

A general method of the initial tensor construction for the TRG as the Steiner tree problem.

[K. N. arXiv:2307.14191]

[K. N., M.Schneider arXiv:2407.14226]

Katsumasa Nakayama (RIKEN)

Manuel Schneider (NYCU)

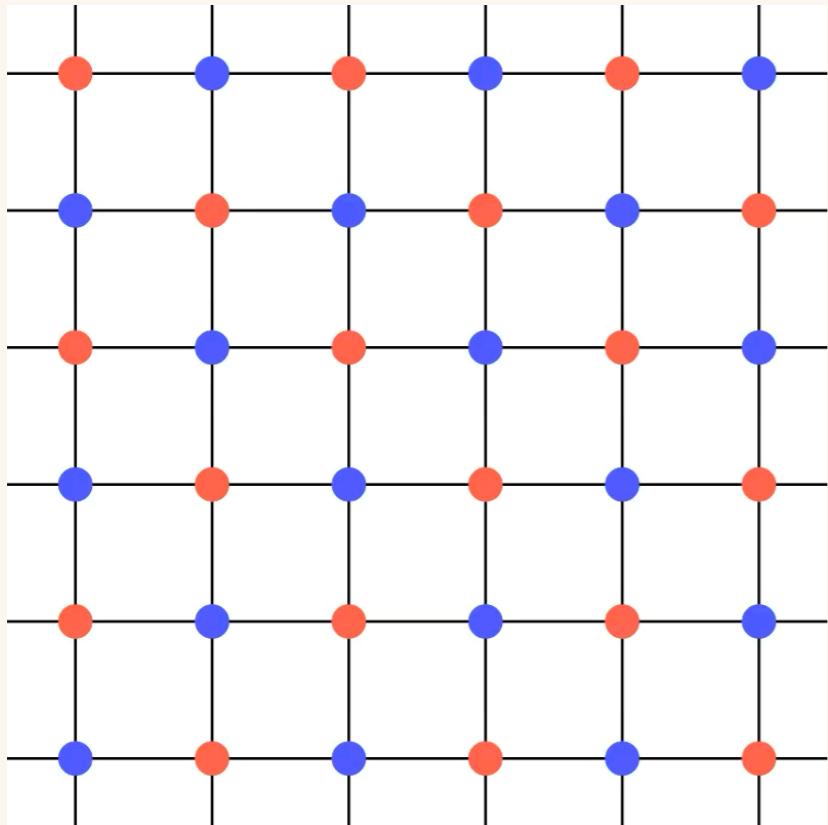
2024/09/25@Mainz Univ., Germany.

● Tensor renormalization group (TRG)

- ◊ What is the TRG?

→ TRG is approximated contraction of

(locally connected) Tensor network.



→ TRG require typical form of the tensor representation.

(Should be represented by graph)

$$Z = \text{Tr} \sum_{i \in \text{lattice}} A_{x_i y_i x'_i y'_i}$$

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

- ◊ What is the Tensor network?

→ Tensors are represented by each lattice points.

→ Indices are represented by line segments.

= Each index is only contained in two tensors.

Initial tensor network construction

● Tensor network rep. of 2dim Ising

- ◊ How to find tensor network representation?

(e.g.): 2dim Ising model (Partition function)

Boltzmann
factor

$$Z = \sum_{\sigma} \prod_{x,y} e^{\sigma_x \sigma_{x+1,y} + \sigma_x \sigma_{y+1}} = \sum_{\sigma} \prod_{x,y} K_{\sigma_x \sigma_{x+1,y} \sigma_{y+1}}$$

→ Tensors $K_{\sigma_x \sigma_{x+1,y} \sigma_{y+1}}$ do not construct tensor network.
(Index σ_x is included in three tensors)

$$K_{\sigma_x \sigma_{x+1,y} \sigma_{y+1}}, K_{\sigma_{x-1,y} \sigma_x \sigma_{x-1,y+1}}, K_{\sigma_{x,y-1} \sigma_{x+1,y-1} \sigma_{x,y}}$$



- ◊ Common method: (Taylor) expansion. and $\sigma^2 = 1$

Tensor network rep. of 2dim Ising

[H.H.Zhao et al. arXiv:1002.1405]

[Z.Y.Xie et al. arXiv:1201.1144] [Y.Liu et al. arXiv:1307.6543]

- Common method: (Taylor) expansion. and $\sigma^2 = 1$

$$e^{\beta\sigma_{x,y}\sigma_{x+1,y}} = \sum_{l_{x,y}=0}^1 (\cosh(\beta))^{1-l_{x,y}} (\sigma_{x,y}\sigma_{x+1,y} \sinh(\beta))^{l_{x,y}} = \sum_{l_{x,y}=0}^1 W_{\sigma_{x,y}l_{x,y}} W_{\sigma_{x+1,y}l_{x,y}}$$

x-direction: $\sigma \rightarrow l$ ↓
y-direction: $\sigma \rightarrow m$ ↓

$$W = \begin{pmatrix} \sqrt{\cosh(\beta)}, \sqrt{\sinh(\beta)} \\ \sqrt{\cosh(\beta)}, -\sqrt{\sinh(\beta)} \end{pmatrix}$$

$$Z = \sum_{\sigma} \prod_{x,y} e^{\sigma_{x,y}\sigma_{x+1,y} + \sigma_{x,y}\sigma_{x,y+1}}$$

$$= \sum_{\sigma,l,m} \prod_{x,y} W_{\sigma_{x,y},l_{x,y}} W_{\sigma_{x,y},l_{x-1,y}} W_{\sigma_{x,y},m_{x,y}} W_{\sigma_{x,y},m_{x,y-1}} = \sum_{l,m} \prod_{x,y} K_{l_{x,y}l_{x-1,y}m_{x,y}m_{x,y-1}}^{(\text{exp})}$$

Taking summation of σ first.

→ Tensors $K_{l_{x,y}l_{x-1,y}m_{x,y}m_{x,y-1}}^{(\text{exp})}$ construct tensor network.

(Index $l_{x,y}$ and $m_{x,y}$ are included in two tensors)

$$K_{l_{x,y}l_{x-1,y}m_{x,y}m_{x,y-1}}^{(\text{exp})}, K_{l_{x+1,y}l_{x,y}m_{x+1,y}m_{x+1,y-1}}^{(\text{exp})}$$

● Tensor network rep. by delta matrix

[K. Nakayama, M.Schneider arXiv:2407.14226]

- ◊ Key point: Expansion produces tensor network rep. using property, $\sigma^2 = 1$.

→ Problem: More complicated Boltzmann factor produces complicated form (difficult to find the tensor network).

- ◊ Our proposal: Index shift by delta matrix.

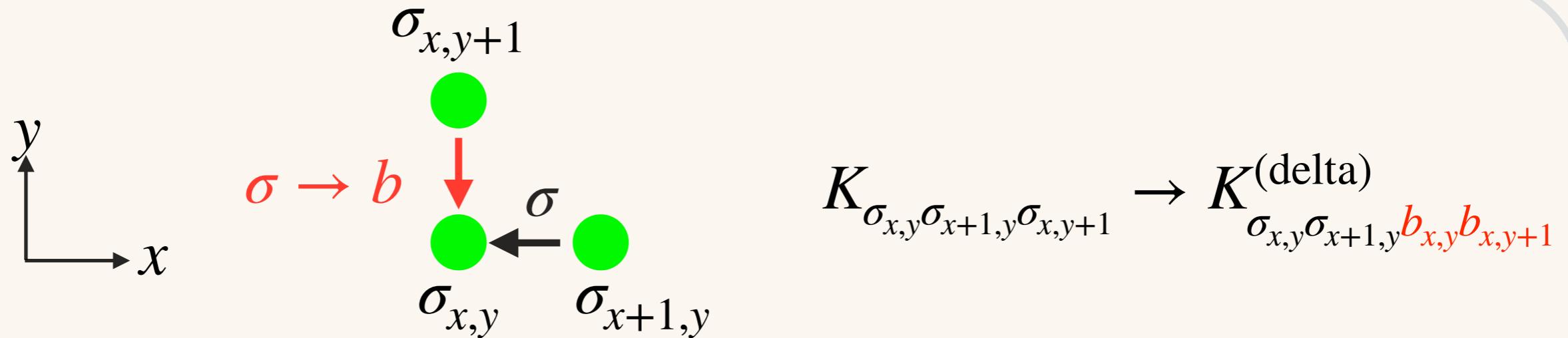
(e.g.): 2dim Ising model (periodic b.c.)

$$\begin{aligned}
 Z &= \sum_{\sigma} \prod_{x,y} K_{\sigma_x, y \sigma_{x+1}, y \sigma_{x, y+1}} = \sum_{\sigma, b} \prod_{x,y} K_{\sigma_x, y \sigma_{x+1}, y} b_{x, y+1} \delta_{b_{x, y+1} \sigma_{x, y+1}} = \sum_{\sigma, b} \prod_{x,y} K_{\sigma_x, y \sigma_{x+1}, y} b_{x, y+1} \delta_{b_{x, y} \sigma_{x, y}} \\
 &= \sum_{\sigma, b} \prod_{x,y} K_{\sigma_x, y \sigma_{x+1}, y}^{(\text{delta})} b_{x, y} b_{x, y+1}
 \end{aligned}$$

◆ index shift ($y + 1 \rightarrow y$) by δ

→ Tensor network constructed by $K_{\sigma_x, y \sigma_{x+1}, y}^{(\text{delta})} \equiv K_{\sigma_x, y \sigma_{x+1}, y} b_{x, y} b_{x, y+1} \times \delta_{b_{x, y} \sigma_{x, y}}$

● Schematic picture of the construction



(1): Dots \leftrightarrow original indices, $\{\sigma_{x,y}, \sigma_{x+1,y}, \sigma_{x,y+1}\}$

(2): Draw arrows to connect all dots.

(3): Arrow (except σ) \leftrightarrow Index shift by δ .

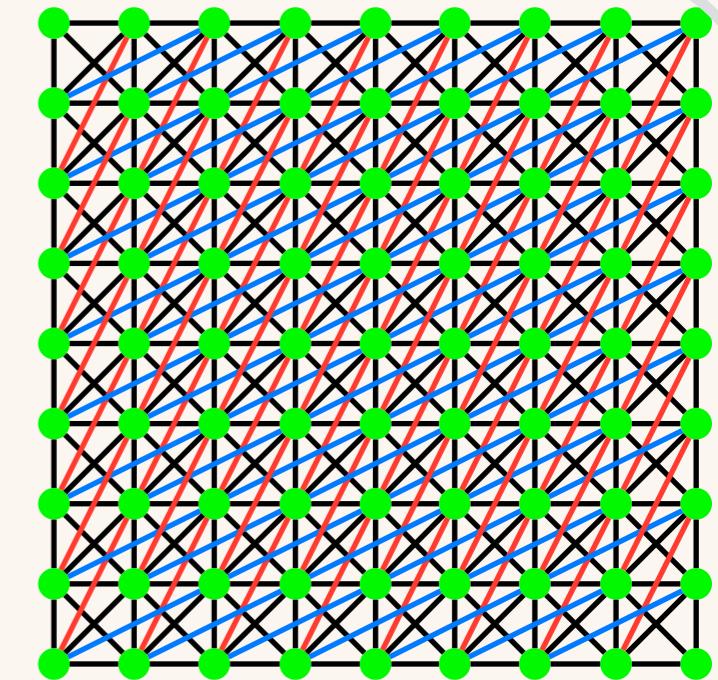
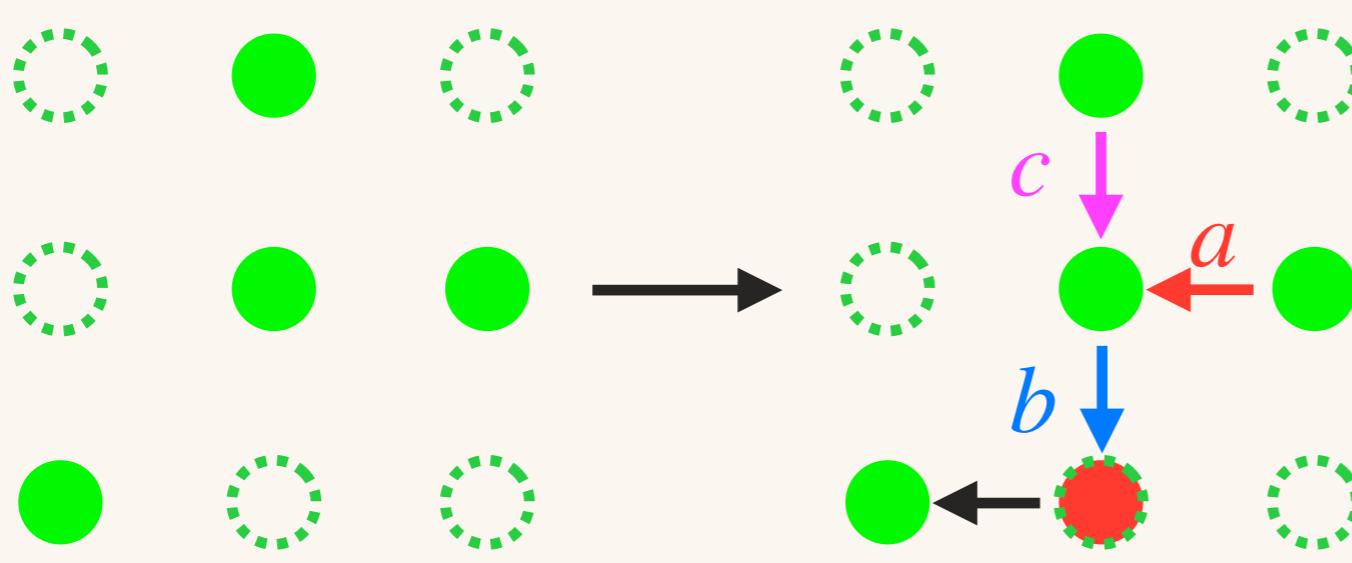


Arrows \leftrightarrow new indices, $\{\sigma, a\}$.

→ This method don't require any properties (equations).

(e.g. $\sigma^2 = 1$, $K_{\sigma_{x,y}\sigma_{x+1,y}\sigma_{x,y+1}} = e^{\sigma_{x,y}\sigma_{x+1,y} + \sigma_{x,y}\sigma_{x,y+1}}$)

Generalization: $J_1 - J_2 + \alpha$



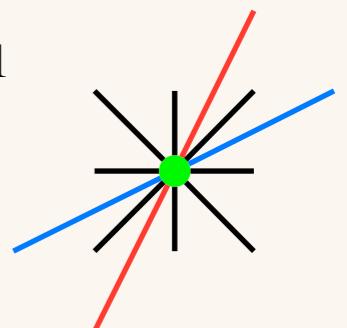
$$K_{\sigma_{x,y}\sigma_{x+1,y+1}\sigma_{x+2,y+1}\sigma_{x+1,y+2}} \rightarrow K''_{[\sigma a]_{x,y}[\sigma a]_{x+1,y}[bc]_{x,y}[bc]_{x,y+1}}$$

$$e^{h(\sigma_{x,y} + \sigma_{x+1,y+1} + \sigma_{x+2,y+1} + \sigma_{x+1,y+2})}$$

$$e^{J_1(\sigma_{x+1,y+1}\sigma_{x+2,y+1} + \sigma_{x+1,y+1}\sigma_{x+1,y+2})} e^{J_2(\sigma_{x,y}\sigma_{x+1,y+1} + \sigma_{x+2,y+1}\sigma_{x+1,y+2})} e^{g_1\sigma_{x,y}\sigma_{x+2,y+1} + g_2\sigma_{x,y}\sigma_{x+1,y+2}}$$

$$e^{t_1\sigma_{x,y}\sigma_{x+2,y+1}\sigma_{x+1,y+2} + t_2\sigma_{x,y}\sigma_{x+1,y+1}\sigma_{x+2,y+1} + t_3\sigma_{x,y}\sigma_{x+1,y+1}\sigma_{x+1,y+2} + t_4\sigma_{x+1,y+1}\sigma_{x+2,y+1}\sigma_{x+1,y+2}}$$

$$e^{e_1\sigma_{x,y}\sigma_{x+1,y+1}\sigma_{x+2,y+1}\sigma_{x+1,y+2}}$$



→ Added red dot is Steiner point.

