計算科学における情報圧縮

Information Compression in Computational Science

2018.1.11

#13:テンソルネットワーク繰り込みと低ランク近似の応用

Tensor network renormalization

理学系研究科　物理学専攻　大久保　毅

Department of Physics, **Tsuyoshi Okubo**

Outline

(Main goals)

- Tensor network representation of a scalar
    - Partition functions in statistical mechanics
    - Exponentially large computational cost

(Share problems)

- Tensor network renormalization
    - Tensor Renormalization Group (TRG) in two dimension
    - Generalization to higher dimensions

(Understand idea of TRG)

- Tensor network renormalization around critical point
    - Fixed point of TRG: Corner double line tensors

(Understand "entanglement structure")

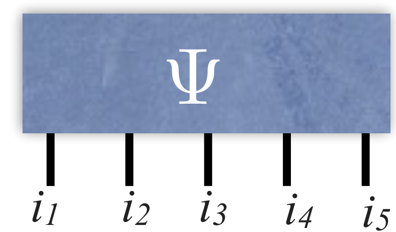
- Report problems

Tensor network representation of a scalar

Tensor network state: approximation for a vector

G.S. wave function: $|\Psi\rangle = \sum_{\{i_1,i_2,\ldots i_N\}} \Psi_{i_1 i_2 \ldots i_N} |i_1 i_2 \ldots i_N\rangle$

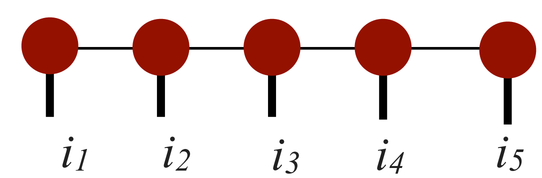
Vector (or N-rank tensor): $\Psi_{i_1 i_2 \ldots i_N}$ =



# of Elements$=a^N$

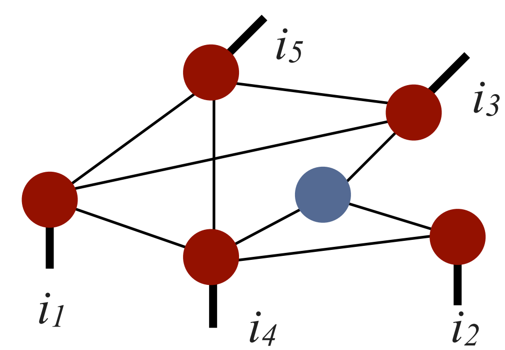
``Tensor network" decomposition

- Matrix Product State (MPS) $A_1[i_1]A_2[i_2]\cdots A_N[i_N]$ =



$A[m]$: Matrix for state m

- General network $\mathrm{Tr}X_1[i_1]X_2[i_2]X_3[i_3]X_4[i_4]X_5[i_5]Y$



X,Y : Tensors

Tr : Tensor network contraction

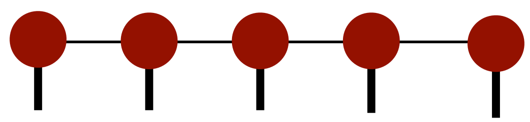
By choosing a ``good" network, we can express G.S. wave function efficiently.

ex. MPS: # of elements $=2ND^2$ D: dimension of the matrix A

Exponential→ Linear *If D does not depend on N…

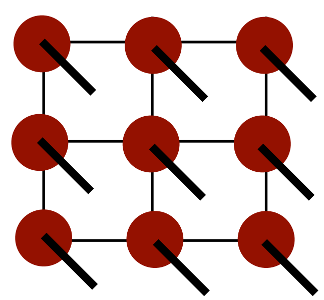
Examples of TNS

MPS:



Good for 1-d gapped systems

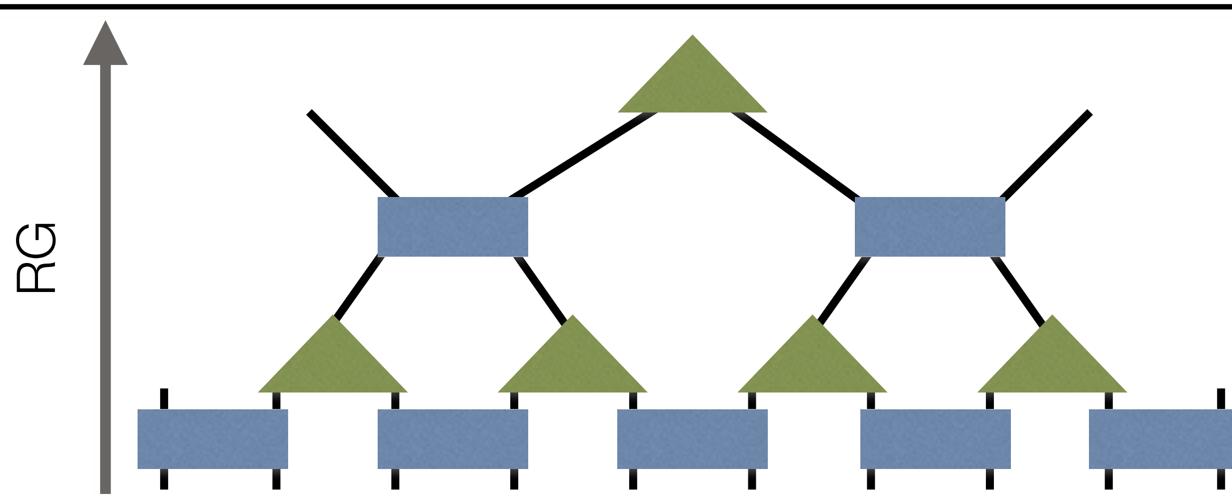
PEPS, TPS:



For higher dimensional systems

Extension of MPS

MERA:

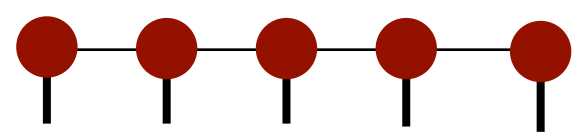
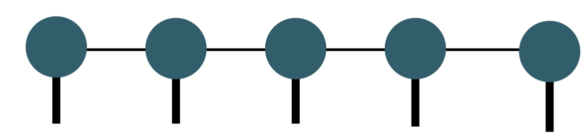


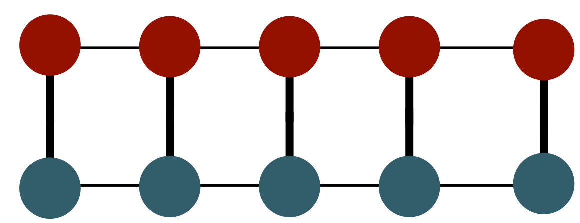
Scale invariant systems

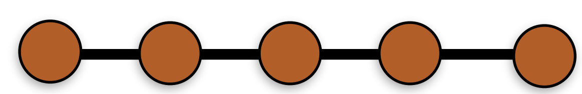
Tensor network representation of a scalar

Example: inner product of two TNSs

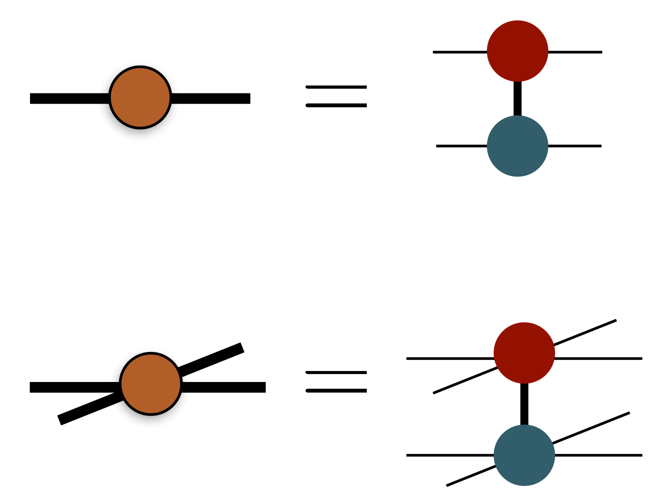
MPS

$\vec{v} =$  $\vec{u} =$ 

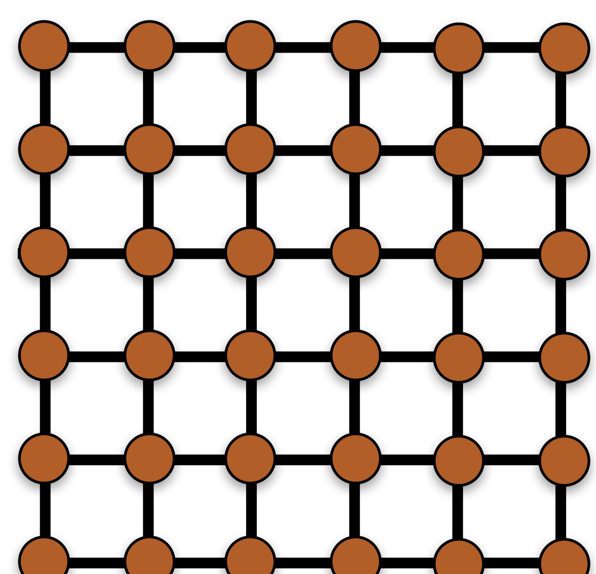
$\vec{v} \cdot \vec{u}^* =$ 

$=$ 

Double layer tensor



TPS (in two dimension)

$\vec{v} \cdot \vec{u}^* =$ 

Statistical mechanics and canonical ensemble

Canonical ensemble:
（カノニカル分布）

$$P(\Gamma) \propto e^{-\beta \mathcal{H}(\Gamma)}$$

Γ ：State (e.g. {S1, S2, ... SL})

