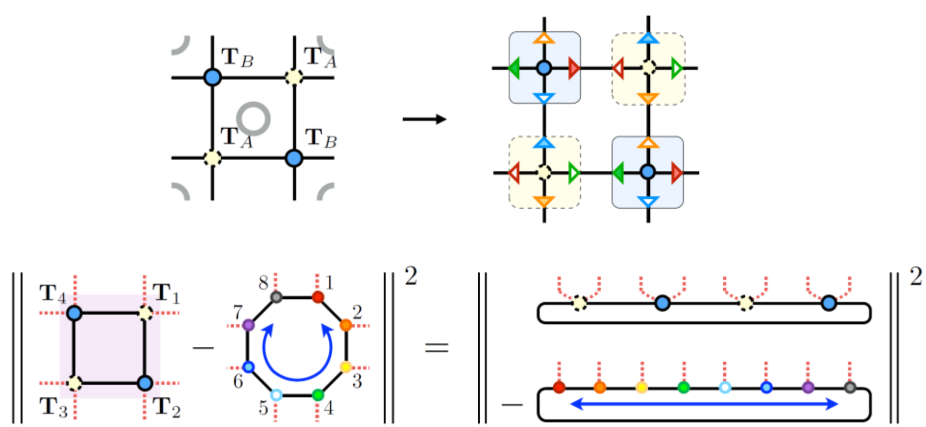
"Entanglement Filtering"

TRG with Entanglement Filtering

- TRG-base methods
  - **TEFT** [Gu, Wen (2009)]
  - **TNR** [Evenbly, Vidal (2015)]
  - **loop-TNR** [Yang, Gu, Wen (2017)]
  - **TNR+** [Bal, et al, (2017)]





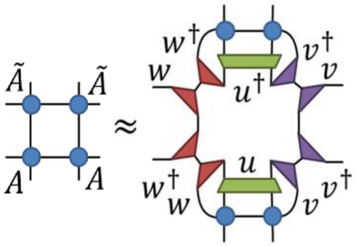


Only for 2-d systems

Entanglement Filtering

- TRG-base methods

Only for 2-d systems



  - TEFT [Gu, Wen (2009)]
  - TNR [Evenbly, Vidal (2015)]
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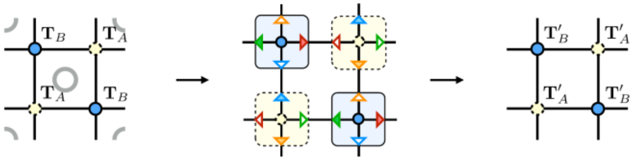
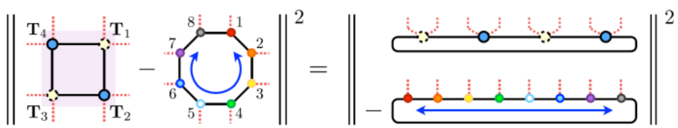
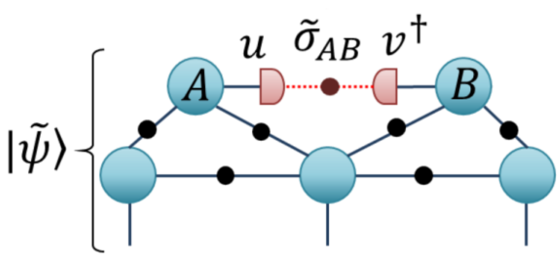


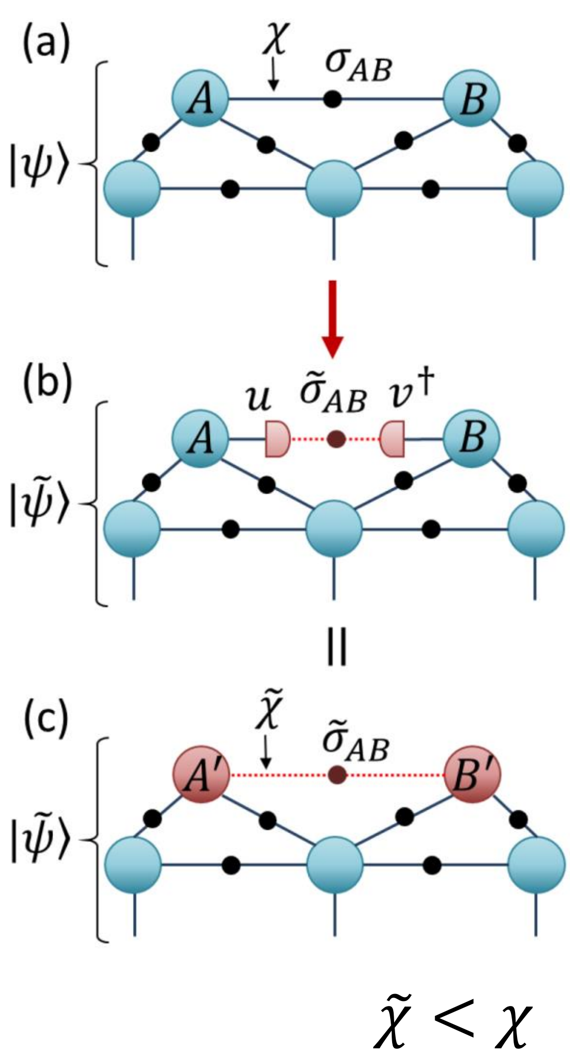


- General methods
  - Graph Independent Local Truncation [Hauru, Delcamp, Mizera (2017)]
  - Tensor Network Skeletonization [Ying (2016)]
  - Entanglement Branching [Harada (2018)]
  - Full Environment Truncation [Evenbly (2018)]



We consider a combination with HOTRG and FET.

Full Environment Truncation (FET)



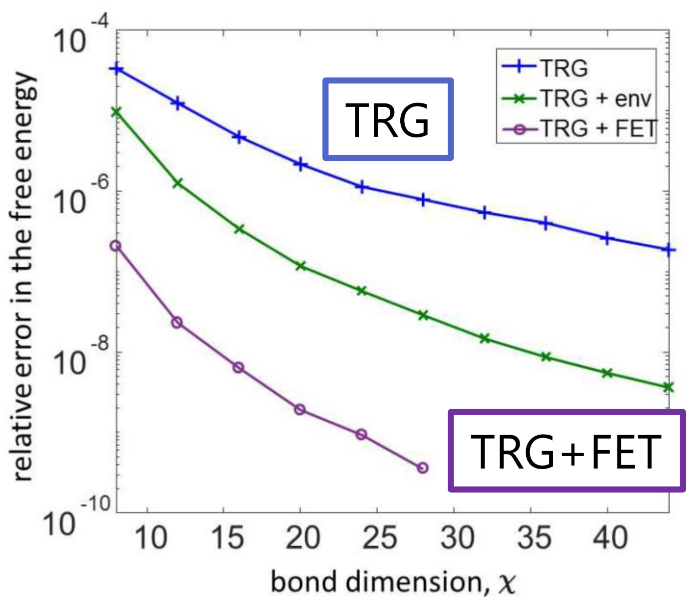
Evenbly (2018)

✓ Simple criterion

Optimize isometries u, v and bond diagonal matrix $\tilde{\sigma}_{AB}$ to minimize the difference

$$\left\| |\psi\rangle - |\tilde{\psi}\rangle \right\|^2$$

✓ TRG + FET



Thank you for your attention!