→ In general: Rectilinear Steiner tree problem
(generalization of the traveling salesman problem).

→ K'' has only $4 \times 4 \times 4 \times 4$ indices.

● J1-J2+ α : Frustrated system with 12 parameters.

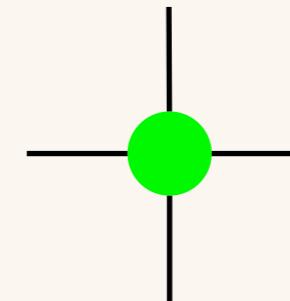
1-spin

$$e^{h(\sigma_{x,y} + \sigma_{x+1,y+1} + \sigma_{x+2,y+1} + \sigma_{x+1,y+2})}$$



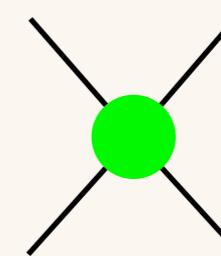
2-spin (J1)

$$e^{J_1^{(x)}\sigma_{x+1,y+1}\sigma_{x+2,y+1} + J_1^{(y)}\sigma_{x+1,y+1}\sigma_{x+1,y+2}}$$



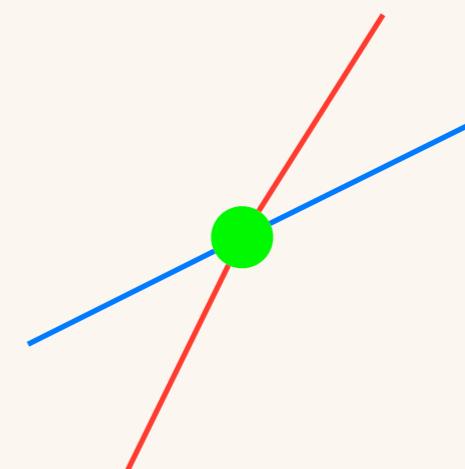
2-spin (J2)

$$e^{J_2^{(a)}\sigma_{x,y}\sigma_{x+1,y+1} + J_2^{(b)}\sigma_{x+2,y+1}\sigma_{x+1,y+2}}$$



2-spin (g1,g2)

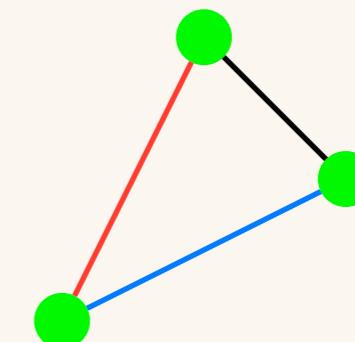
$$e^{g_1\sigma_{x,y}\sigma_{x+2,y+1} + g_2\sigma_{x,y}\sigma_{x+1,y+2}}$$



● J1-J2+ α : Frustrated system with 12 parameters.

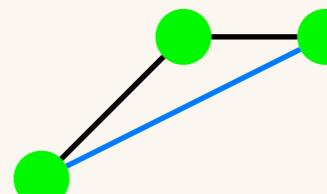
3-spin t1

$$e^{t_1 \sigma_{x,y} \sigma_{x+2,y+1} \sigma_{x+1,y+2}}$$



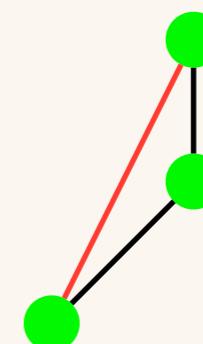
3-spin t2

$$e^{t_2 \sigma_{x,y} \sigma_{x+1,y+1} \sigma_{x+2,y+1}}$$



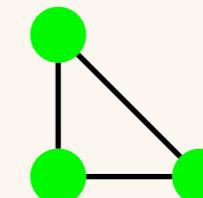
3-spin t3

$$e^{t_3 \sigma_{x,y} \sigma_{x+1,y+1} \sigma_{x+1,y+2}}$$



3-spin t4

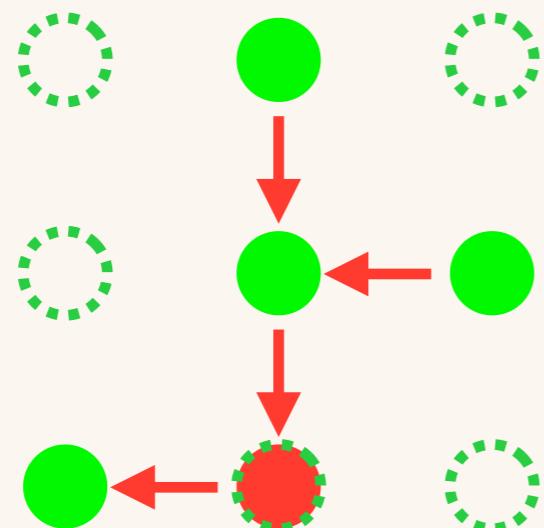
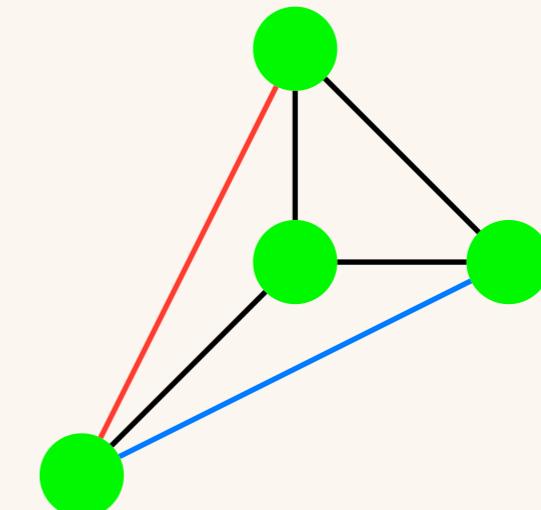
$$e^{t_4 \sigma_{x+1,y+1} \sigma_{x+2,y+1} \sigma_{x+1,y+2}}$$



● J1-J2+ α : Frustrated system with 12 parameters.

4-spin

$$e^{e_1 \sigma_{x,y} \sigma_{x+1,y+1} \sigma_{x+2,y+1} \sigma_{x+1,y+2}}$$



$$= K''_{[\sigma a]_{x,y} [\sigma a]_{x+1,y} [bc]_{x,y} [bc]_{x,y+1}}$$

◊ Num. of kind of interaction (parameters):

$$\left(\sum_{k=2}^4 {}_4C_k \right) + 1 = 2^4 - 4 = 12$$

→ K'' has only $4 \times 4 \times 4 \times 4$ indices.

● Note: Traveling salesman problem.

- ◊ Traveling salesman problem (famous NP-hard):
Find shortest line segments (roads) between dots (towns)
to connect every dots.



- ◊ Steiner tree problem:
Traveling salesman + we can freely add dots (town)



- ◊ Rectilinear Steiner tree problem: (NP-hard (complete))
Steiner tree on the lattice.
...dots on lattice points, line segments only on the links.

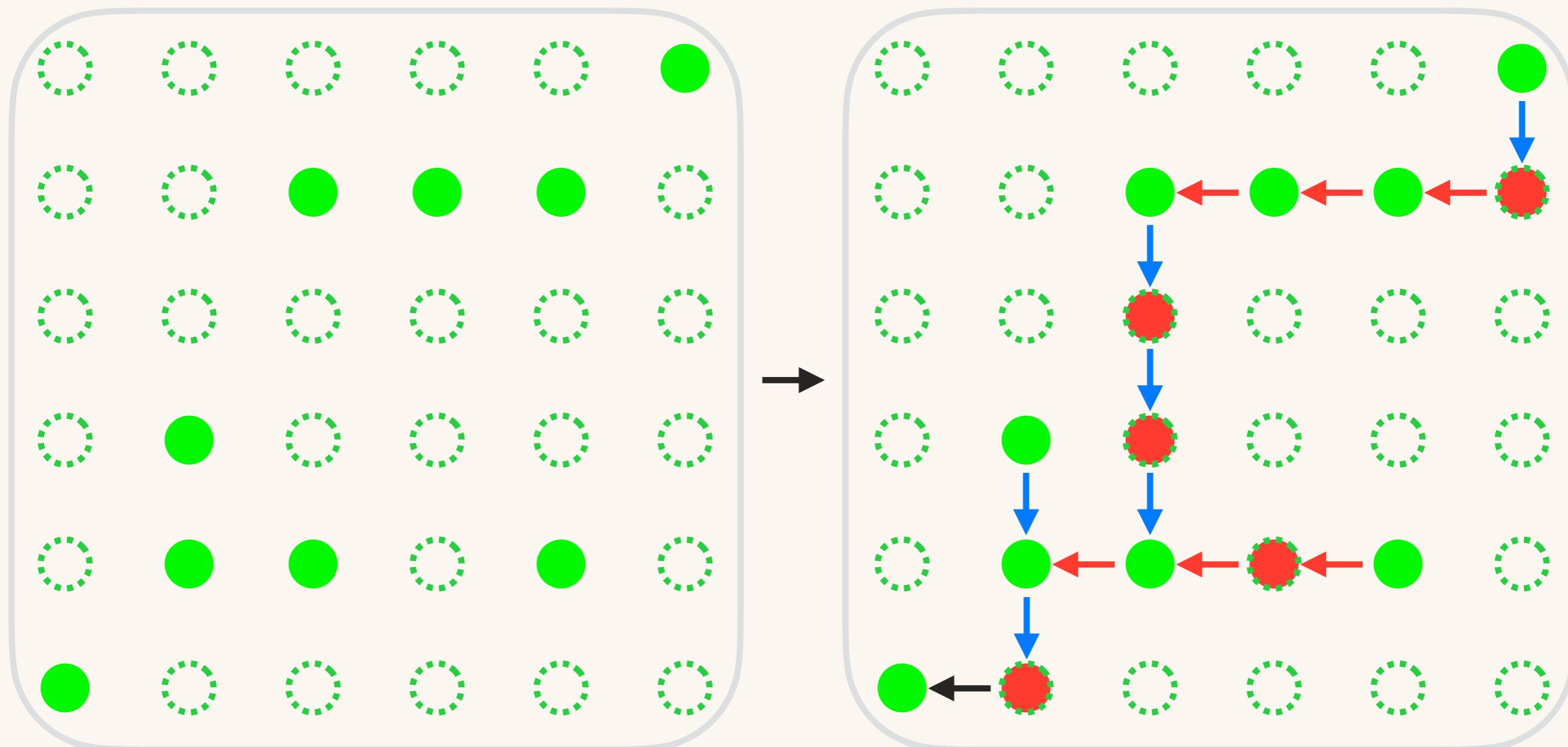
→ Index size of tensor = $D_{\text{ini}}^{(\text{Road length})}$

→ Long range interaction becomes harder.

→ Mild long ranges (e.g. plaquette, clover, etc.) are not hard.¹²

● Note: (Rectilinear) Steiner tree problem

- ◊ Rectilinear Steiner tree problem: Find shortest line segment on the lattice between dots with additional dots.

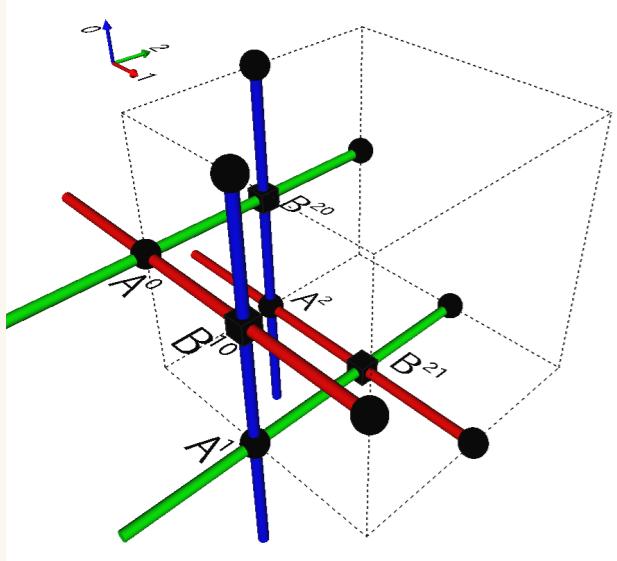


→ Num. of interaction (parameters) order $\sim O(\sum {}_9 C_k = 2^9)$
 → K'' has $2^6 \times 2^6 \times 2^7 \times 2^7$ indices.

Tensor network rep. of 3dim Z2 gauge theory

[Y.Liu et al. arXiv:1307.6543] [Y.Kuramashi, Y.Yoshimura, arXiv:1808.08025]

- Common method: (Taylor) expansion. and $\sigma^2 = 1$



$$Z = 2^{-3V} \sum_{\sigma} \prod_{n, \mu > \nu} e^{-\beta \sigma_{n,\mu} \sigma_{n+\hat{\mu},\nu} \sigma_{n+\hat{\nu},\mu} \sigma_{n,\nu}}$$

$$e^{-\beta \sigma_{n,\mu} \sigma_{n+\hat{\mu},\nu} \sigma_{n+\hat{\nu},\mu} \sigma_{n,\nu}} = \cosh \beta \sum_{p=0}^1 (\tanh \beta)^p (\sigma_{n,\mu} \sigma_{n+\hat{\mu},\nu} \sigma_{n+\hat{\nu},\mu} \sigma_{n,\nu})^p$$

$$A_{pqrs} = \text{mod}(1 + p + q + r + s, 2)$$

$$B_{pqrs} = (\tanh \beta)^{(p+q+r+s)/4} \delta_{pq} \delta_{pr} \delta_{rs}$$

$$Z = \sum_{g,h,i,j,k,l} \prod_n T_{[gh]_{x,y,z} [gh]_{x+1,y,z} [ij]_{x,y,z} [ij]_{x,y+1,z} [kl]_{x,y,z} [kl]_{x,y,z+1}}^{(\text{exp})}$$

$$T_{[xX][x'X'][yY][y'Y'][zZ][z'Z']}^{(\text{exp})} = (\cosh \beta)^3 \sum_{a,b,c,d,e,f} A_{cyZe} A_{fzx b} A_{dYXa} B_{bx'y'c} B_{aX'Z'e} B_{fz'Y'd}$$

- In general: Any kind of expansion produces tensor network.