$P(\Gamma)$: Probability to appear state Γ

$\beta = \frac{1}{k_B T}$: Inverse temperature

$\mathcal{H}$ ：Hamiltonian

Partition function（分配関数）

＝Normalization factor of the canonical ensemble

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

Relation to the free energy in thermodynamics

$$F = -k_B T \ln Z$$

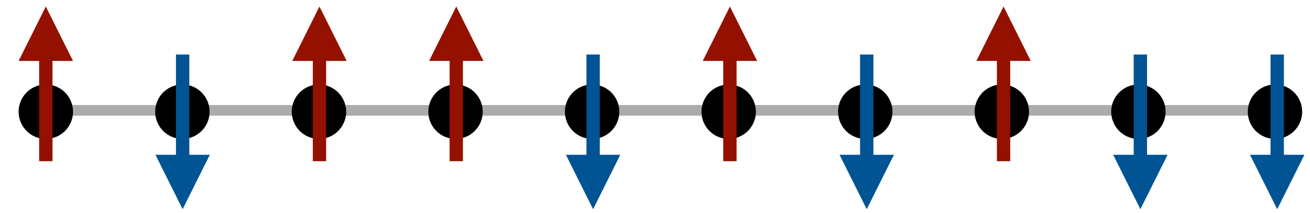
log of the partition function＝Free energy

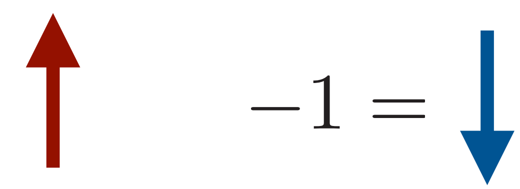
Tensor network representation of partition function

Classical Ising model on a chain

$$\mathcal{H} = -J\sum_{i=1}^{L-1} S_i S_{i+1}$$

$$S_i = 1, -1$$





Partition function:

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

$$= \sum_{\{S_i=\pm 1\}} \prod_{i=1}^{L-1} e^{\beta J S_i S_{i+1}}$$

$$= \sum_{S_1=\pm 1, S_L=\pm 1} \left(T^{L-1}\right)_{S_1, S_L}$$

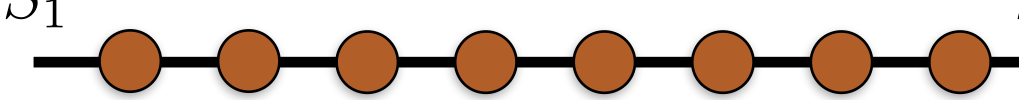
Transfer matrix (転送行列)

$$T_{S_i, S_{i+1}} = e^{\beta J S_i S_{i+1}}$$

$$T = \begin{array}{cc} +1 & -1 \\ \end{array}$$

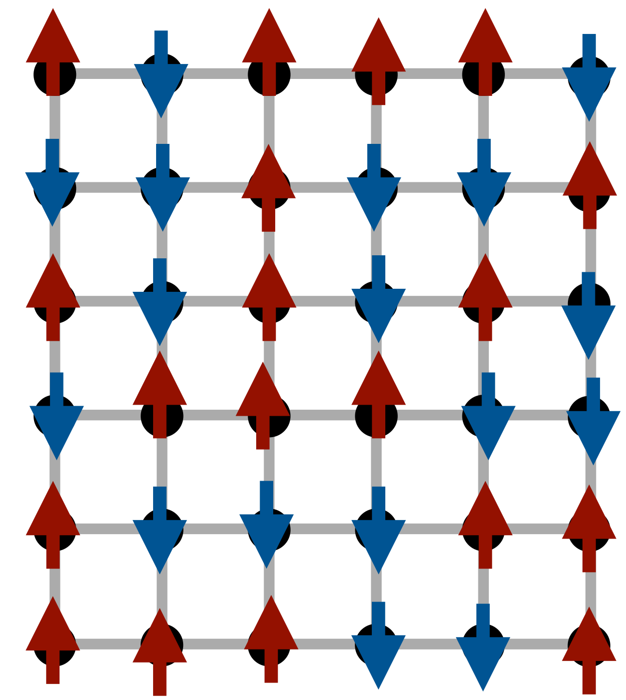
$$T = \begin{pmatrix} e^{\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} \end{pmatrix} \begin{array}{c} +1 \\ -1 \end{array}$$

$$\sum_{S_1=\pm 1, S_L=\pm 1}$$



Tensor network representation in two dimension

Classical Ising model on the square lattice



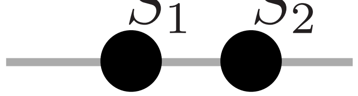
$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j \quad (S_i = \pm 1 = \uparrow, \downarrow)$$

$$\Rightarrow \quad Z = \sum_{\{S_i = \pm 1\}} e^{\beta J \sum_{\langle i,j \rangle} S_i S_j}$$

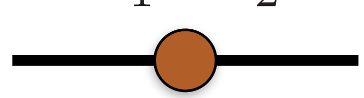
We can use a tensor instead of the transfer matrix.

$$e^{\beta J S_1 S_2} = T_{S_1 S_2}$$

$\Rightarrow$ Tensor?

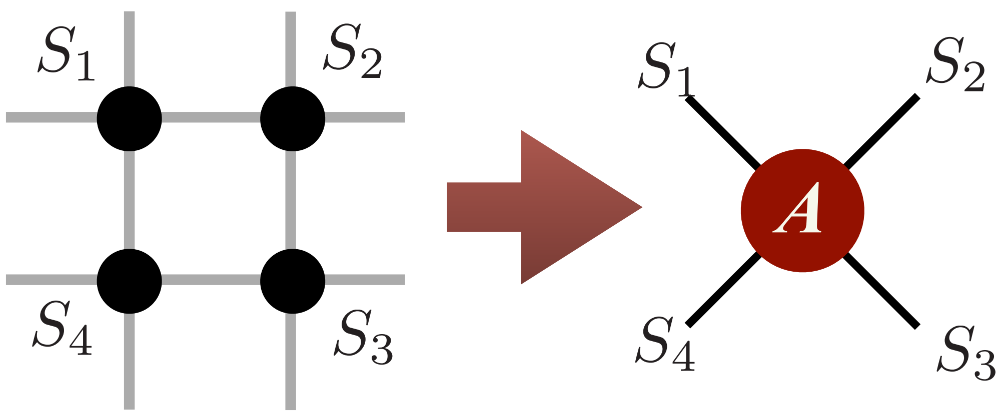


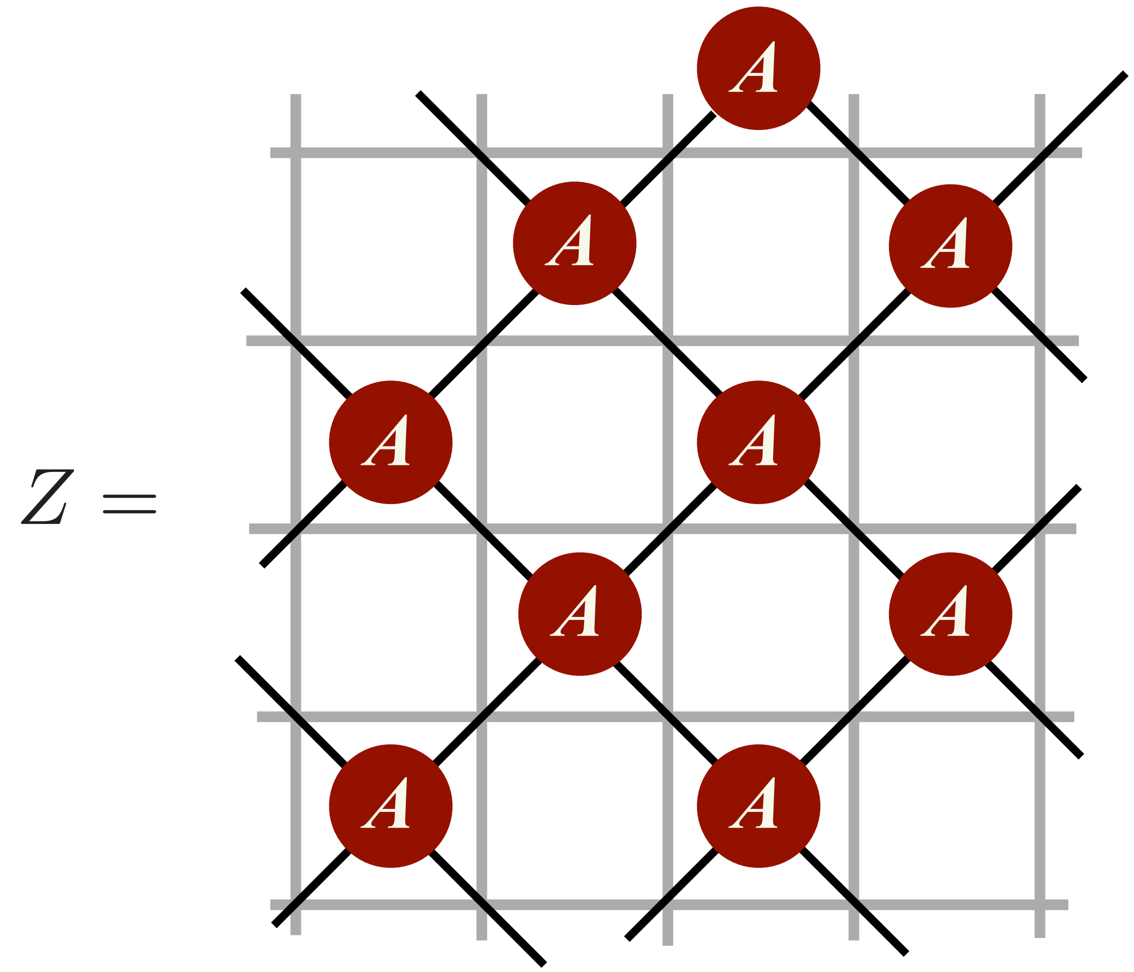
$\Rightarrow$



Tensor network representation in two dimension

$$e^{\beta J(S_1S_2+S_2S_3+S_3S_4+S_4S_1)} = A_{S_1S_2S_3S_4}$$





Partition function = Tensor network of tensor A

Square lattice Ising model→Square lattice tensor network rotating 45 degrees.