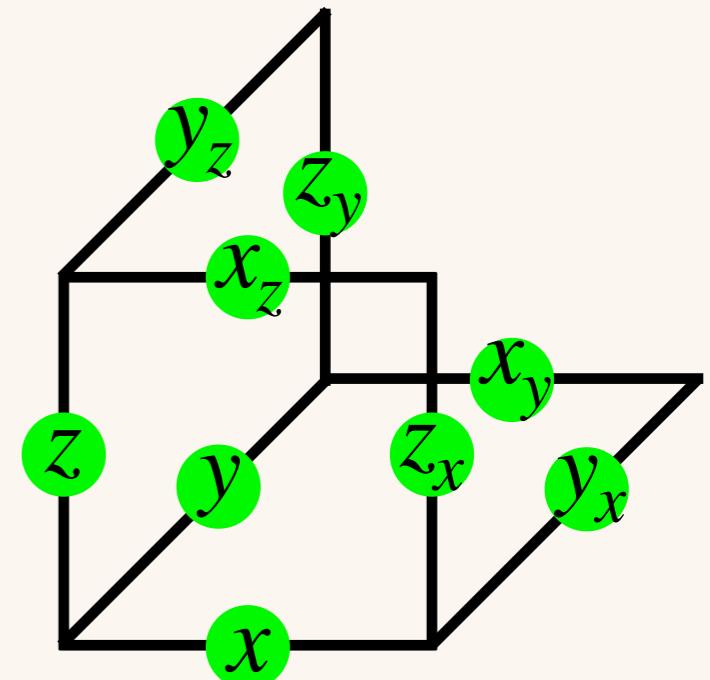
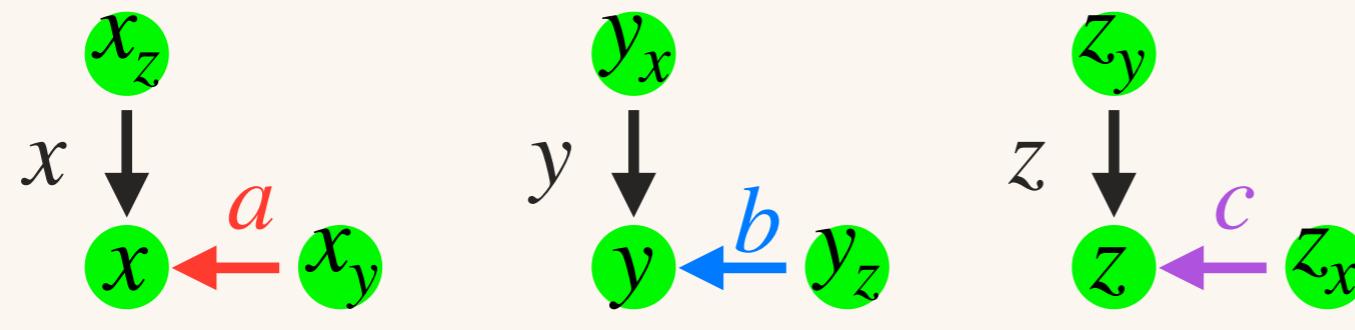
(Character for gauge theory, Orthogonal function, Taylor...) 14

● Tensor network rep. of 3dim Z2 gauge theory

- ◇ Our proposal: Index shift by delta matrix.

$$Z = 2^{-3V} \sum_{\sigma} \prod_{n, \mu > \nu} e^{-\beta \sigma_{n,\mu} \sigma_{n+\hat{\mu},\nu} \sigma_{n+\hat{\nu},\mu} \sigma_{n,\nu}} = \sum_{\sigma} \prod_{n, \mu > \nu} e^{-\beta(x x_{\hat{y}} y y_{\hat{x}} + x x_{\hat{z}} z z_{\hat{x}} + y y_{\hat{z}} z z_{\hat{y}})}/8$$

→ x, y, z are independent with each other.

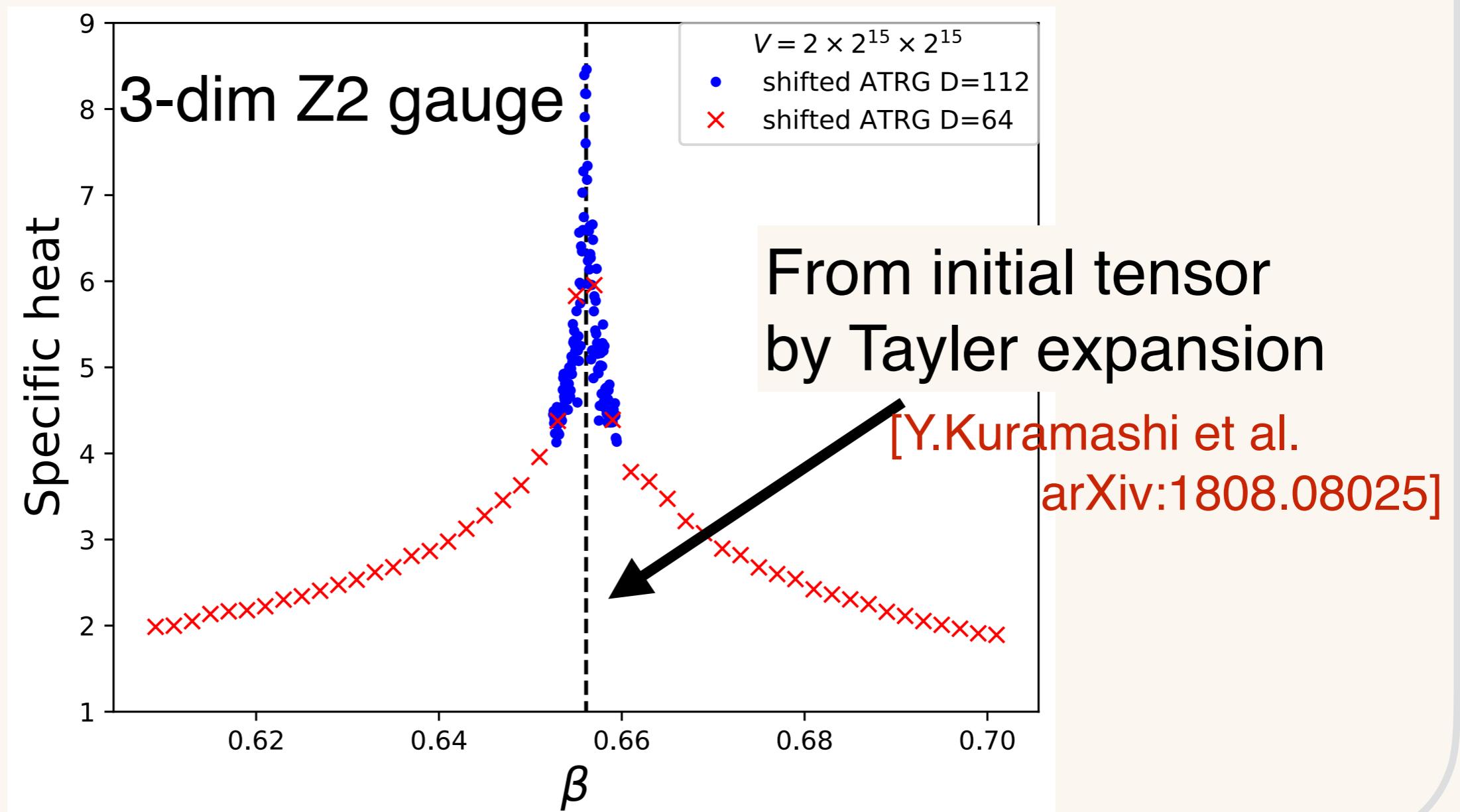


$$K_{x x_y x_z y y_z y_x z z_x z_y} \rightarrow K''_{[x \textcolor{blue}{b}] [x \textcolor{blue}{b}]_z [y \textcolor{magenta}{c}] [y \textcolor{magenta}{c}]_x [z \textcolor{red}{a}] [z \textcolor{red}{a}]_y}$$

→ K'' has only $4 \times 4 \times 4 \times 4 \times 4 \times 4$ indices.

● Critical temperature of 3dim Z2 gauge theory

- ◊ Numerical calc. by (modified) ATRG + impurity method



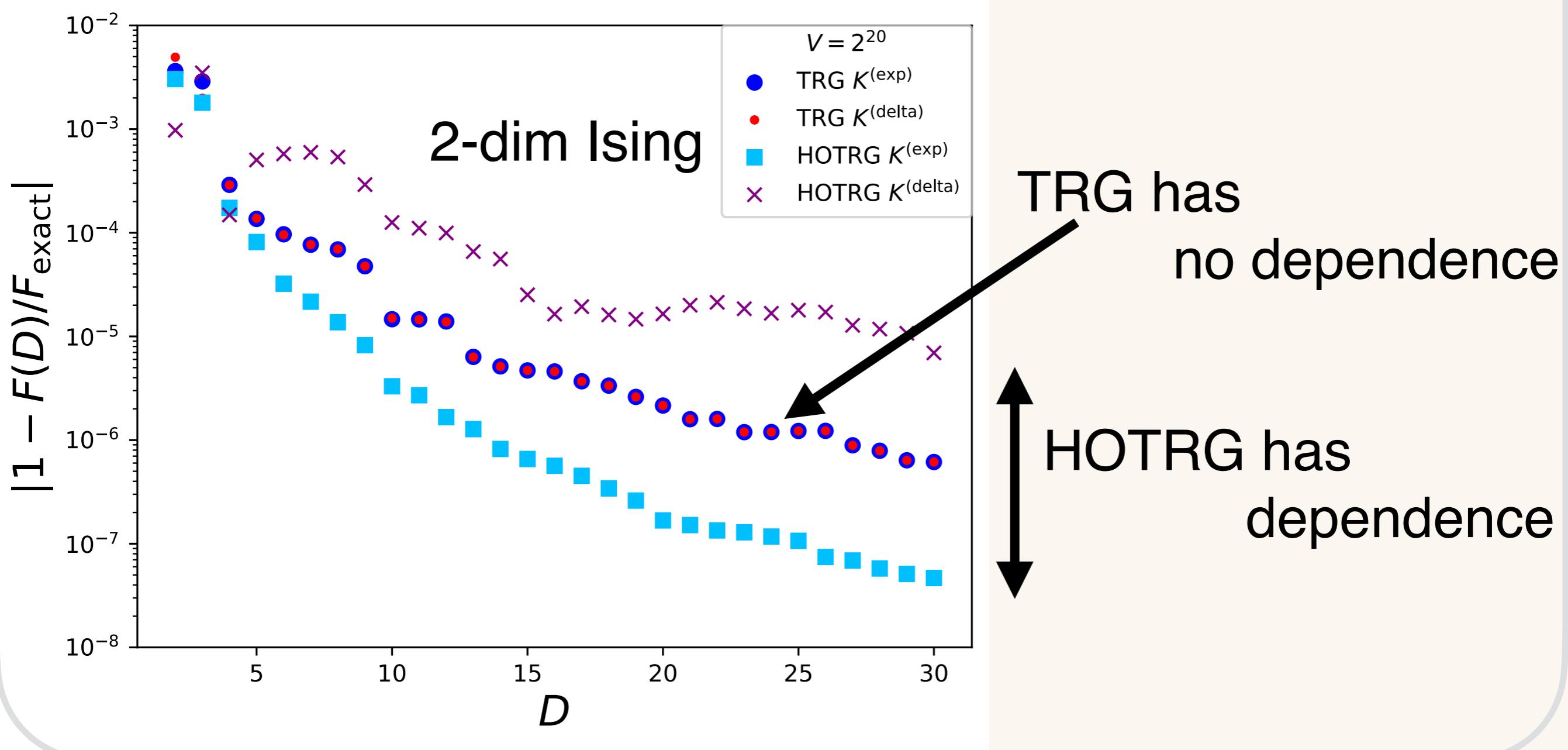
→ Our method produces correct result for critical temperature.

Initial tensor network dependence

Initial tensor dependence

- Now we can construct initial tensor by simple method.

→ We did not say our method produces best precision.



→ But we can eliminate this initial tensor dependence.

● Boundary TRG

[S. Iino et al. arXiv:1905.02351]

[K. N., M. Schneider arXiv:2407.14226]

- ◊ Original HOTRG: choose U or V by minimizing the norm.

$$C_U = \left\| \begin{array}{c} K \\ \text{---} \\ K \end{array} - \begin{array}{c} U^{\dagger(\text{HOTRG})} \\ \text{---} \\ U^{(\text{HOTRG})} \end{array} \right\|^2$$

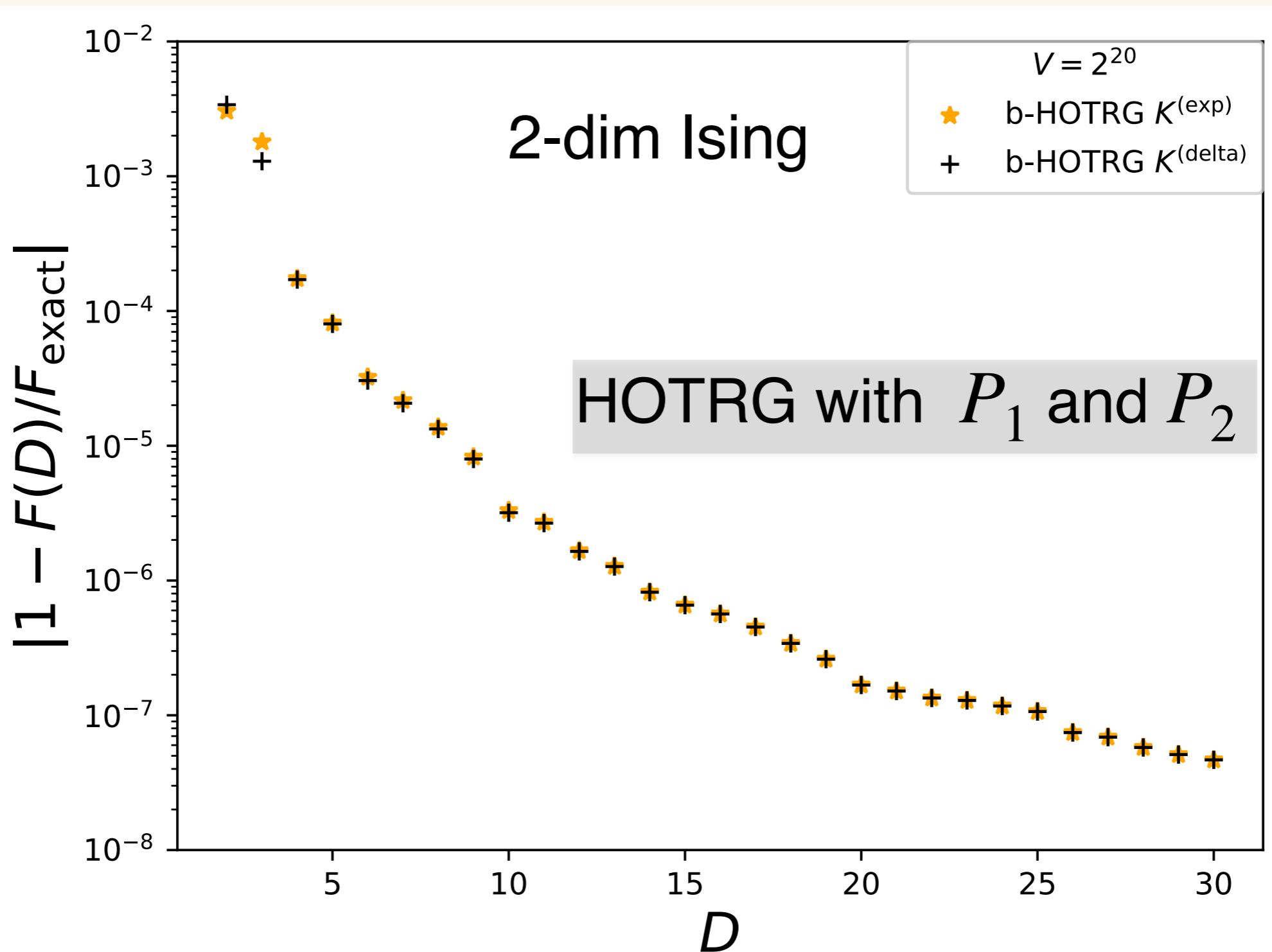
$$C_V = \left\| \begin{array}{c} K \\ \text{---} \\ K \end{array} - \begin{array}{c} V^{(\text{HOTRG})} \\ \text{---} \\ V^{\dagger(\text{HOTRG})} \end{array} \right\|^2$$

- ◊ HOTRG with boundary TRG:
construct P_1, P_2 by U and V .

$$C_{P_1, P_2} = \left\| \begin{array}{c} K \\ \text{---} \\ K \end{array} - \begin{array}{c} P_1^{(\text{bHOTRG})} \\ \text{---} \\ P_2^{(\text{bHOTRG})} \end{array} \right\|^2$$

→ Generalization from U or V to P_1 and P_2 can be done
for any other TRG methods.¹⁹

Boundary HOTRG



→ HOTRG with P_1 and P_2 is initial tensor independent.

Boundary TRG for ATRG and MDTRG

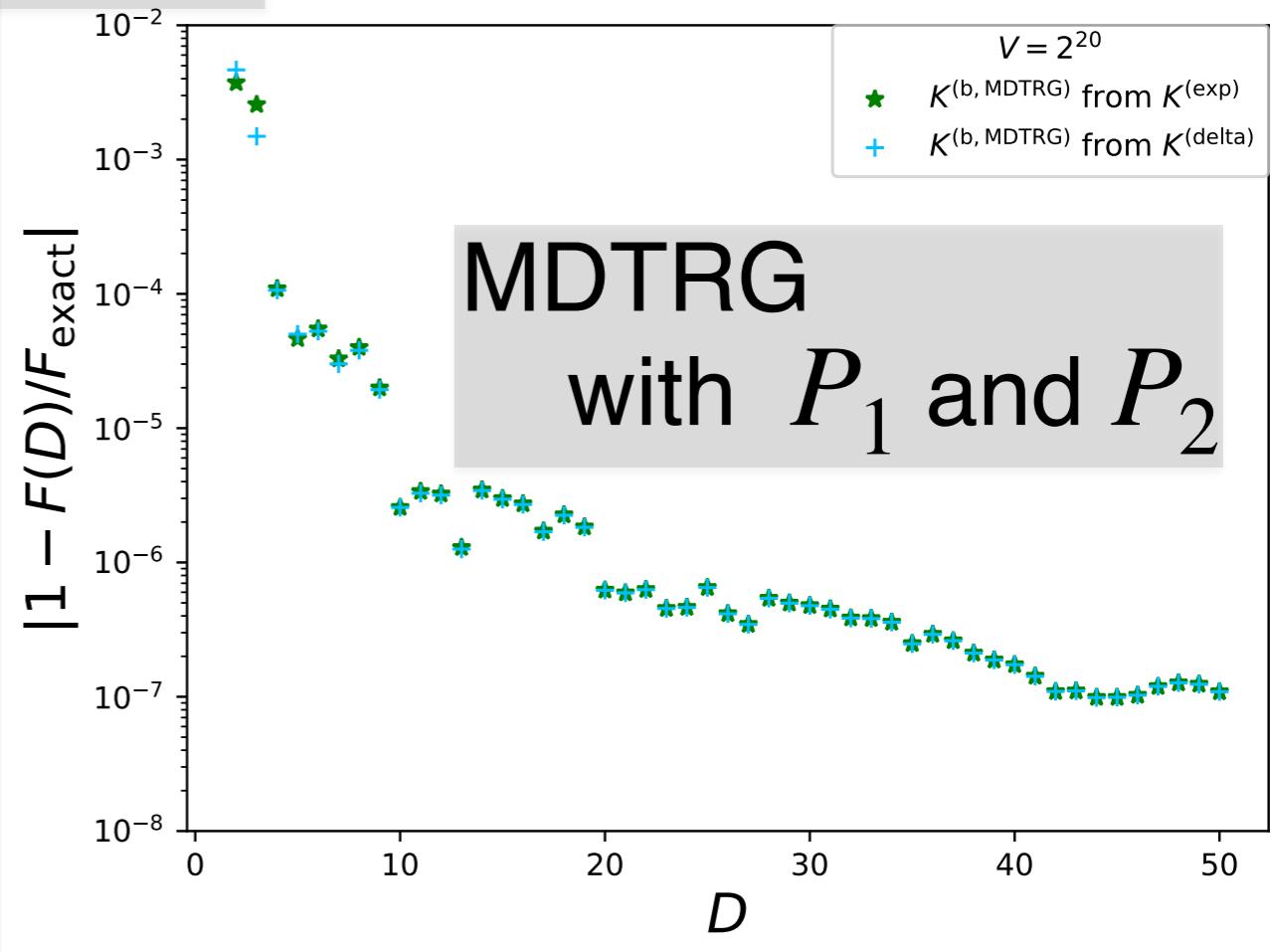
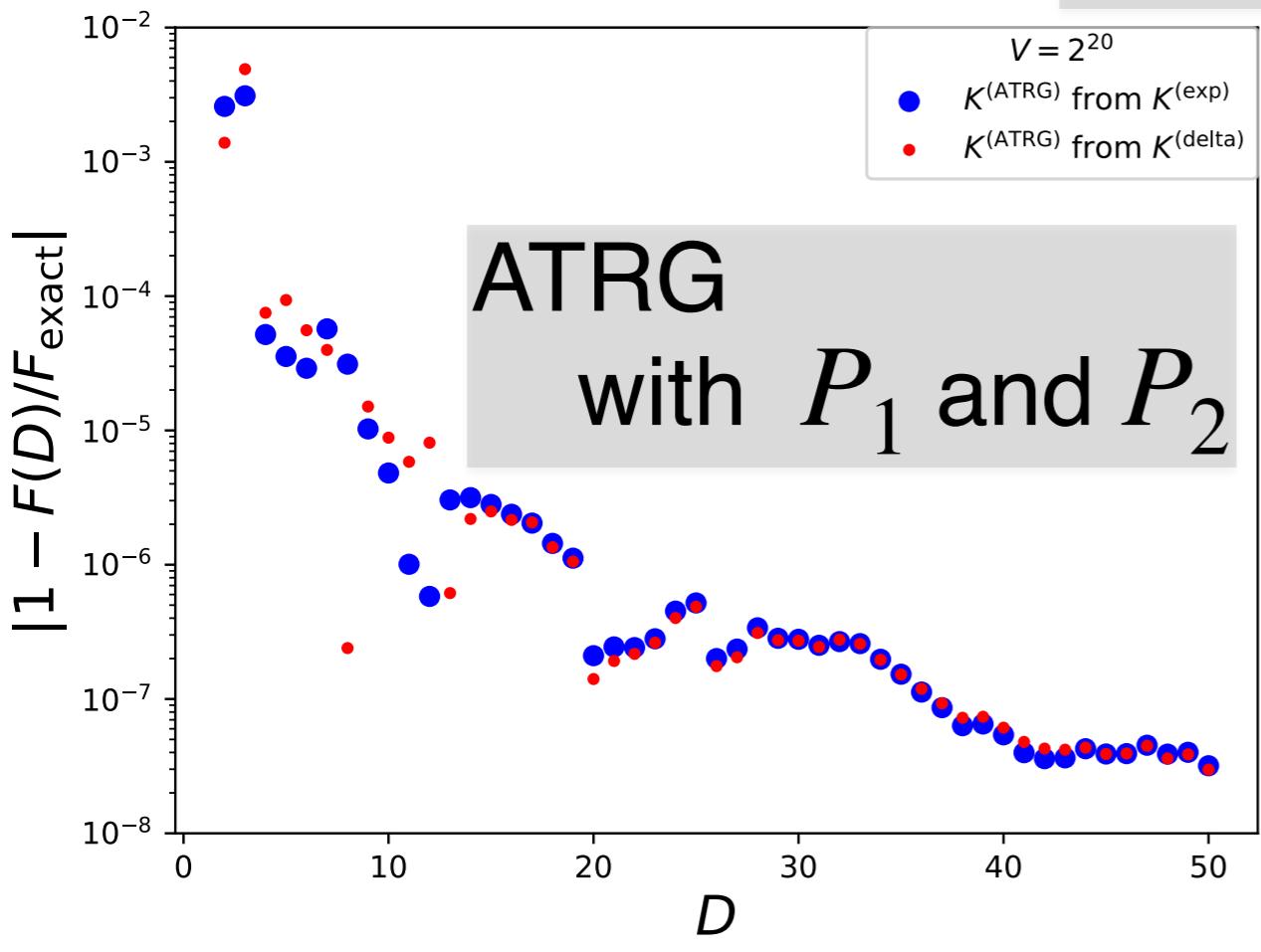
[D. Adachi et al. arXiv:1906.02007]

[D. Kadoh, K.N. arXiv:1912.02414] [K.N. arXiv:2307.14191]

- Many method (ATRG, TriadTRG, MDTRG) can use isometry (U or V) or P_1 and P_2 .

[K. N., M. Schneider arXiv:2407.14226]

2-dim Ising



→ TRG methods with P_1 and P_2 are initial tensor independent.

→ Our construction can also produce compatible result.

● Summary

[main]

- ◊ We propose a general method to construct the initial tensor network from Boltzmann factor representation.
- ◊ We can eliminate initial tensor dependence by using boundary TRG method for isometry.

[details]

- ◊ This relates to the rectilinear Steiner tree problem
(generalized traveling salesman problem)
- ◊ We test our construction in the 2-dim Ising model and 3-dim Z2 gauge theory, and reproduce results.

→ Our method could be a simple, good choice for first study. ₂₂

Backup

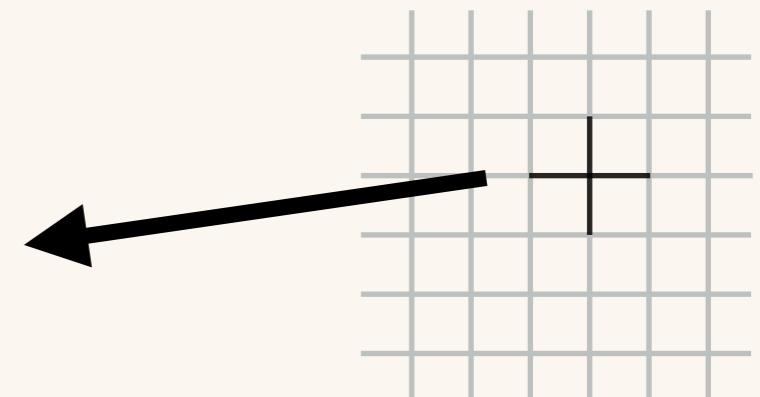
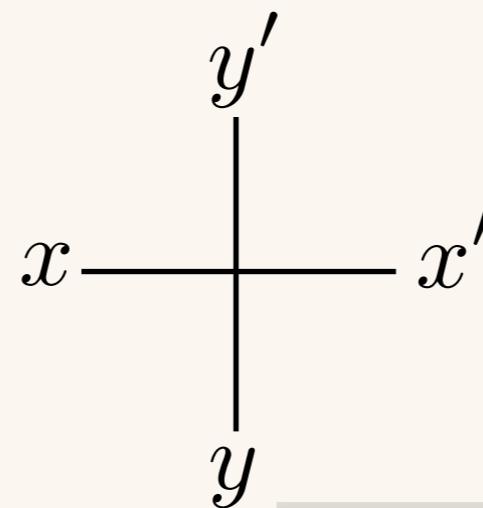
Tensor renormalization group (TRG)

[M. Levin, C. P. Nave. arXiv:cond-mat/0611687]

- ◇ TRG calculate the physical quantity as trace of tensors.

$$Z = \text{Tr} \prod_{i \in \text{lattice}} A_{x_i y_i x'_i y'_i} \quad \int D\bar{\psi} D\psi \left[- \sum_x \mathcal{L}(\bar{\psi}_x, \psi_x) \right]$$

$$A_{xyx'y'} =$$



- Sign problem
- Another representation

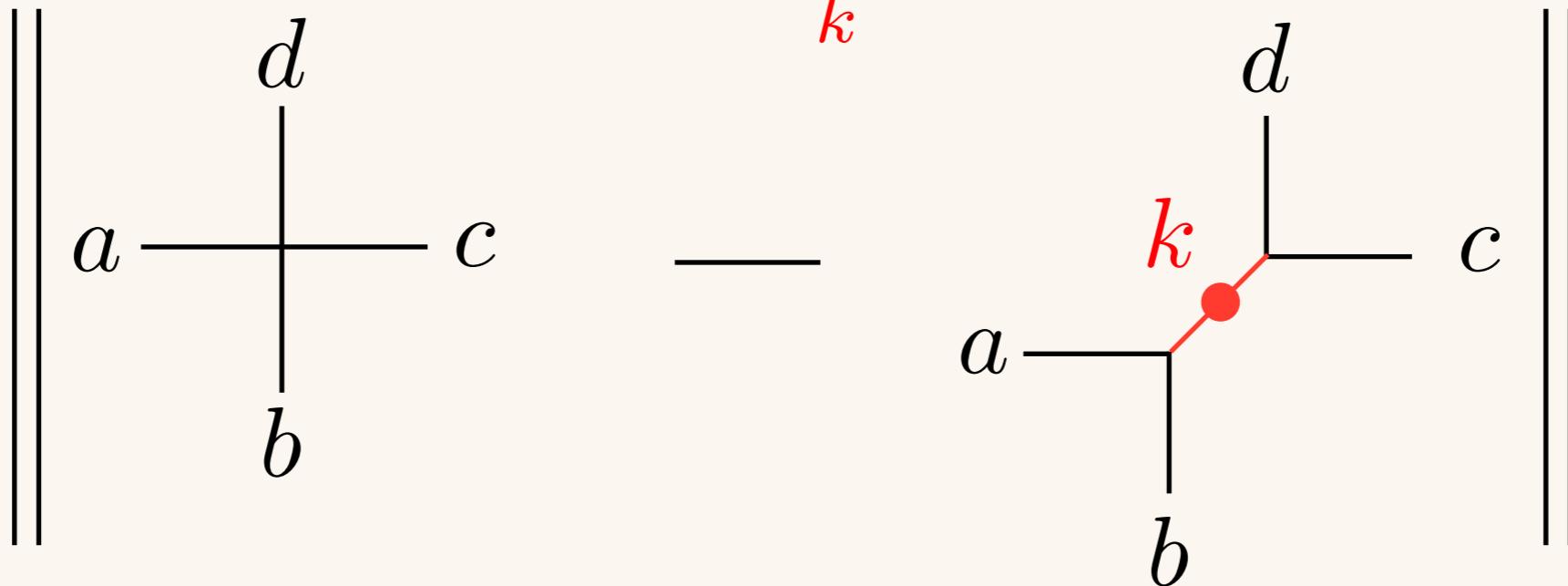
✗ High cost ($\dim \geq 3$)
 △ Systematic error

How can we take whole contraction approximately?