*We can construct a tensor network where tensors are on the nodes of original lattice.

Calculation cost of "classical" tensor network

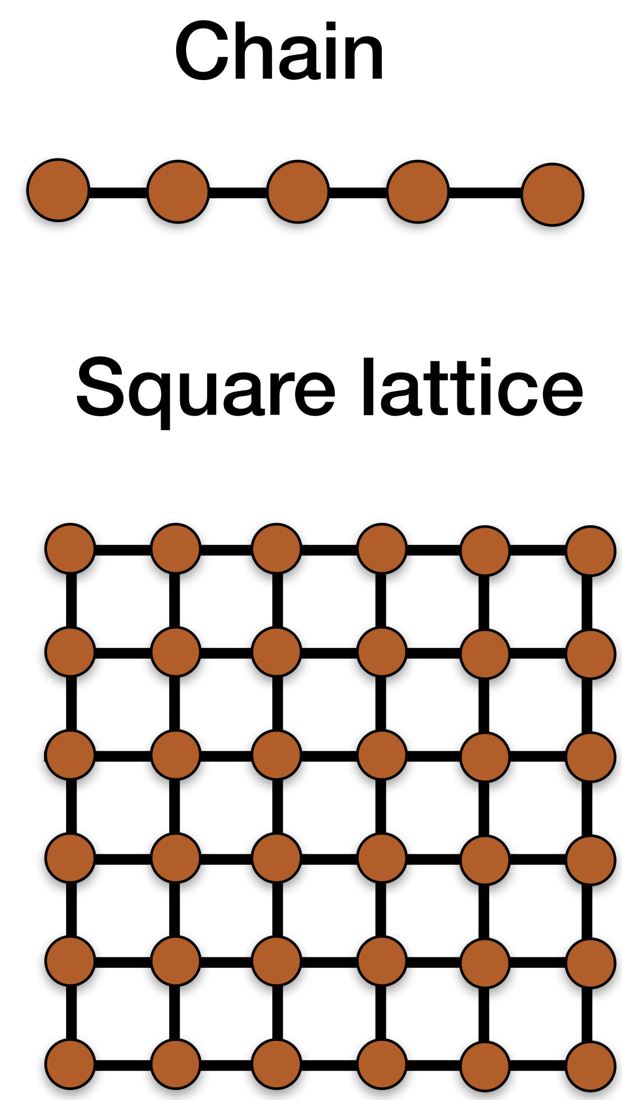
Cost of tensor network contraction:

d-dimensional cubic lattice $N = L^d$

Chain: $O(ND^2)$ (Open)
$O(ND^3)$ (Periodic)

Square: $O(D^L)$ (Open)
$O(D^{2L})$ (Periodic)

d-dimensional cubic: $O(D^{L^{d-1}})$



It is impossible to perform exact contraction.

→ We need efficient approximations for the contraction.

Tensor network renormalization

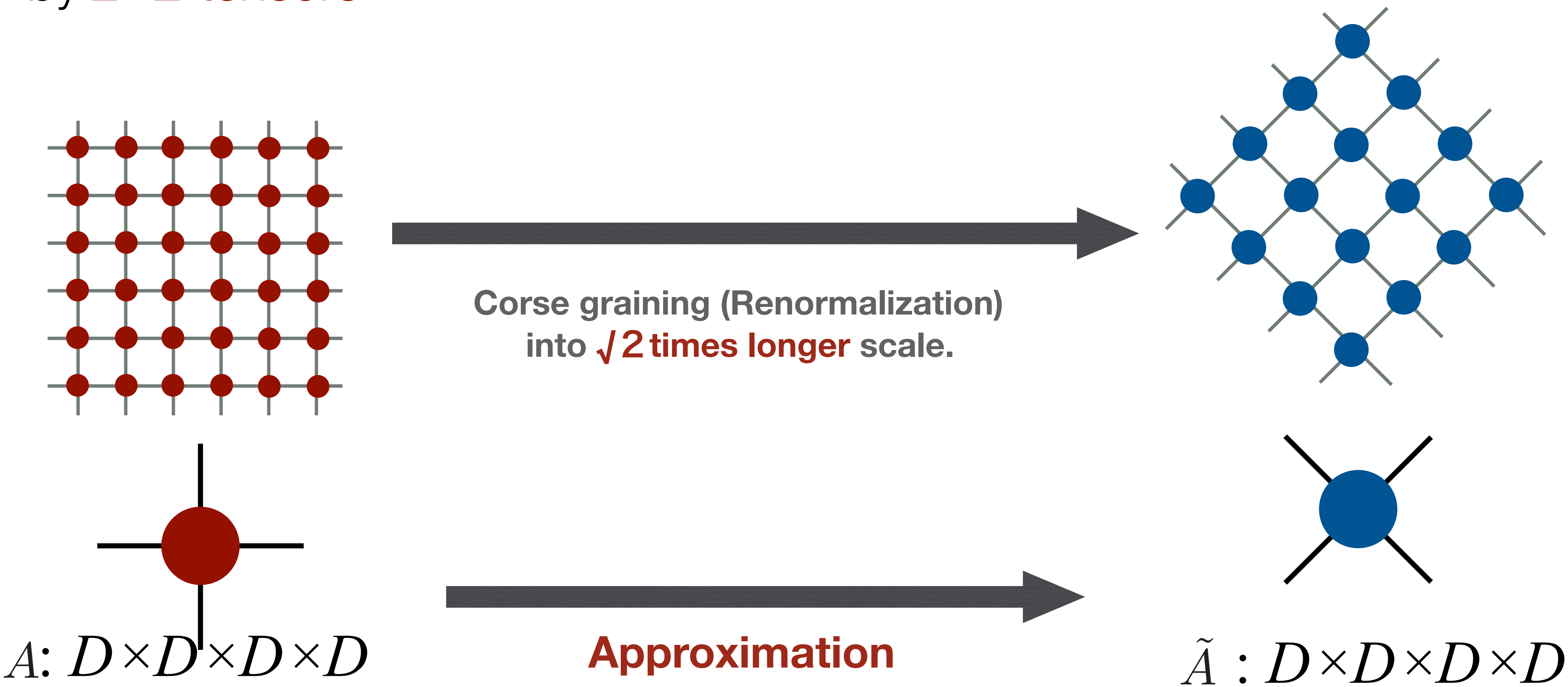
Tensor network renormalization
（テンソルネットワーク繰り込み）

- Approximate calculation of a tensor network contraction by using "coarse graining" （粗視化）of the network
  - Coarse graining $\longleftrightarrow$ Real space renormalization
  - （粗視化） $\longleftrightarrow$ （実空間繰り込み）
- It can be applicable to (basically) any lattices, and the idea (algorithm) is independent on "models" represented by tensor networks.
  - Potential application to wide range of the science.

Outline of tensor network renormalization

Scaler represented by $L \times L$ tensors

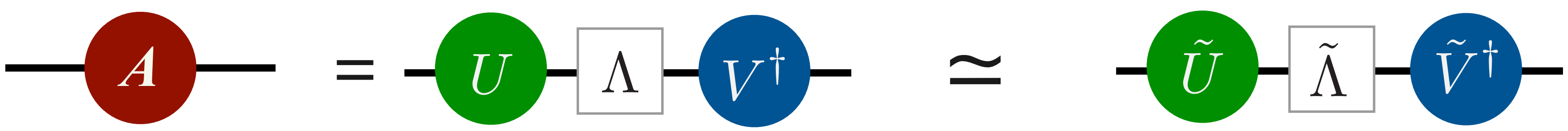
$(L \times L)/2$ tensors



Reduce the number of tensors
keeping their size constant

Key technique: low rank approximation by SVD

Best low-rank approximation of a matrix = SVD

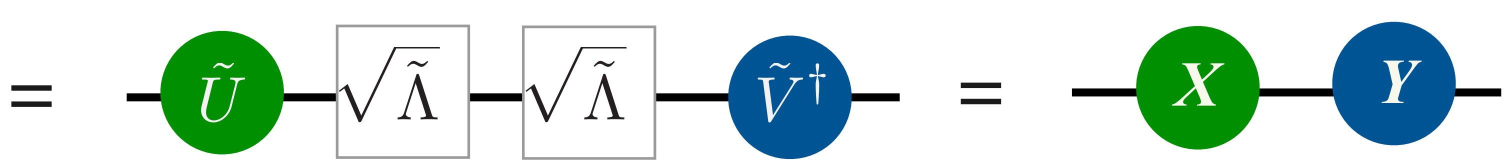


$A : M \times N$
(M ≦ N)

$\Lambda : M \times M$
(Diagonal matrix)
$U, V : (\mathrm{M,N}) \times M$

$\tilde{\Lambda} : R \times R$
(Keeping the R largest singular values)
$\tilde{U}, \tilde{V} : (\mathrm{M,N}) \times R$

In addition,



$\sqrt{\tilde{\Lambda}}$:Diagonal matrix
those elements are $\sqrt{\lambda}$

$X = \tilde{U}\sqrt{\tilde{\Lambda}}$ $:\mathrm{M} \times R$

$Y = \sqrt{\tilde{\Lambda}}\tilde{V}^\dagger$ $:\mathrm{R} \times M$

By SVD, we can decompose a matrix into a product of "small" matrices.