→ Singular value decomposition (Frobenius norm)

● SVD and corresponding cost function

$$T_{abcd} = \sum_k^D A_{ab}{}^k \lambda^k B_{cd}{}^k$$

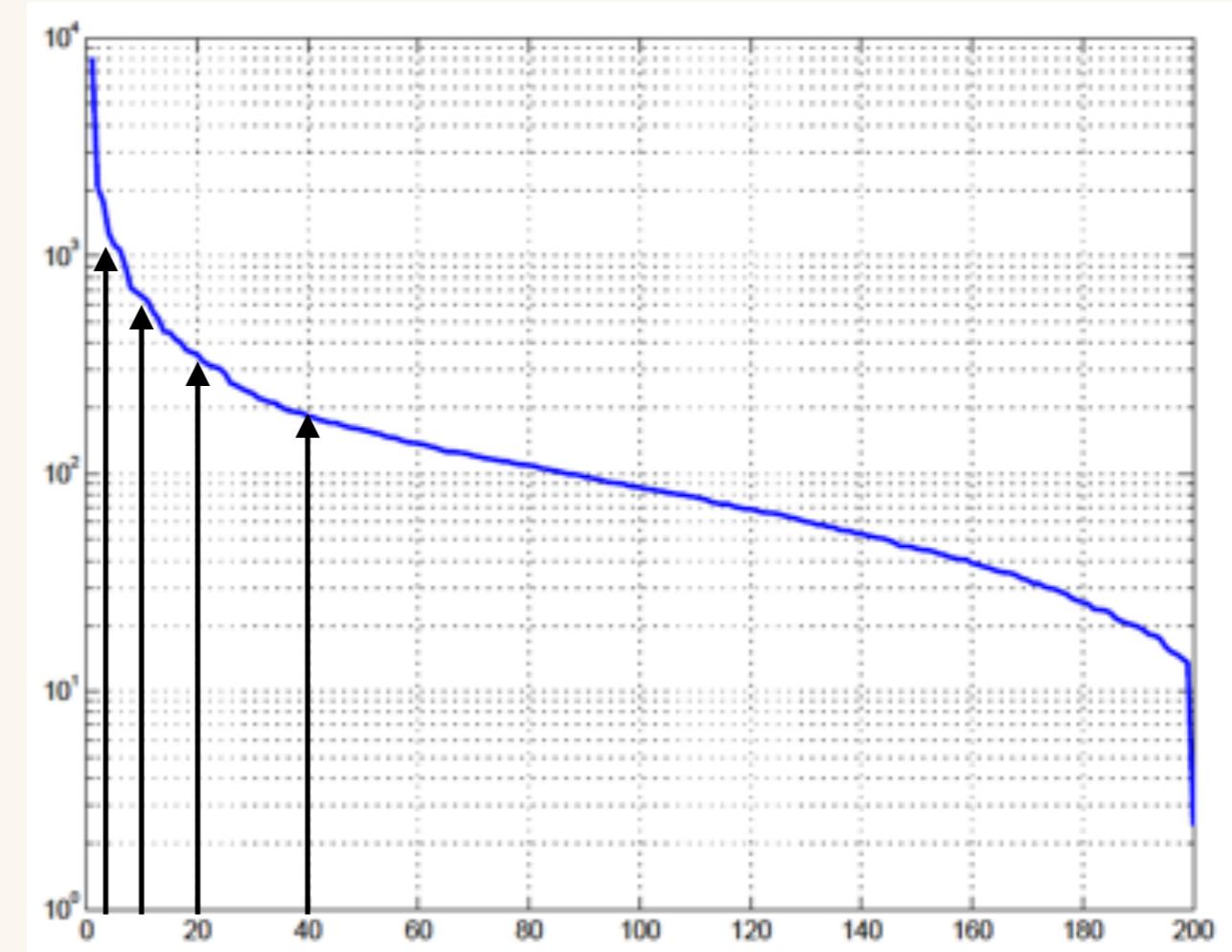
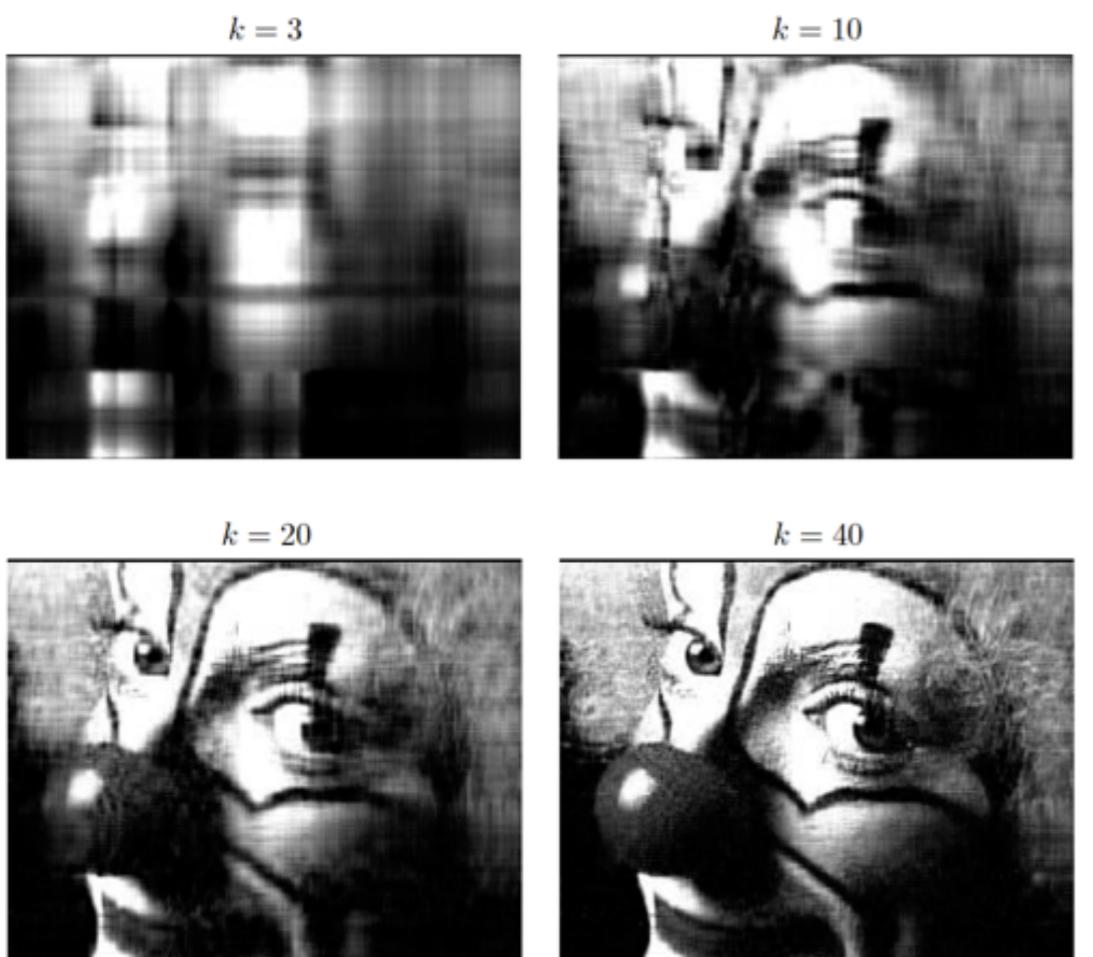


◊ truncation of the SVD minimize the cost function

→ k is truncated

$$\dim(k) = \dim(a)\dim(b) \rightarrow D$$

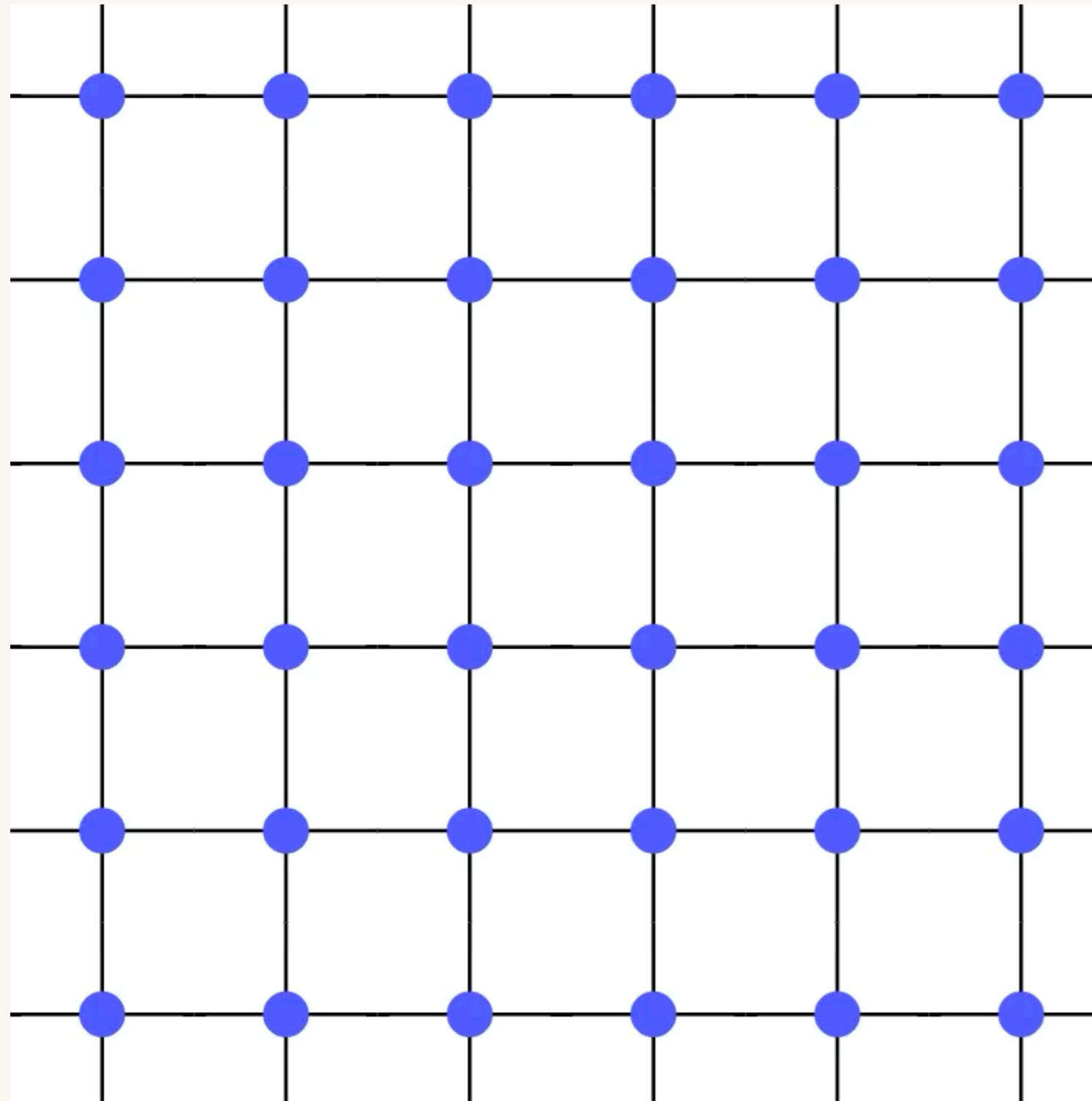
● SVD for a coarse graining (e.g. Image)



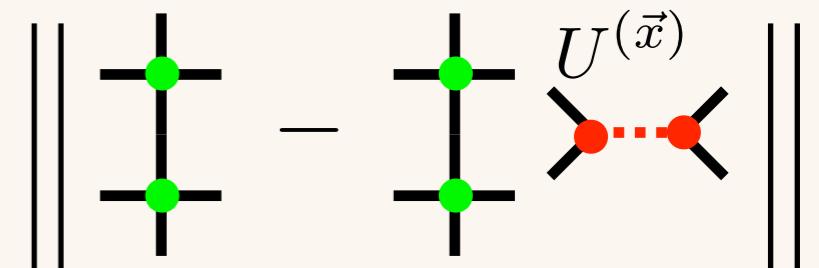
[<http://www.na.scitec.kobe-u.ac.jp/~yamamoto/lectures/cse-introduction2009/cse-introduction090512.PPT>]

- Cause-graining by HOTRG

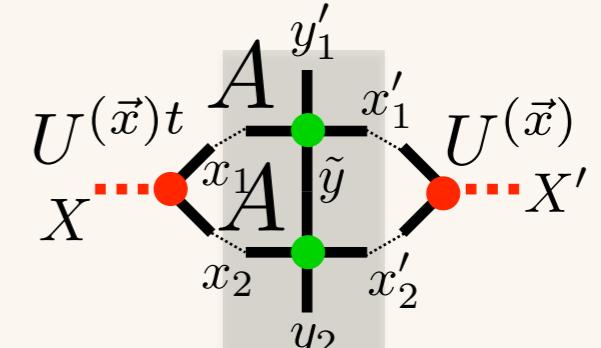
- ◇ Contraction by projection operator U (isometry)



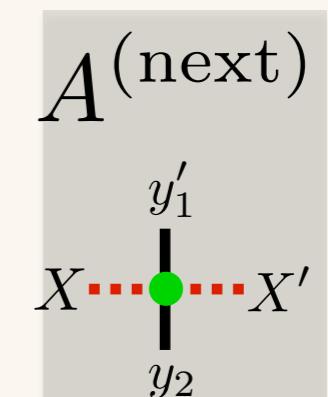
- ◇ Cost function



→ Find U (Isometry).

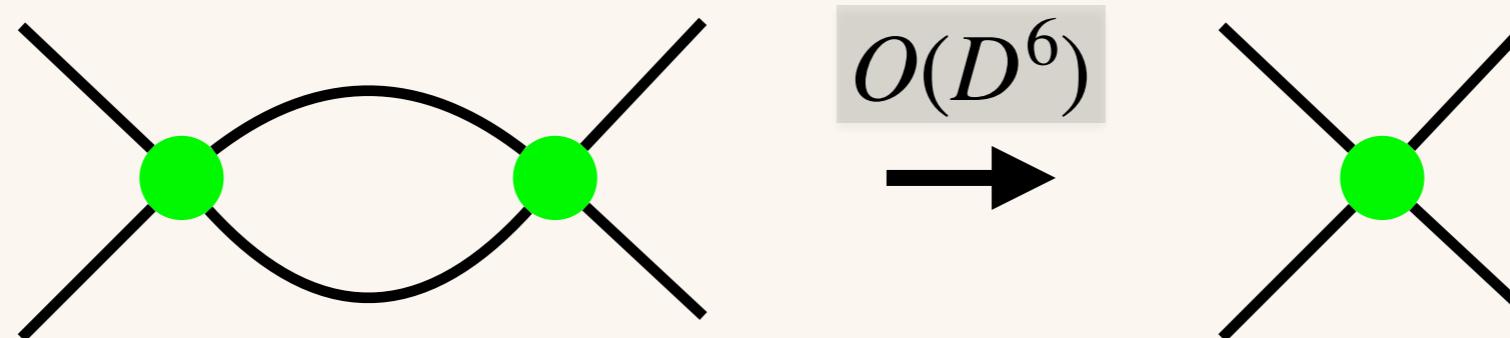


$O(D^{4\dim-1})$

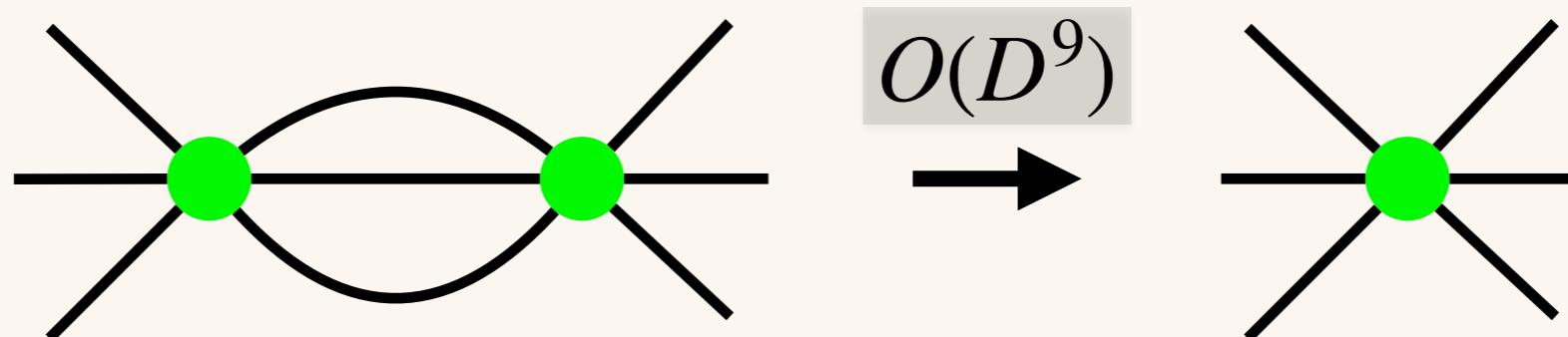


● Computational cost for contraction

- ◊ $(D^2 \times D^2)$ matrix- $(D^2 \times D^2)$ matrix product $\rightarrow O(D^6)$

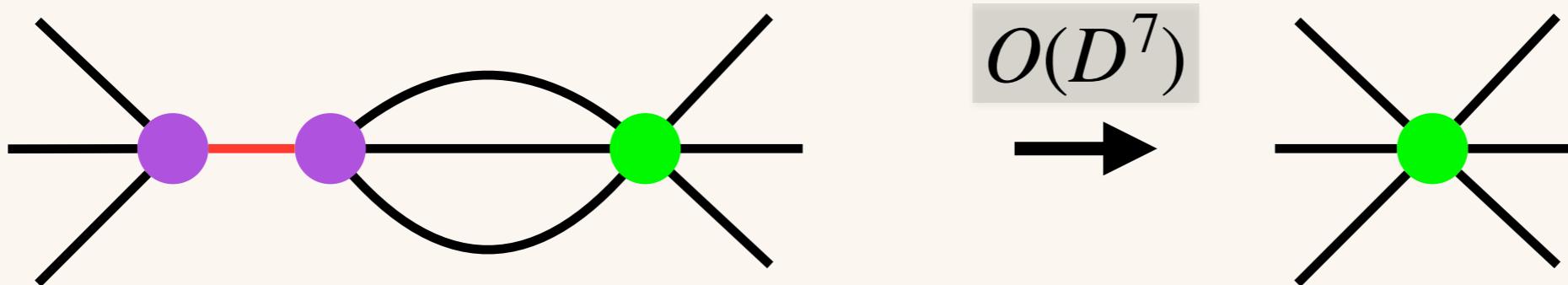


→ Higher order tensor contraction needs larger cost.