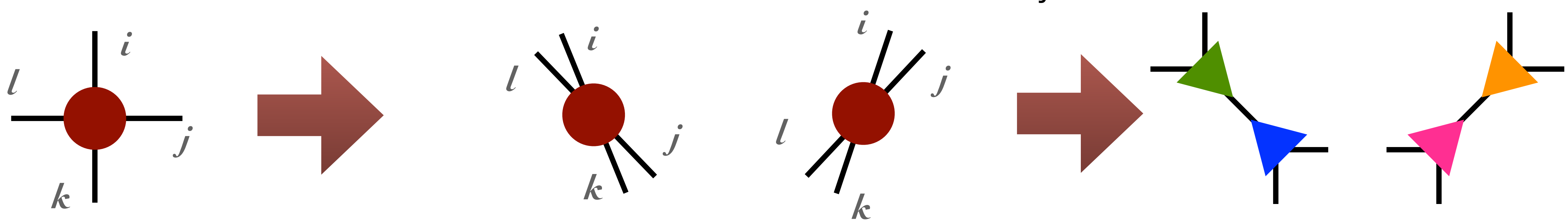
Recipe of Tensor Renormalization Group (TRG)

M. Levin and C. P. Nave, Phys. Rev. Lett. **99**, 120601 (2007)
Z.-C. Gu, M. Levin and X.-G. Wen, Phys. Rev. B **78**, 205116 (2008)

1. Decomposition

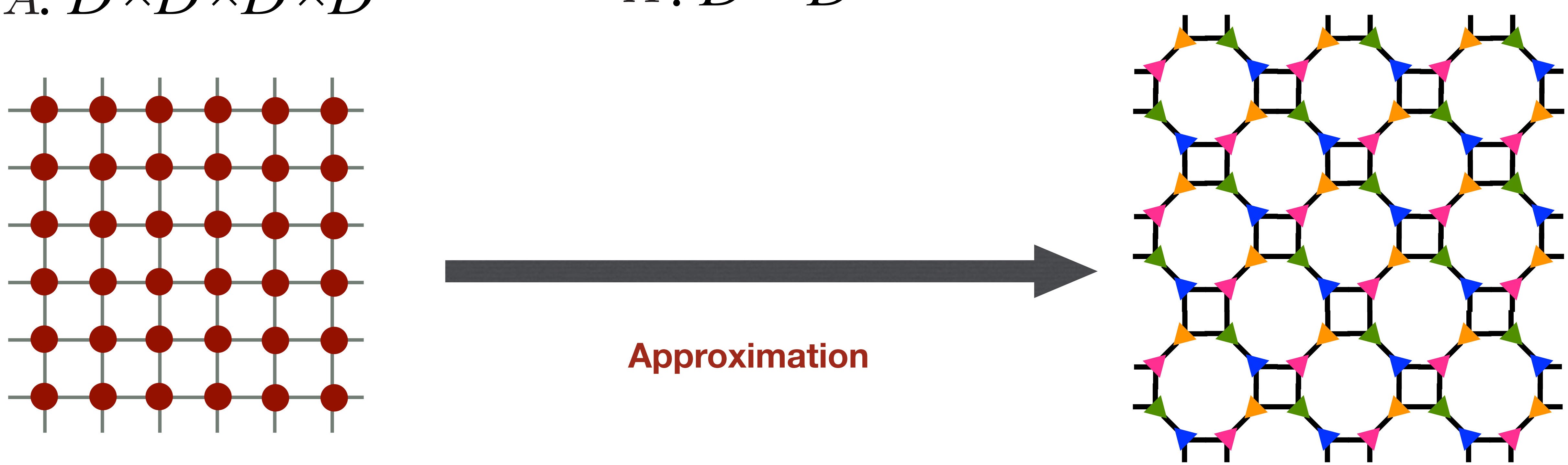
Regard a tensor as a matrix

D-rank approximation by SVD



$A_{i,j,k,l}$ $\quad$ $A_{(i,l),(j,k)}$ $\quad$ $A_{(i,j),(k,l)}$

A: $D \times D \times D \times D$ $\qquad$ $A: D^2 \times D^2$



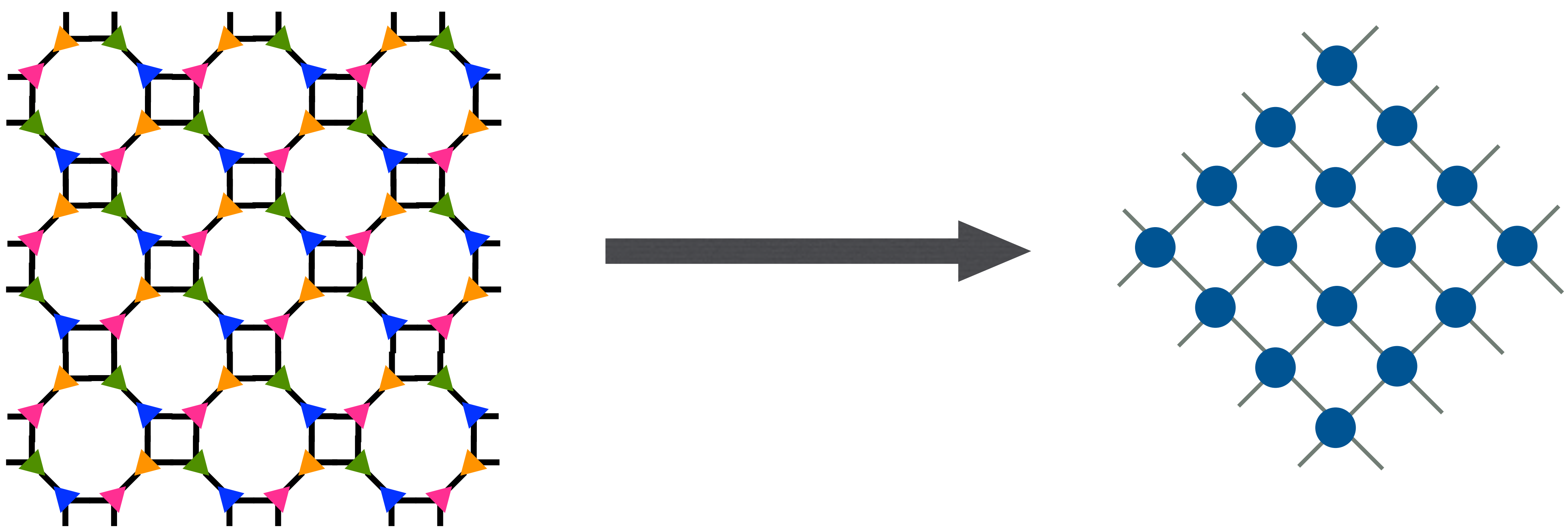
Recipe of Tensor Renormalization Group (TRG)

M. Levin and C. P. Nave, Phys. Rev. Lett. **99**, 120601 (2007)
Z.-C. Gu, M. Levin and X.-G. Wen, Phys. Rev. B **78**, 205116 (2008)

2. Coarse graining

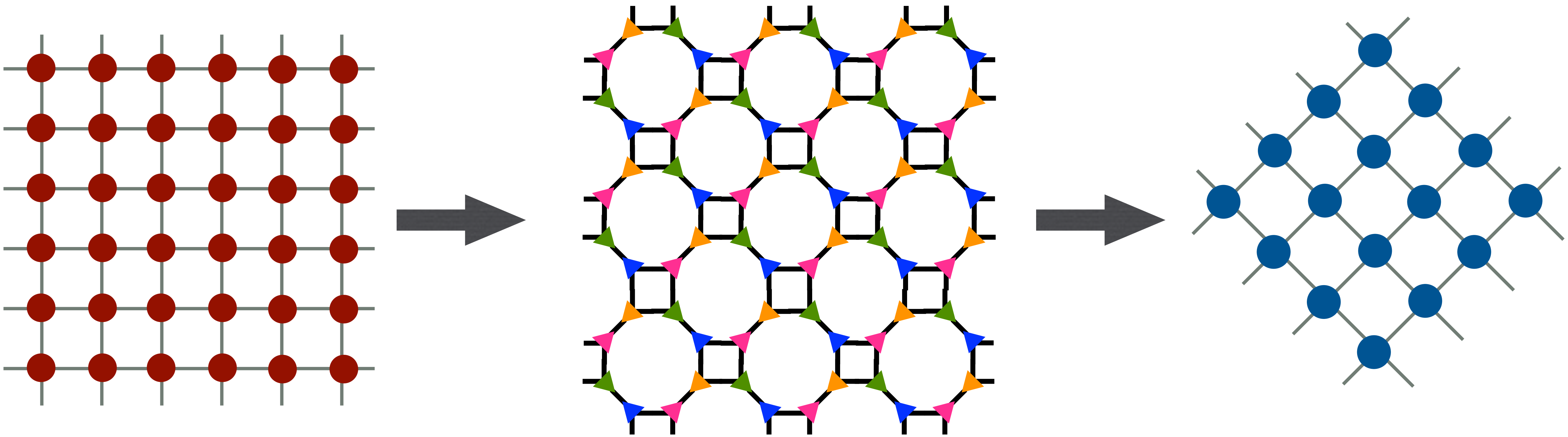
$$\tilde{A} : D \times D \times D \times D$$

In total, two original tensors are coarse grained into a new tensor.



Recipe of Tensor Renormalization Group (TRG)

M. Levin and C. P. Nave, Phys. Rev. Lett. **99**, 120601 (2007)
Z.-C. Gu, M. Levin and X.-G. Wen, Phys. Rev. B **78**, 205116 (2008)



Calculation cost: SVD= $O(D^6)$

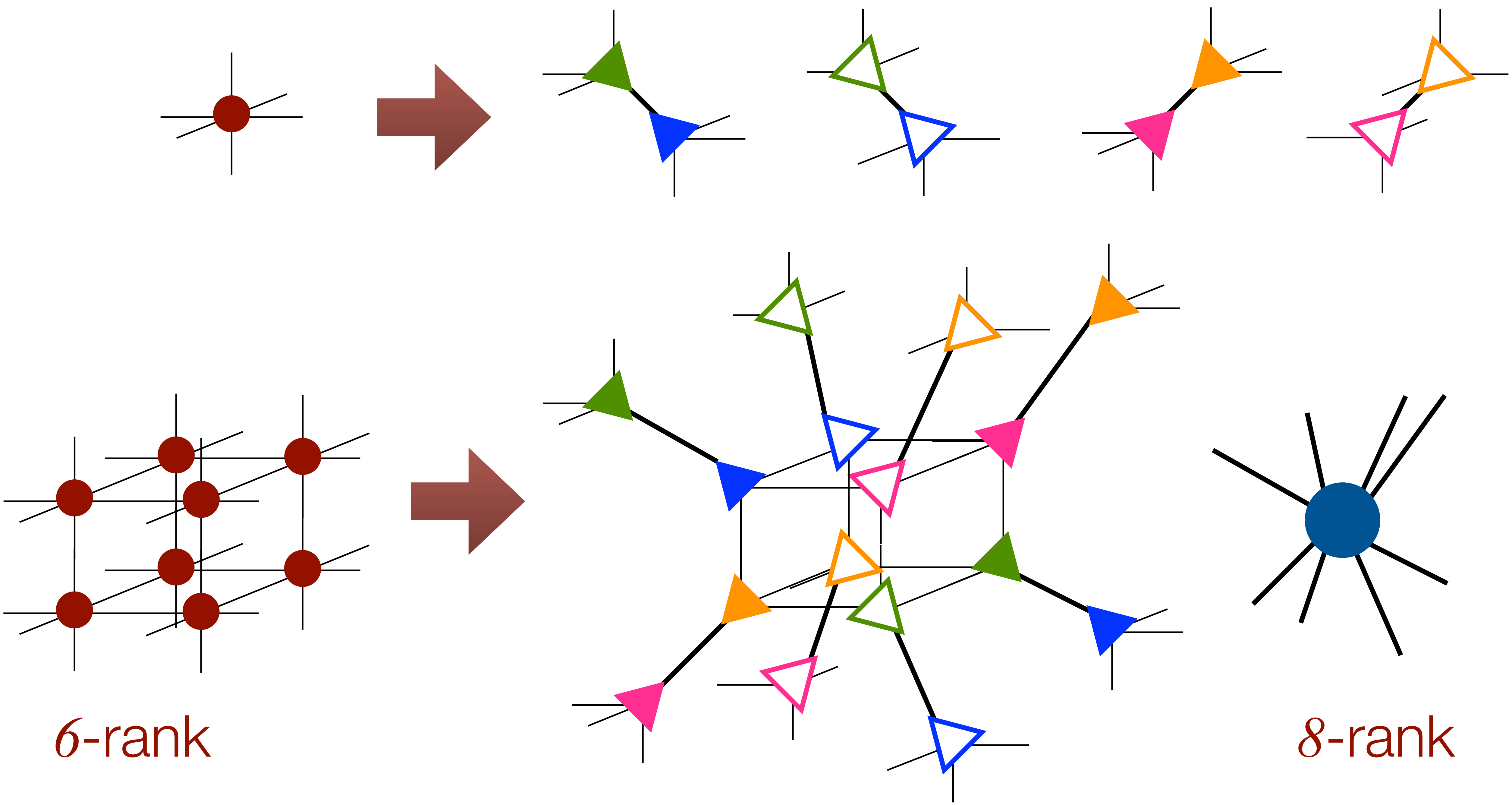
Contraction= $O(D^6)$ (per tensor)

*By one TRG step, # of tensors is reduced by 1/2.

We can calculate the contraction in polynomial cost!

Tensor renormalization group for higher dimensions

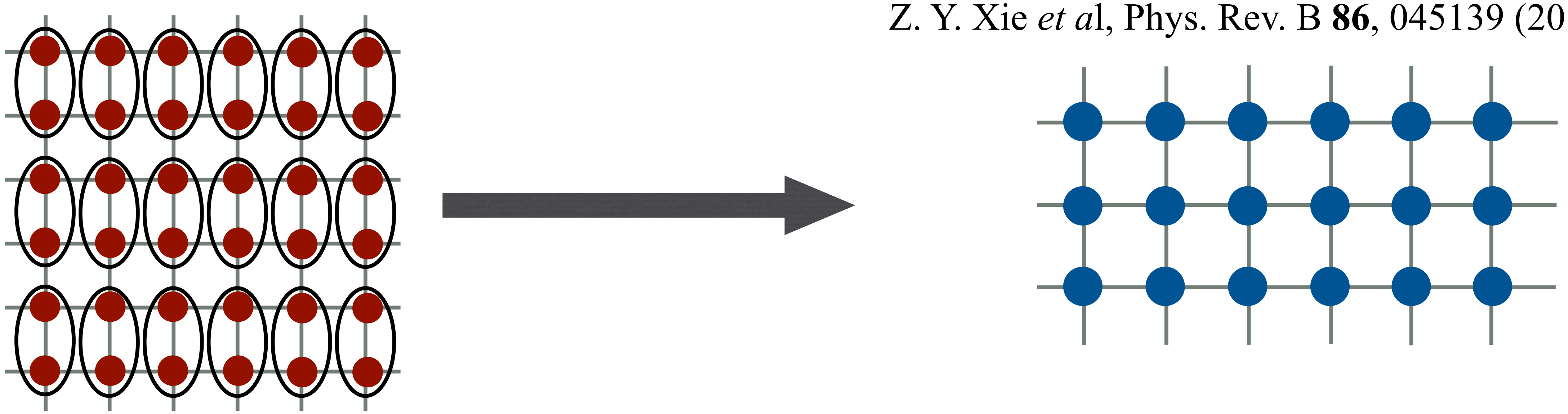
Simple generalization of TRG to cubic lattice (three dimension)



Tensor renormalization group by using HOSVD

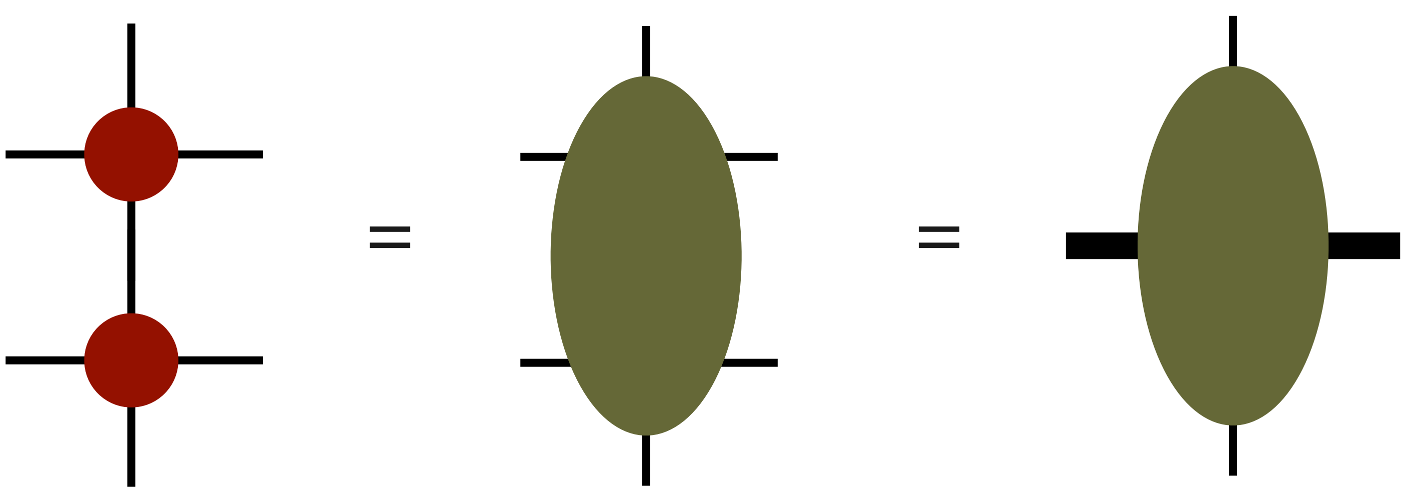
Anisotropic coarse graining by using HOSVD instead of SVD