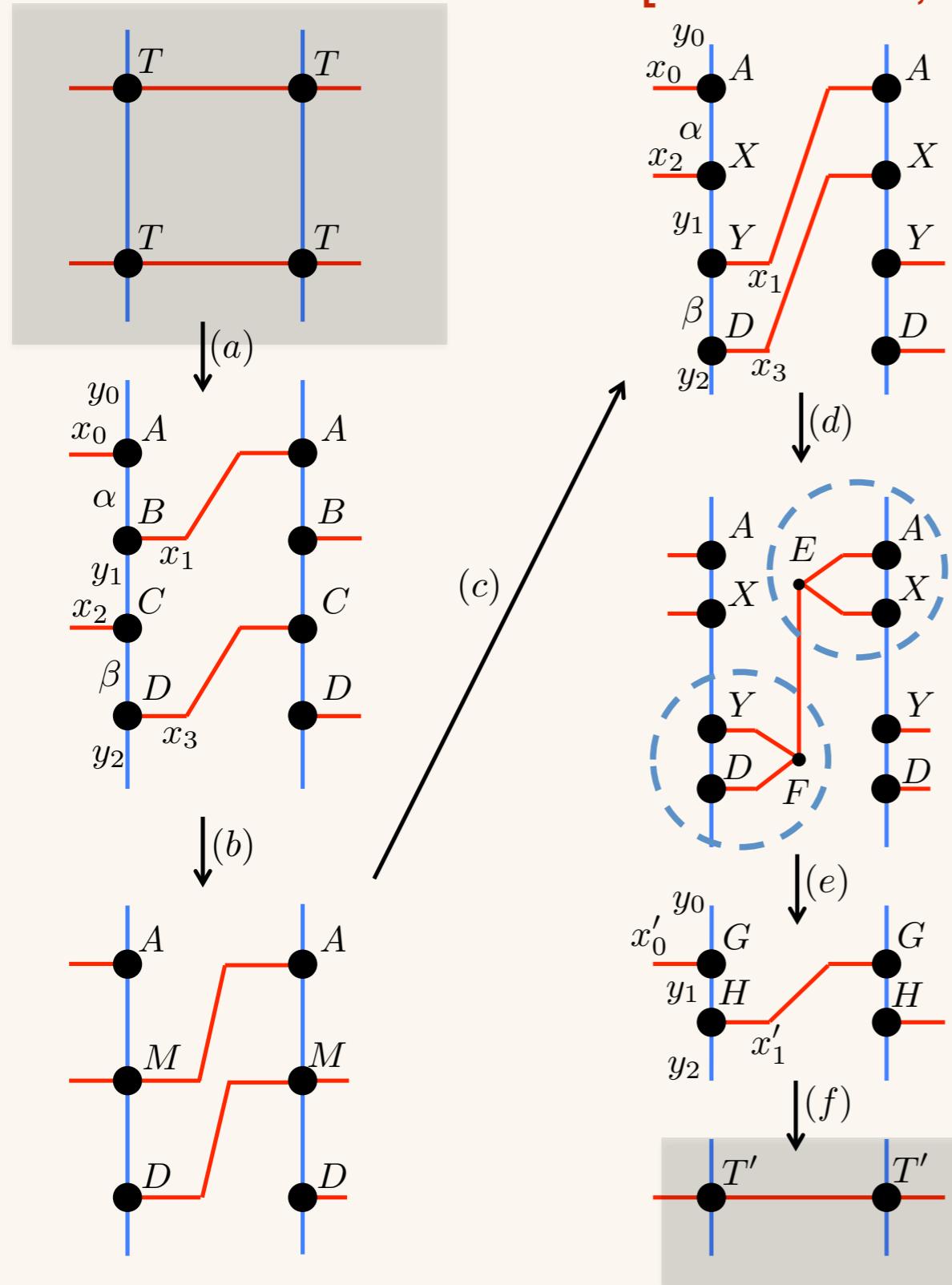
- ◊ Cost reduction = Low order approximation of tensor

(and/or parallel computing)



● Anisotropic TRG (ATRG)

[D. Adachi, T. Okubo, and S. Todo. arXiv:1906.02007]



◇ Auxiliary SVD before SVD
(In order to reduce indeces)

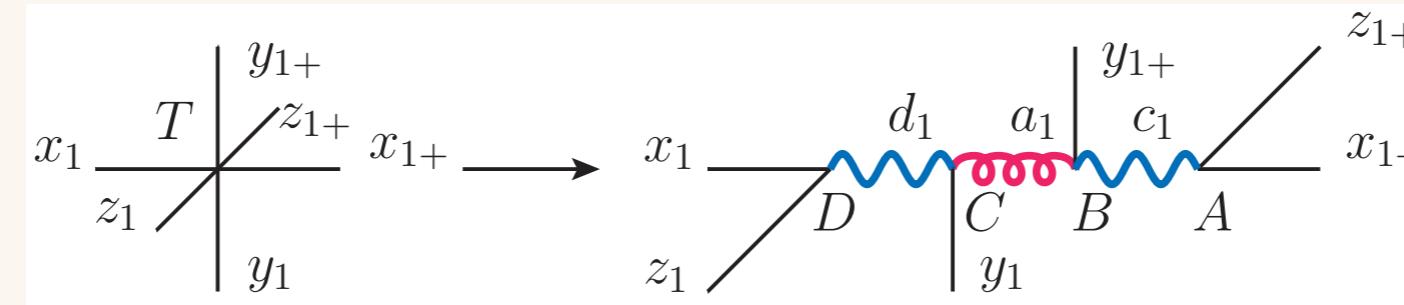
$$O(D^{4\dim-1}) \rightarrow O(D^{2\dim+1})$$

$$\begin{array}{ccc} d & & d \\ \text{---} & = & \text{---} \\ a & c & a & c \\ | & | & | & | \\ b & & b & \\ \end{array}$$

● Triad RG

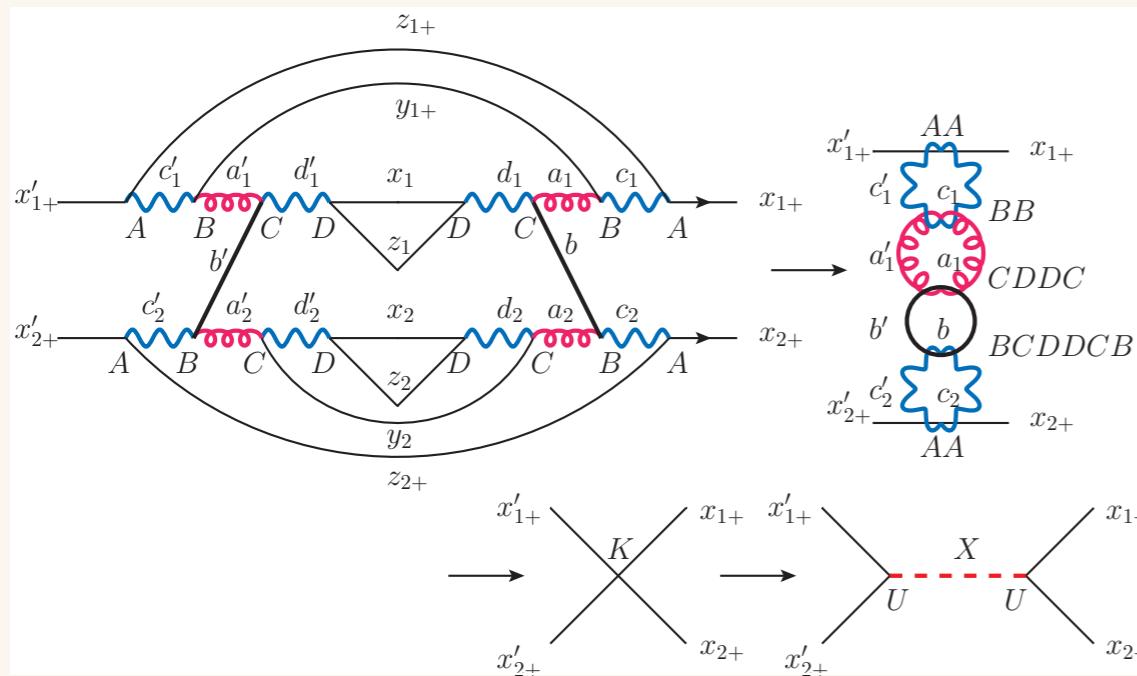
[D. Kadoh and K.N. arXiv:1912.02414]

- ◇ Using the Triad (Rank-3) tensor as a fundamental tensor

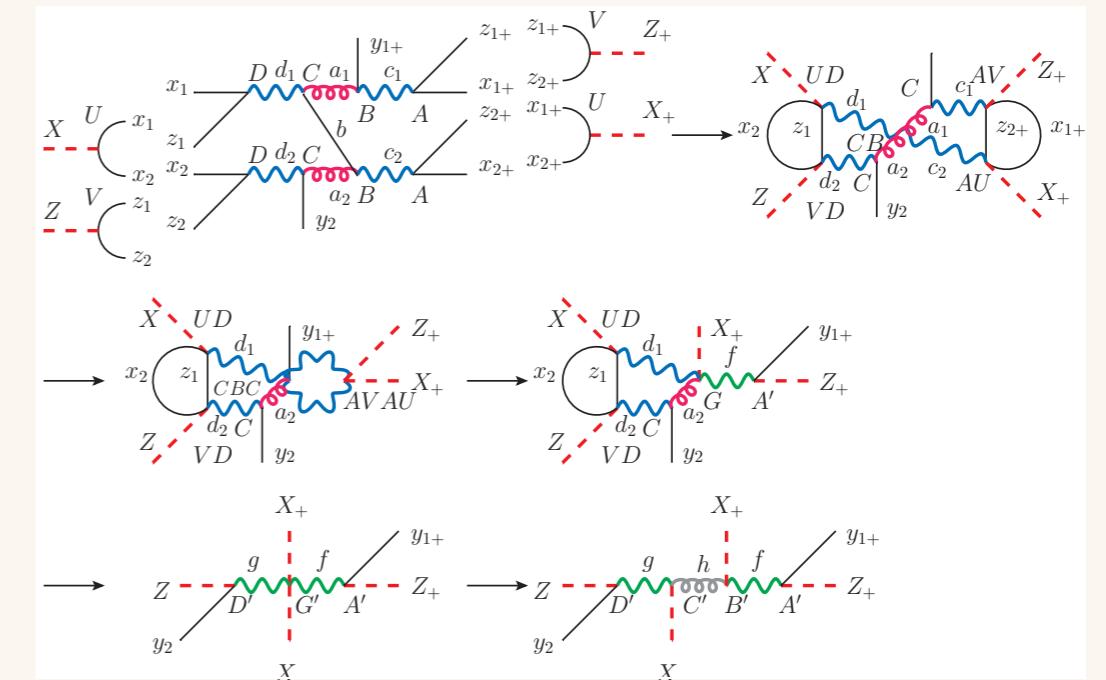


→ We apply HOTRG-like procedure to Triad tensor rep.

- ◇ projection operator U



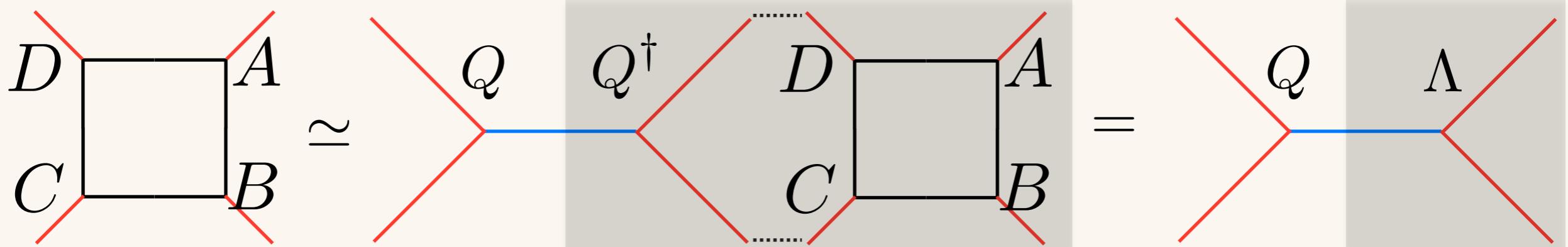
- ◇ contraction part



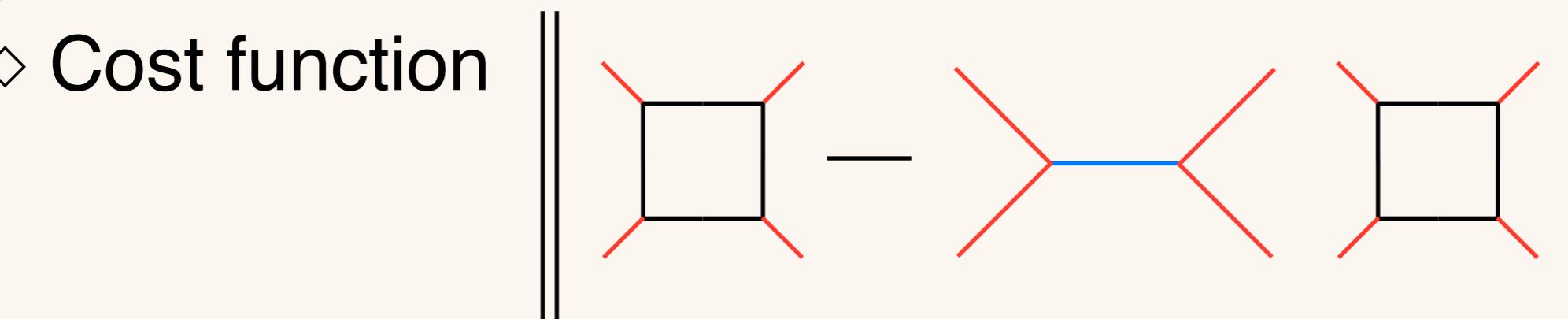
● Randomized-SVD

[N. Halko, et al. arXiv:0909.4061]
 [S. Morita, et al. arXiv:1712.01458]

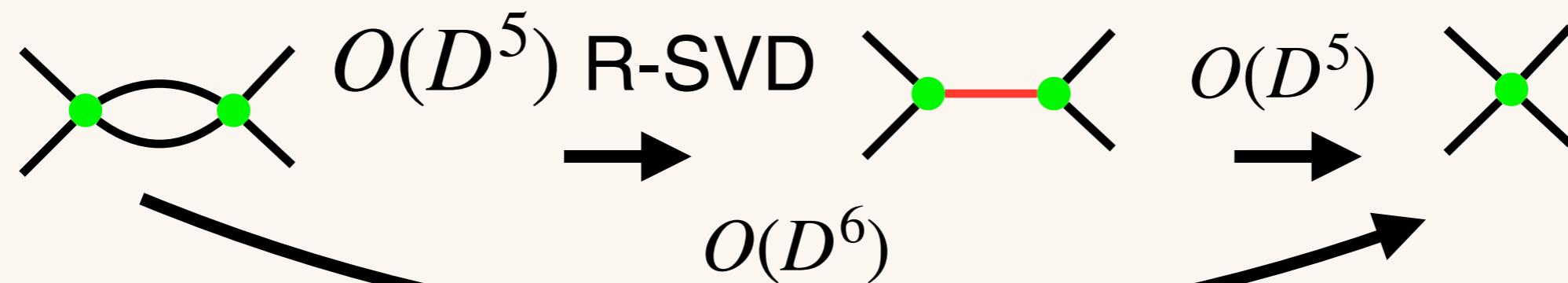
- ◊ Approximated contraction by orthogonal matrix Q



- ◊ Cost function



→ Approximated CONTRACTION of tensor network.