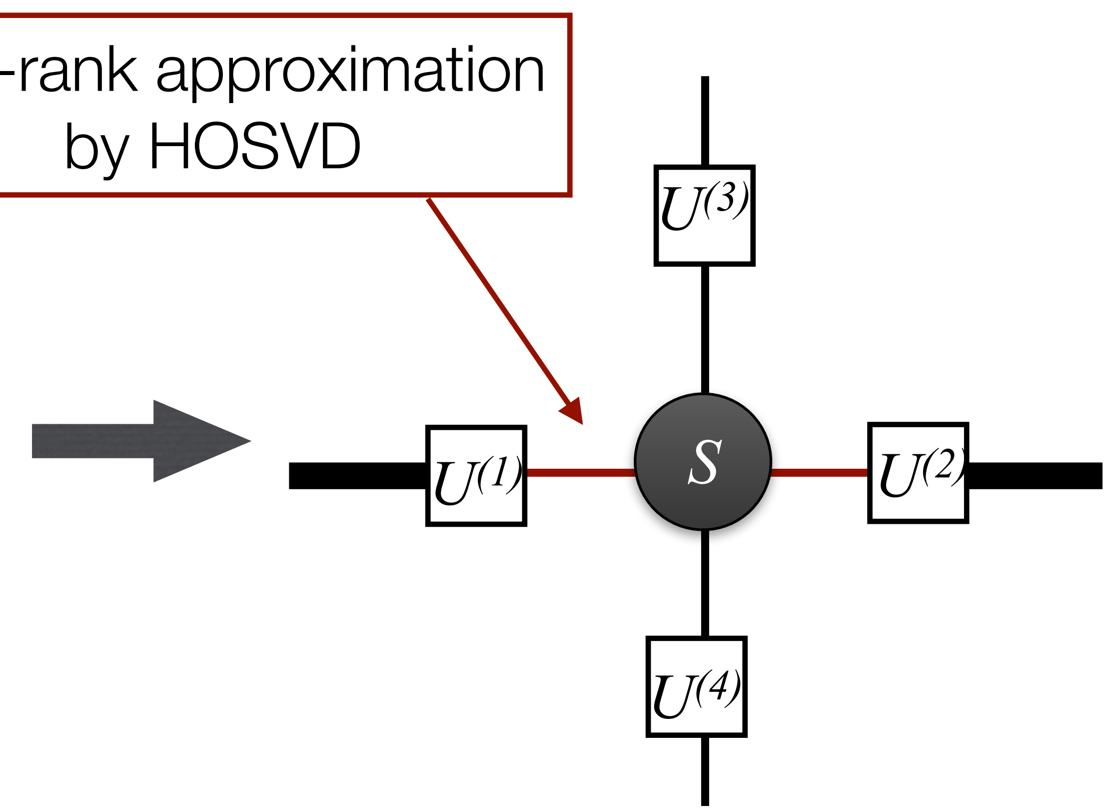
Z. Y. Xie *et al*, Phys. Rev. B **86**, 045139 (2012)



Basic idea of HOTRG algorithm:

(For details, see the original paper.)



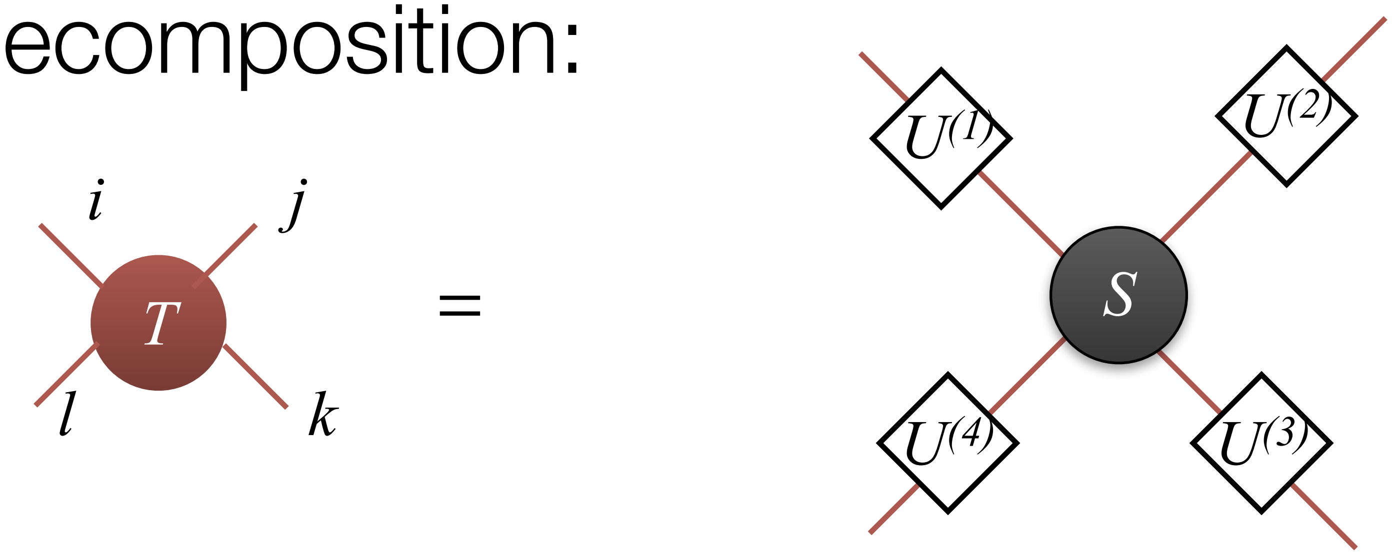


(Reference of HOSVD)

Tucker decomposition: generalization of SVD

Review: T. G. Kolda et al, SIAM Review **51**, 455 (2006)

Tucker decomposition:



$U^{(i)}$: Factor matrix (usually unitary)

S :Core tensor

$$T_{ijkl} = \sum_{i'=1}^{I}\sum_{j'=1}^{J}\sum_{k'=1}^{K}\sum_{l'=1}^{L} S_{i'j'k'l'} U^{(1)}_{ii'} U^{(2)}_{jj'} U^{(3)}_{kk'} U^{(4)}_{ll'}$$

Low "rank" approximation

$$T_{ijkl} \simeq \sum_{i'=1}^{\color{red}{I'}}\sum_{j'=1}^{\color{red}{J'}}\sum_{k'=1}^{\color{red}{K'}}\sum_{l'=1}^{\color{red}{L'}} S_{i'j'k'l'} U^{(1)}_{ii'} U^{(2)}_{jj'} U^{(3)}_{kk'} U^{(4)}_{ll'}$$

$I' < I, \quad J' < J, \quad K' < K, \quad L' < L$

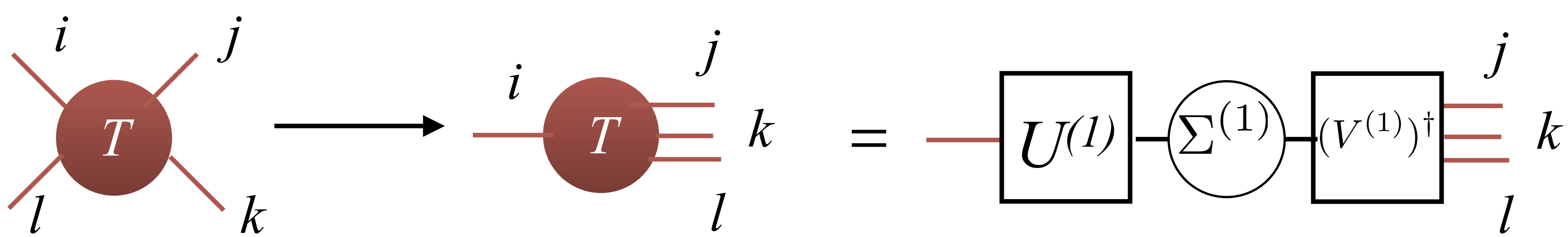
rank-(I',J', K', L') approximation

(Reference of HOSVD)

Higher order SVD (HOSVD)

L. De Lathauwer et al, SIAM J. Matrix Anal. & Appl., **21**, 1253 (2000)

Define a factor matrix from matrix SVD:



Core tensor is calculated as

$$S_{i'j'k'l'} \equiv \sum_{ijkl} T_{ijkl} (U^{(1)})^{\dagger}_{i'i} (U^{(2)})^{\dagger}_{j'j} (U^{(3)})^{\dagger}_{k'k} (U^{(4)})^{\dagger}_{l'l}$$

Properties of the core tensor

$$S^{*}_{:,i_n=\alpha,:,:} \cdot S_{:,i_n=\beta,:,:} = \begin{cases} 0 & (\alpha \neq \beta) \\ (\sigma^{(n)}_{\alpha})^2 & (\alpha = \beta) \end{cases}$$

Dot product

$$A \cdot B \equiv \sum_{i,j,k,l} A_{ijkl} B_{ijkl}$$

Generalization of the diagonal matrix Σ in matrix SVD.

* Low-rank approximation based on HOSVD is not optimal.

Power of the HOTRG

Advantage:

- HOTRG does not change the network structure.
  - We can easily generalize it to higher dimensions.
- Low-rank approximation is based on the cluster of two tensors.
  - At the approximation, we take into account more information.
  - More efficient than TRG where SVD is done for a single tensor.

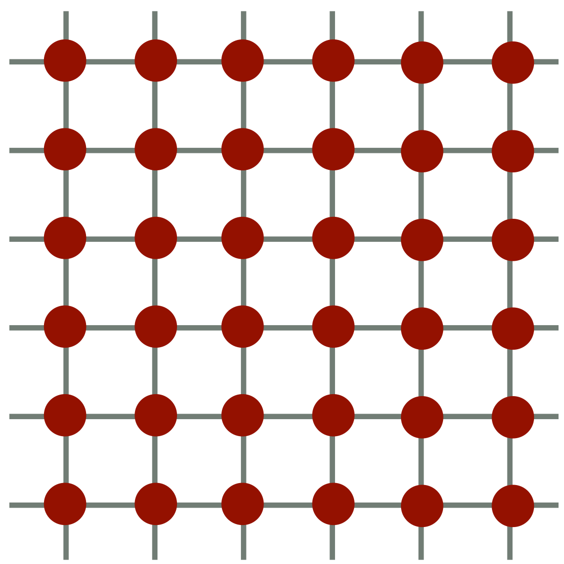
Disadvantage:

- HOTRG needs higher cost than TRG.
  - $\mathrm{O}(D^7)$ in HOTRG $\longleftrightarrow$ $\mathrm{O}(D^6)$ in TRG

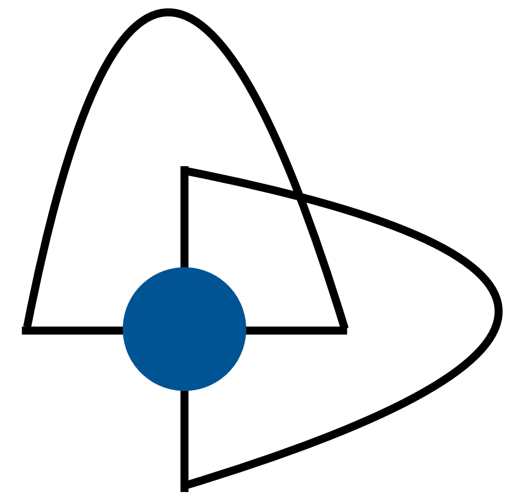
Application to a classical partition function

Partition function

(Periodic boundary condition)

$Z =$ 

Repeat TRG step until only a few tensors remain.



We can easily calculate physical quantities from Z.

Free energy: $F = -k_B T \ln Z$

Energy: $E = -\dfrac{\partial \ln Z}{\partial \beta}$ (Use difference approximation)

Specific heat: $C = \dfrac{1}{k_B T^2} \dfrac{\partial^2 \ln Z}{\partial \beta^2}$ (Use difference approximation)

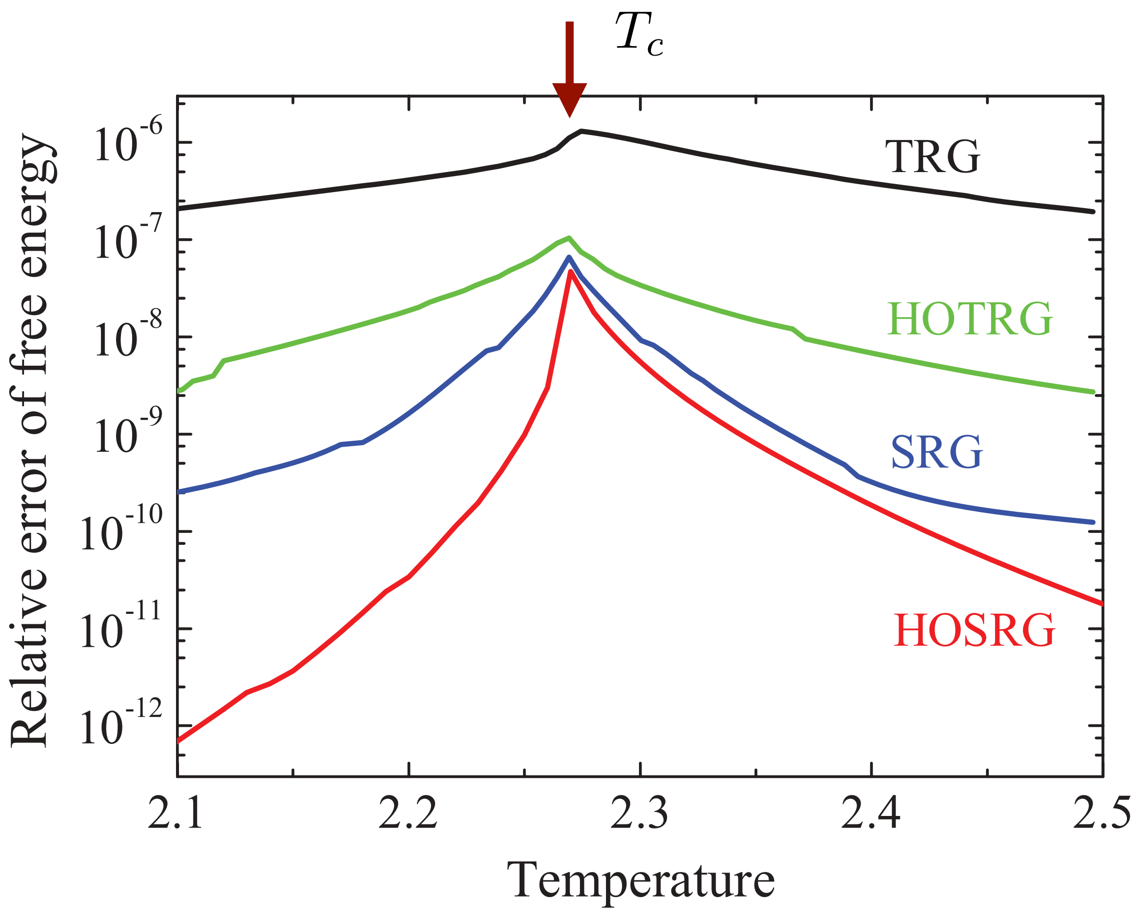
Example of calculation

Ising model in infinite size

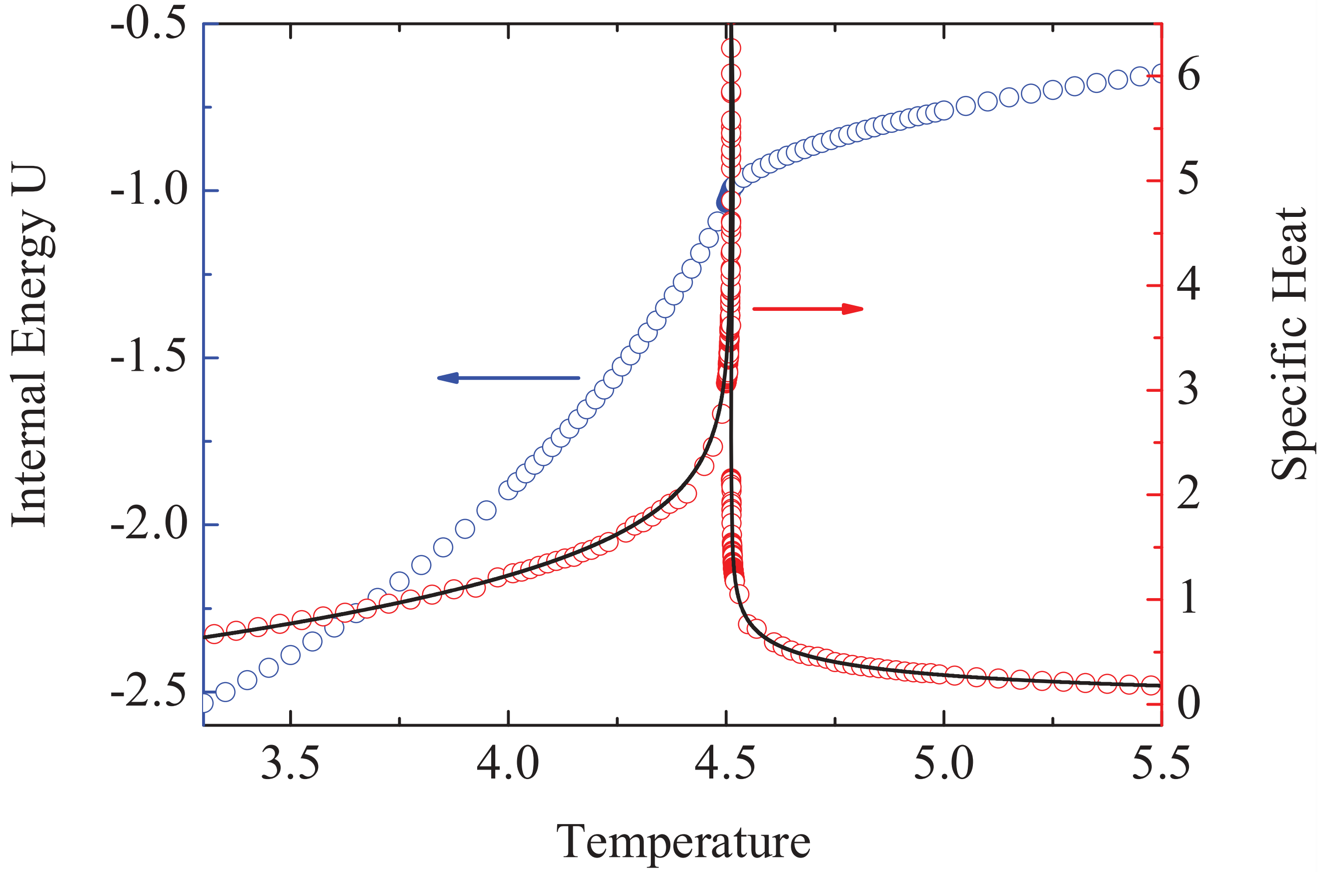
$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j$$

Z. Y. Xie *et a*l, Phys. Rev. B **86**, 045139 (2012)

Error of free energy for 2D Ising model



Energy and specific heat of 3D Ising model



$$T_c/J = \frac{2}{\ln(1+\sqrt{2})} \simeq 2.269$$

Tensor network renormalization at the critical point

— When the accuracy of TRG becomes worse?