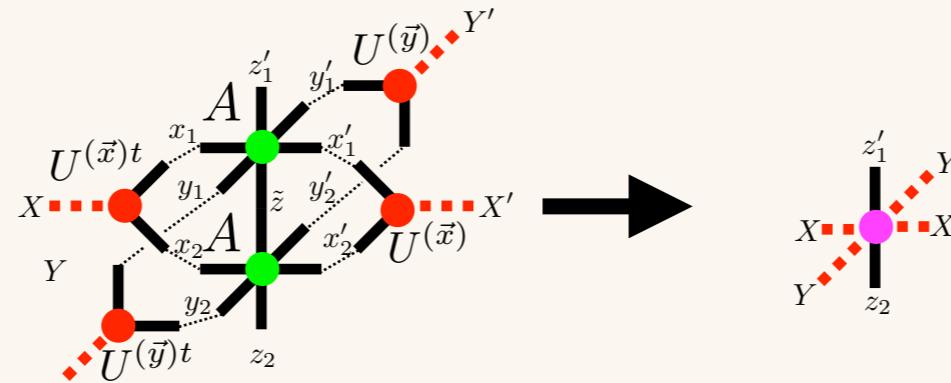


NOTE: R-SVD provides approximation of ABCD.

HOTRG

[Z.Y. Xie, J. Chen, et al. arXiv:1201.1144]

$$U^{(\vec{y})t} U^{(\vec{x})t} A A U^{(\vec{x})} U^{(\vec{y})} \rightarrow A^{(\text{next})}$$

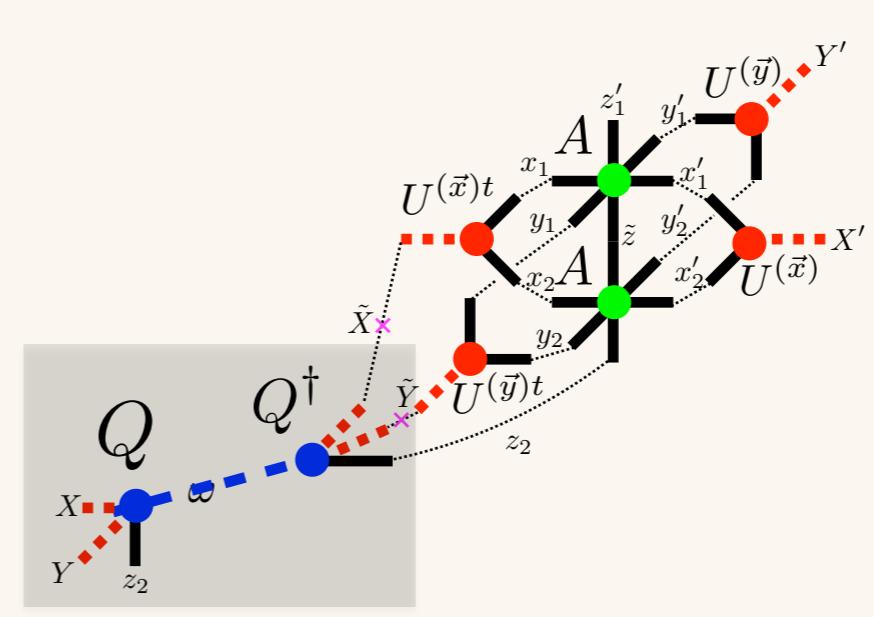
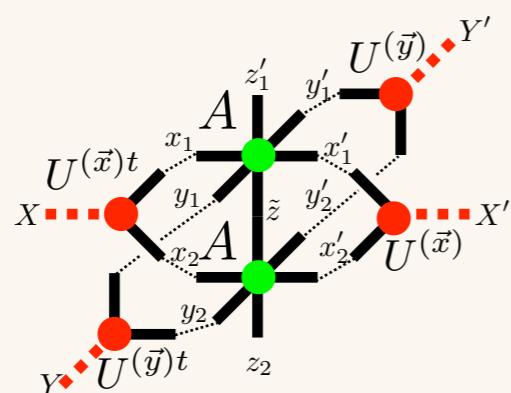


HOTRG with R-SVD

[K.N. arXiv:2307.14191]

[D. Kadoh, K.N. arXiv:1912.02414]

$$Q Q^\dagger U^{(\vec{y})t} U^{(\vec{x})t} A A U^{(\vec{x})} U^{(\vec{y})} \simeq A^{(\text{next})}$$

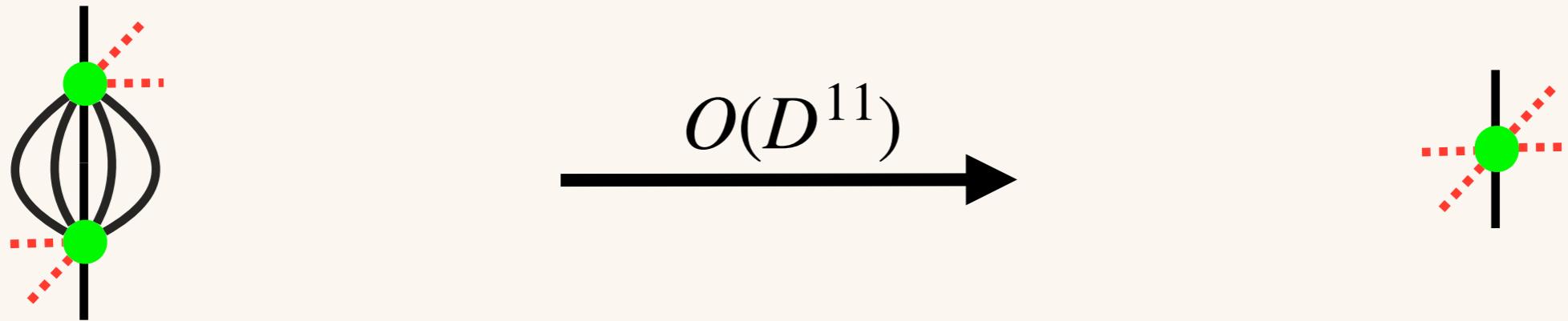


→ Contraction with R-SVD

$$O(D^{4d-1}) \rightarrow O(D^{3d})$$

● HOTRG

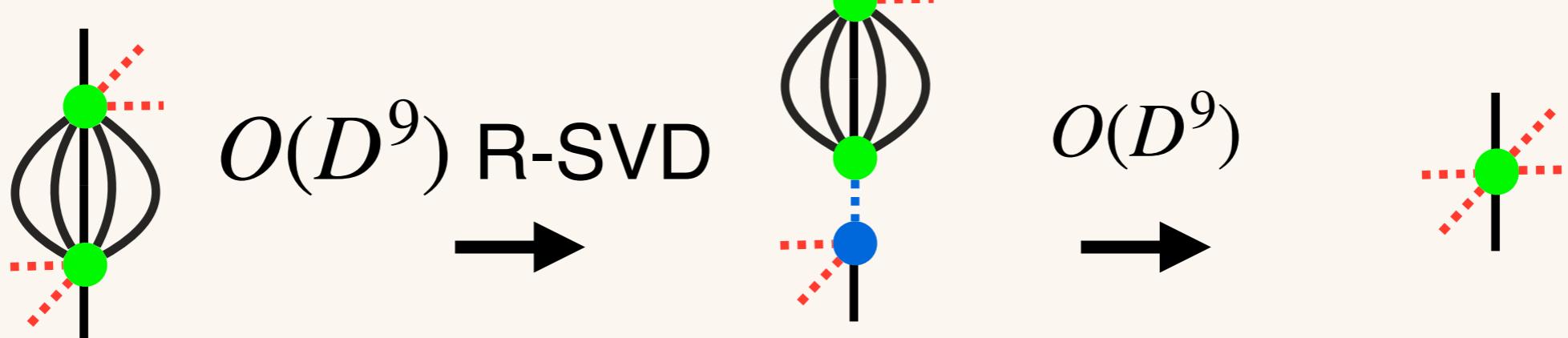
[Z.Y. Xie, J. Chen, et al. arXiv:1201.1144]



● HOTRG with R-SVD

[K.N. arXiv:2307.14191]

[D. Kadoh, K.N. arXiv:1912.02414]



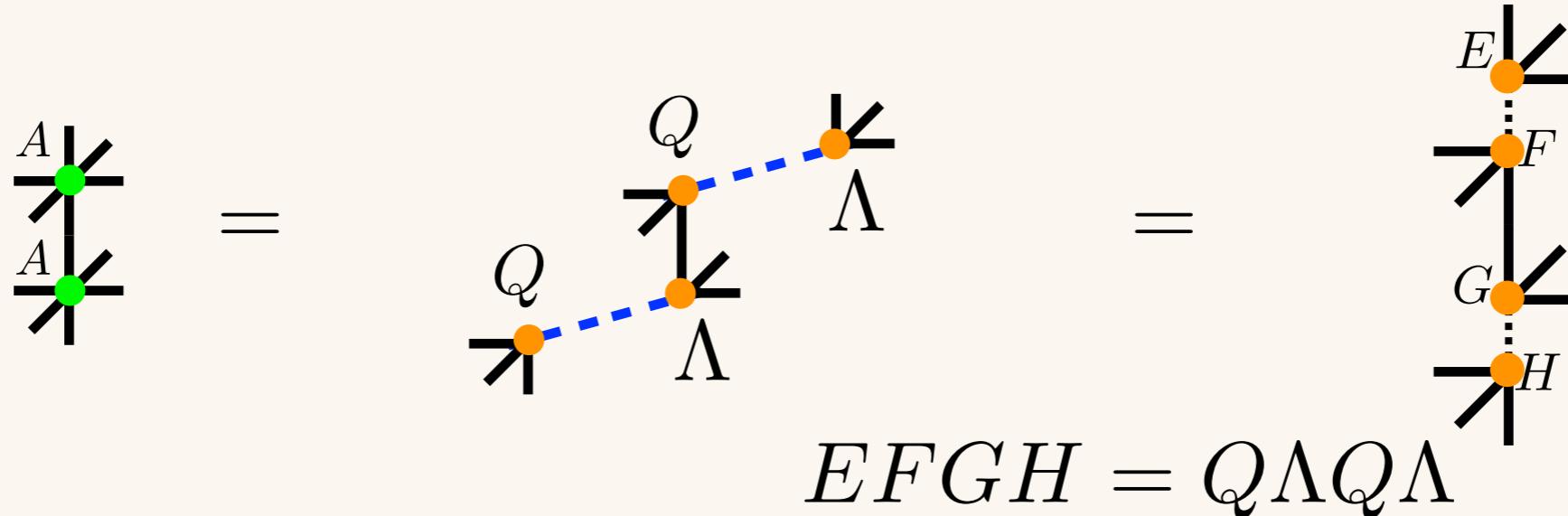
→ Contraction with R-SVD

$O(D^{4d-1}) \rightarrow O(D^{3d})$

● Minimally-decomposed TRG(MDTRG)

[K.N. arXiv:2307.14191]

→ We already have tensor of order d+1 rep.



A :Order 2d

E, F, G, H :Order d+1

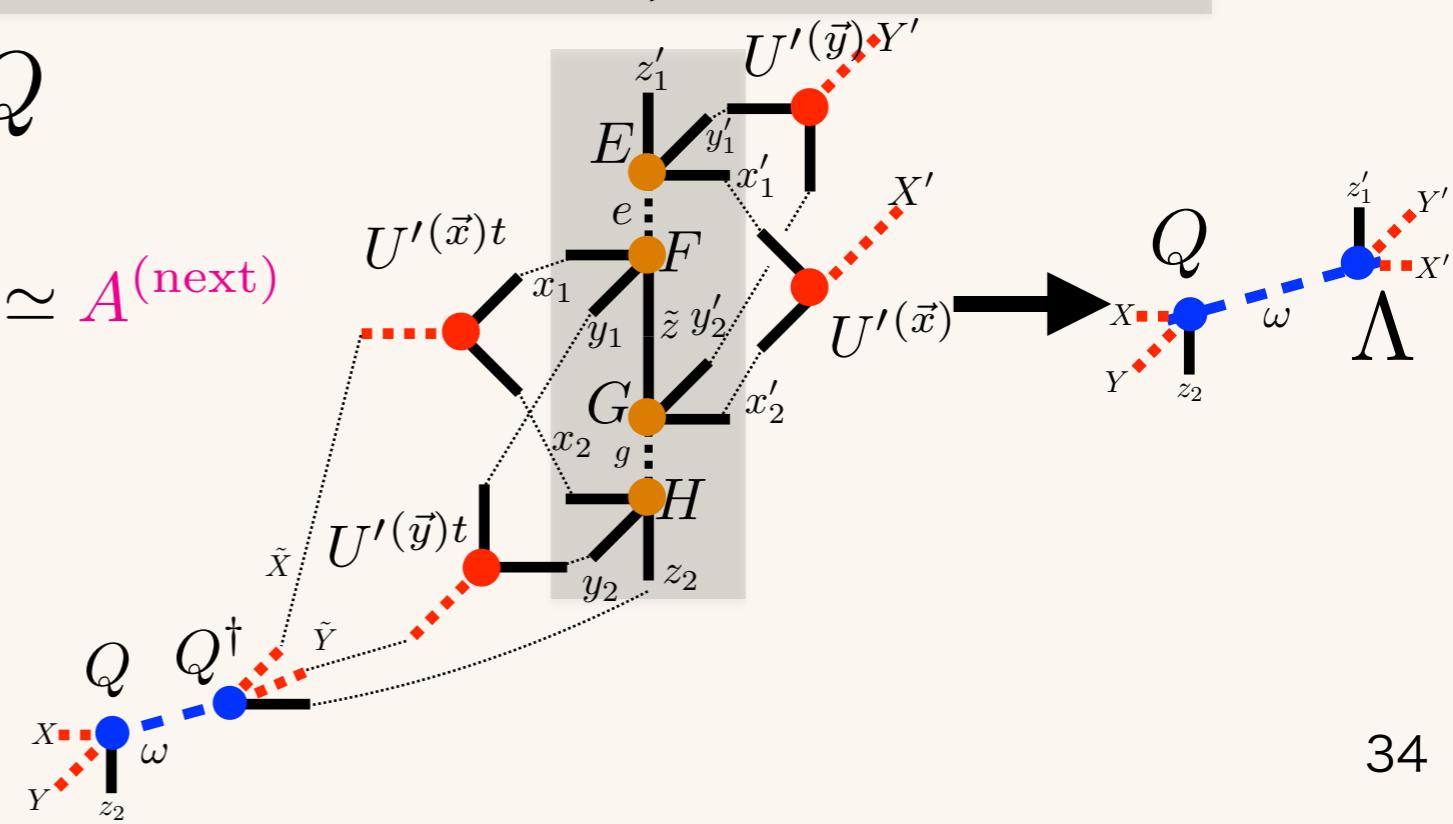
Q, Λ :Order d+1

◇ Contraction with $EFGH, Q$

$$QQ^\dagger U'(\vec{y})^t U'(\vec{x})^t EFGH U'(\vec{x}) U'(\vec{y}) = Q\Lambda \simeq A^{(\text{next})}$$

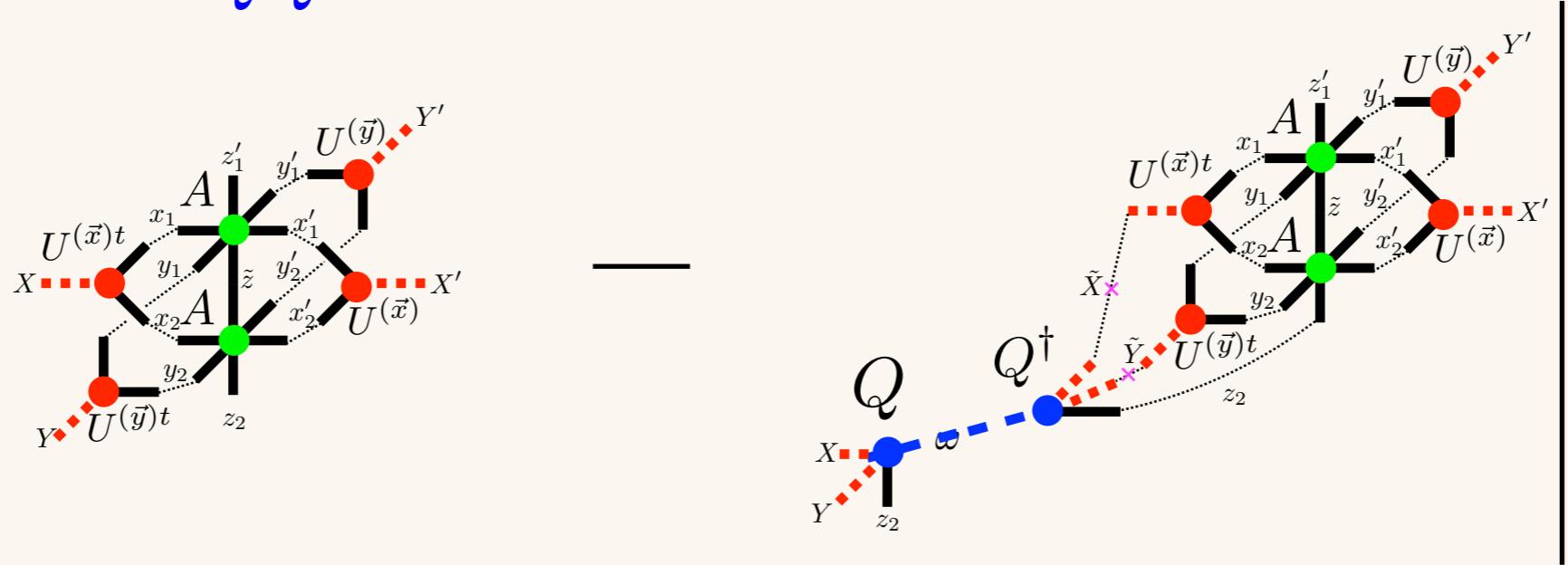
◇ Cost reduction

$$O(D^{3d}) \rightarrow O(D^{2d+1})$$



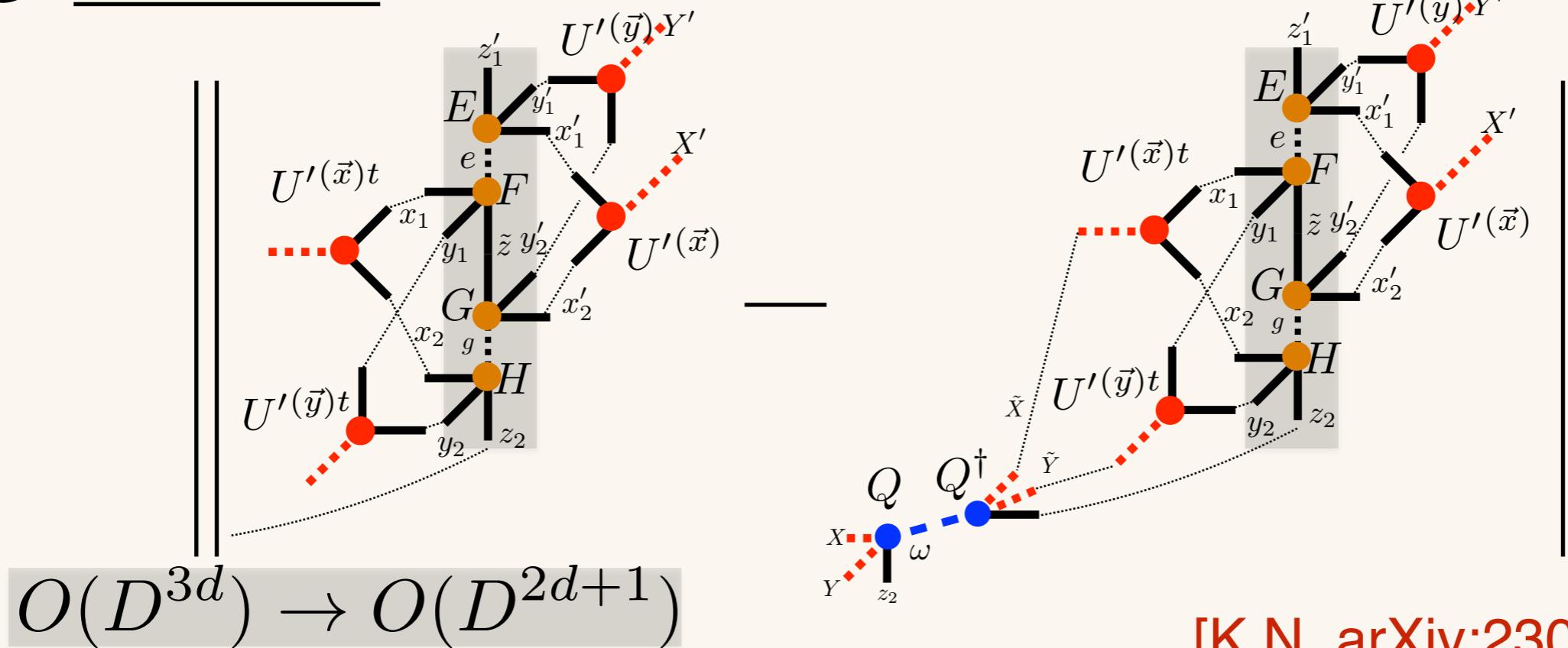
HOTRG with R-SVD

$$QQ^\dagger U^{(\vec{y})t} U^{(\vec{x})t} AAU^{(\vec{x})} U^{(\vec{y})} \simeq A^{(\text{next})}$$



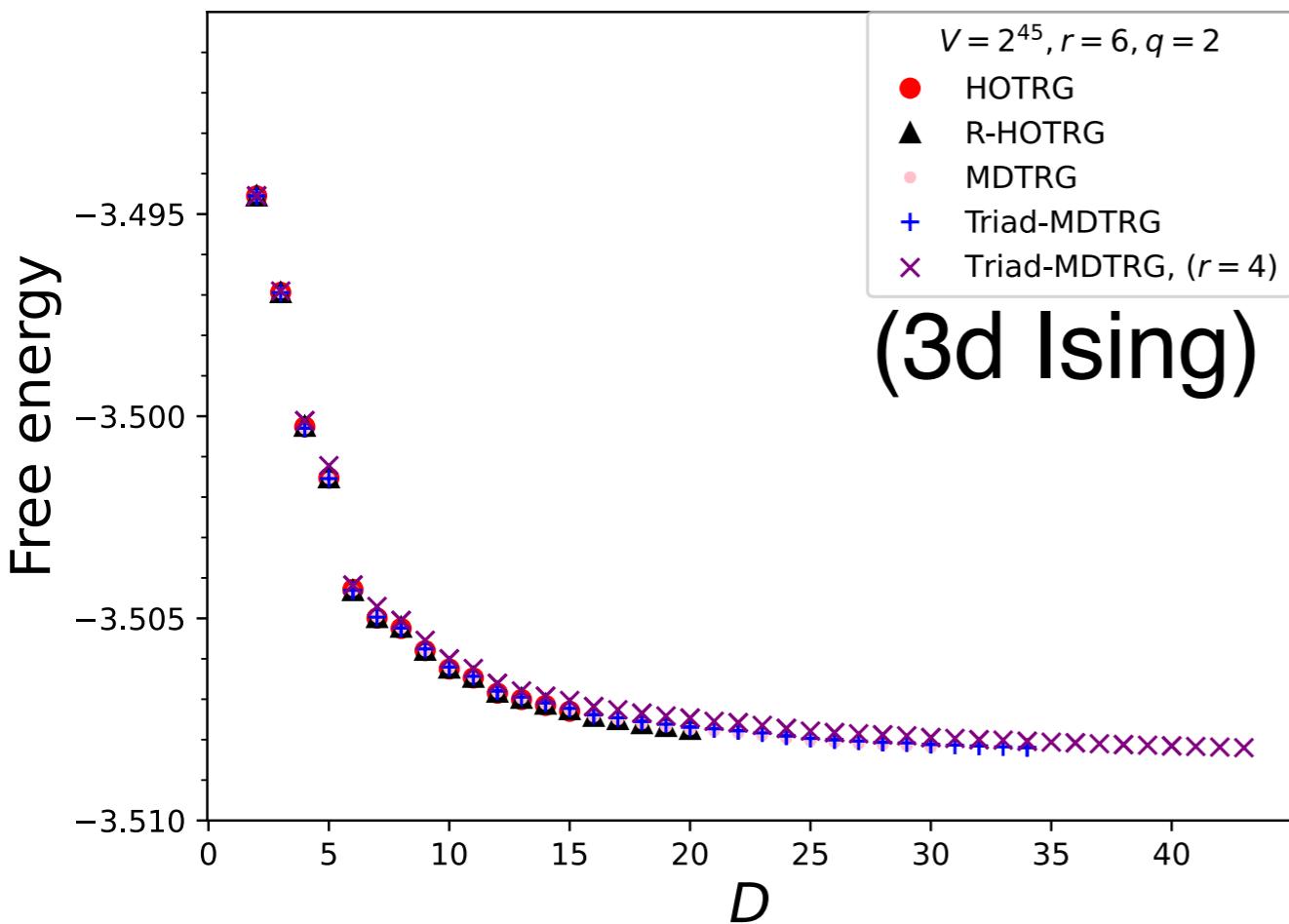
MDTRG

$$QQ^\dagger U'^{(\vec{y})t} U'^{(\vec{x})t} EFGHU'^{(\vec{x})} U'^{(\vec{y})} = Q\Lambda \simeq A^{(\text{next})}$$

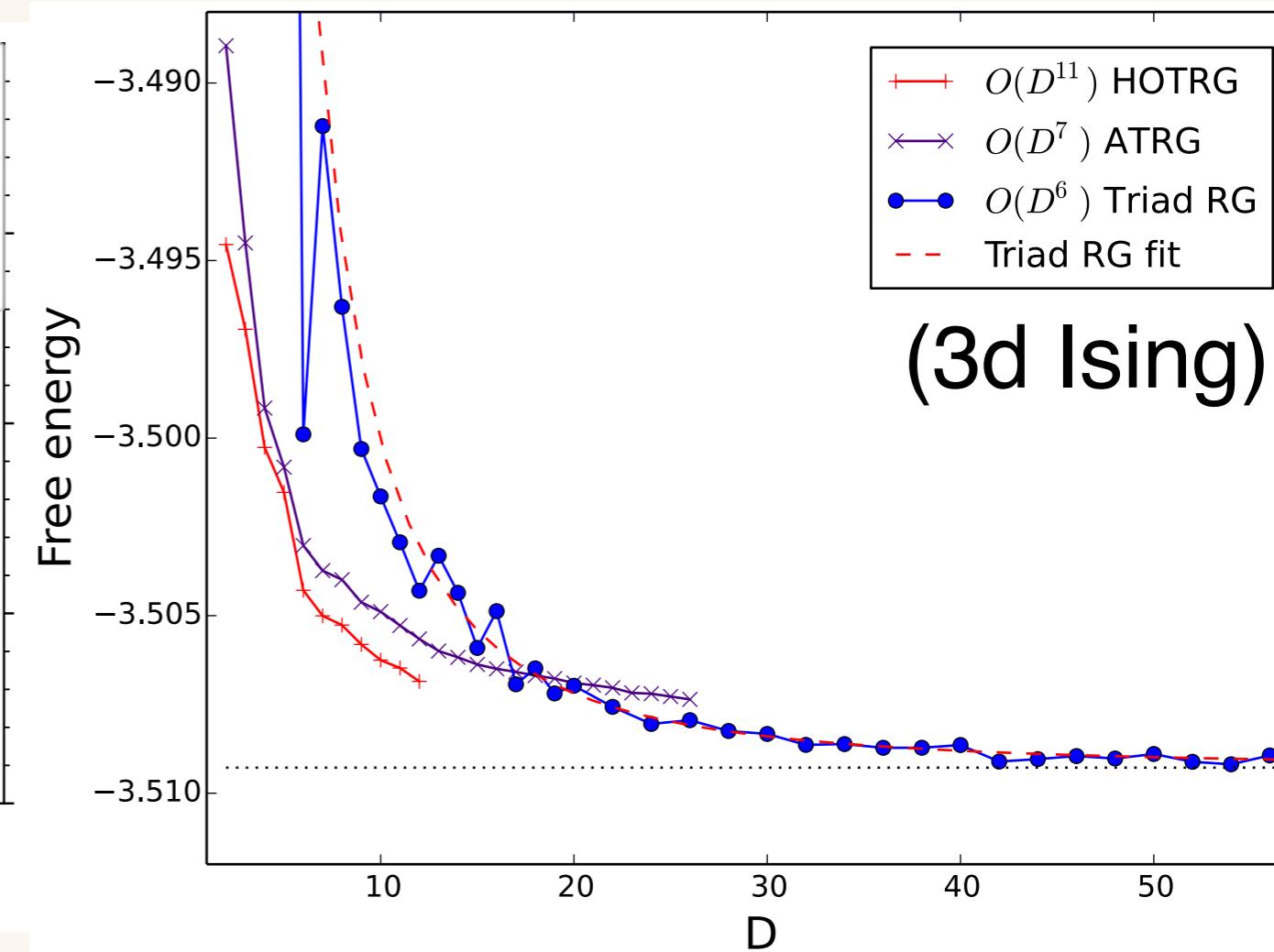


Free energy density of 3d-Ising model

[K.N. arXiv:2307.14191]



[D. Kadoh, K.N. arXiv:1912.02414]



→ R-HOTRG, MDTRG, Triad-MDTRG results are consistent with HOTRG (additional systematic error is not dominant).

● Summary

- ◊ How about HOTRG with Randomized-SVD?

	with R-SVD	w/o R-SVD	unit-cell order
◊ HOTRG	$O(D^{3d})$	$O(D^{4d-1})$	$\nleq 2d$
◊ MDTRG	$O(D^{2d+1})$	$O(D^{3d})$	$\nleq d+1$
◊ Triad-MDTRG	$O(D^{d+3})$	$O(D^{3d})$	$\nleq d+1$

- ◊ Can we reduce the systematic error from decomposition?

- R-HOTRG, MDTRG, and Triad-MDTRG produce consistent result with the HOTRG. The dominant systematic error is the truncation of the isometry.
- We have to pay attention to the cost function.