Correlation (entanglement) within a tensor

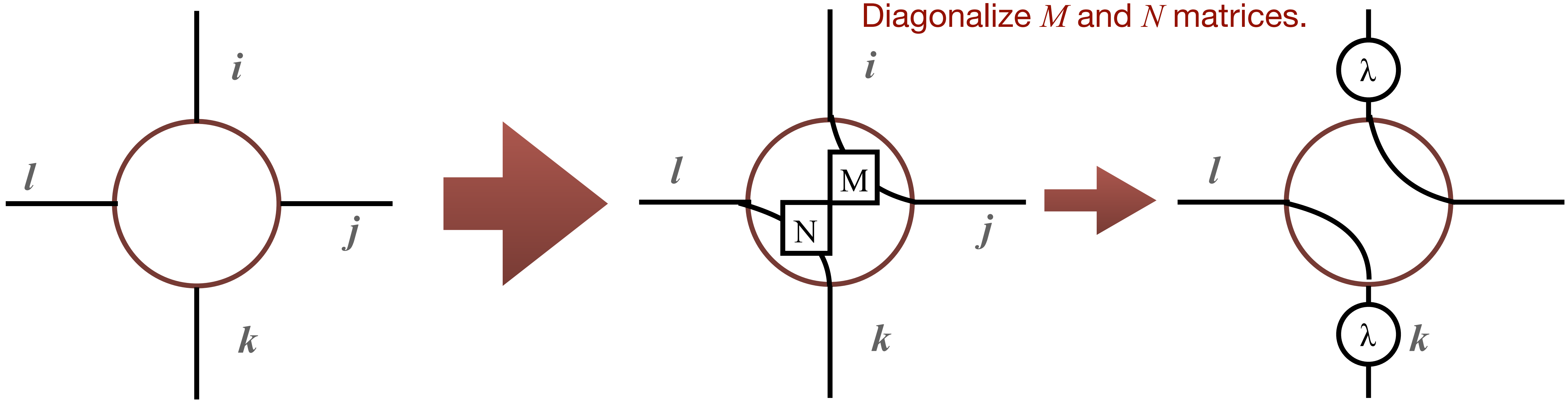
General tensor

$$A_{ijkl}$$

Eg. *Correlation* in (i,j) and (k,j)

$$A_{ijkl} = M_{ij} N_{kl} \quad \Rightarrow \quad A_{ijkl} = \lambda_i^{(M)} \lambda_k^{(N)} \delta_{ij} \delta_{kl}$$

Diagonalize M and N matrices.



New rule for representation of the correlation:

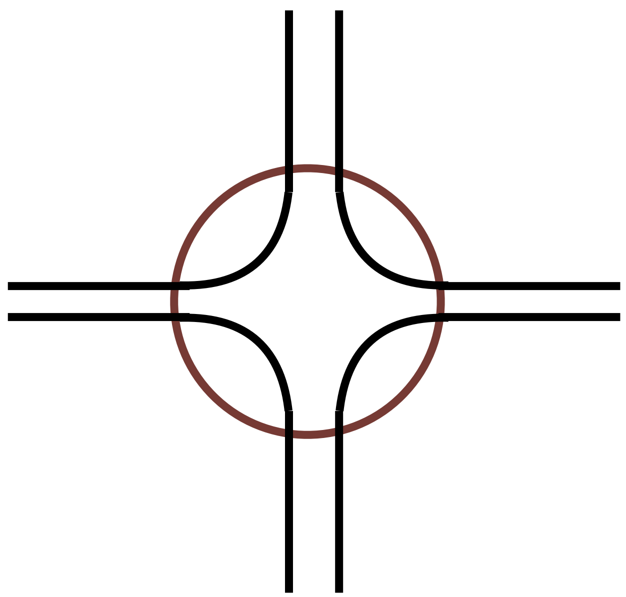
$$i \;\text{———}\; j = \delta_{ij}$$

(+ we neglect eigenvalues in the graph.)

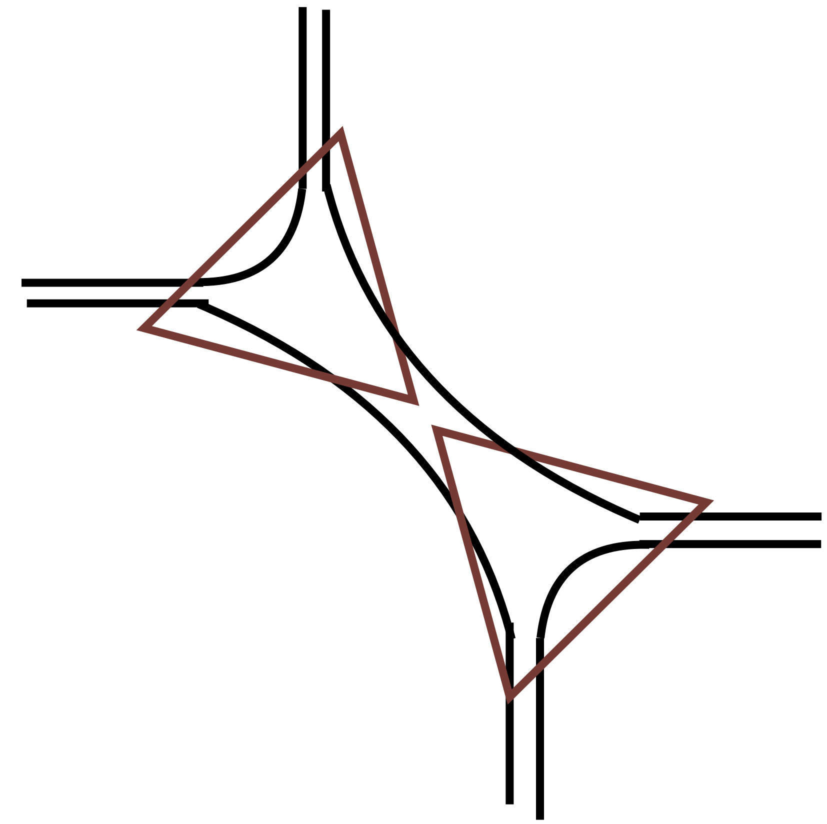
Fixed point of TRG: Corner Double Line tensor (固定点)

Corner Double Line (CDL) tensor:

There are correlations among the nearest legs.



SVD



Original bond dimension = D

Degree of freedoms connecting two tensors.

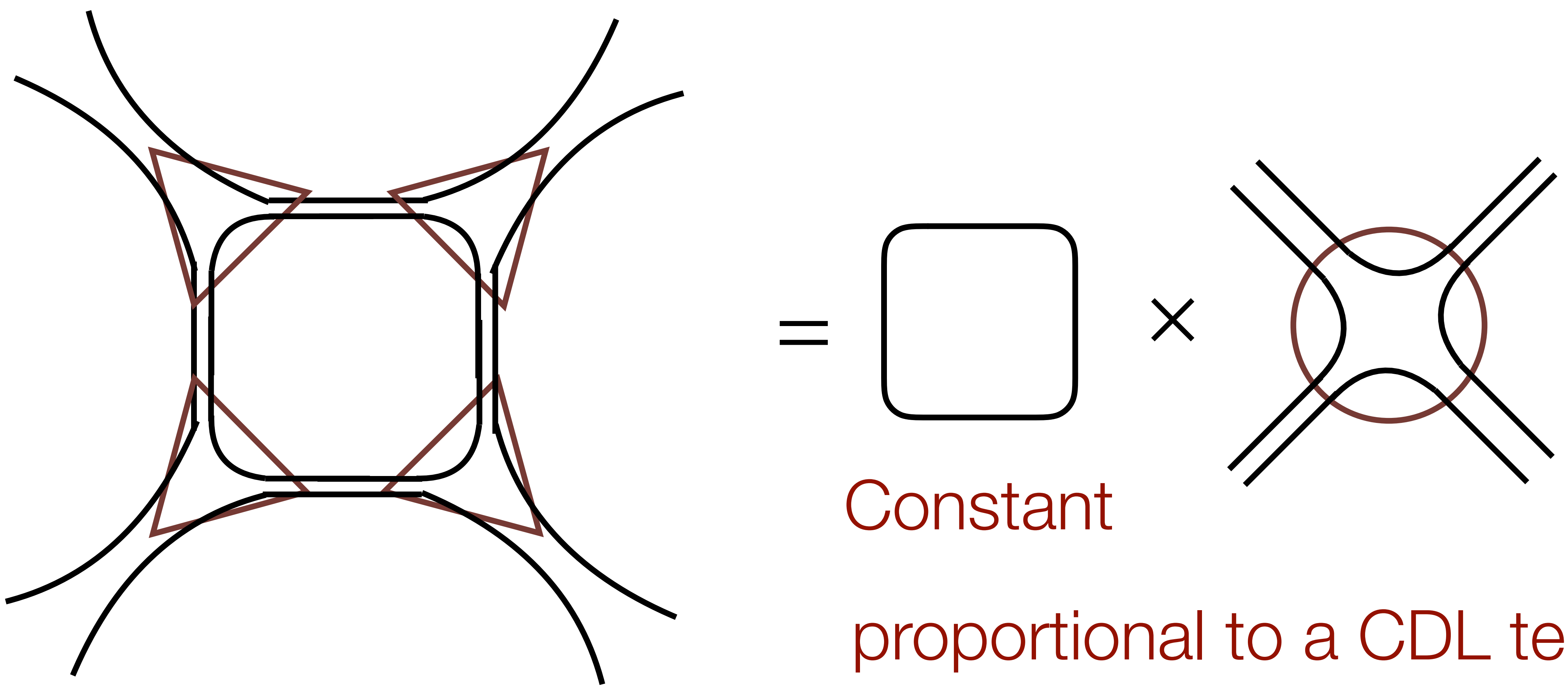
Two lines = D

Single line: bond dimension $\sqrt{D}$

No truncation error at SVD
(Original rank = D)

Fixed point of TRG: Corner Double Line tensor

Contraction of four tensors in TRG:



proportional to a CDL tensor!

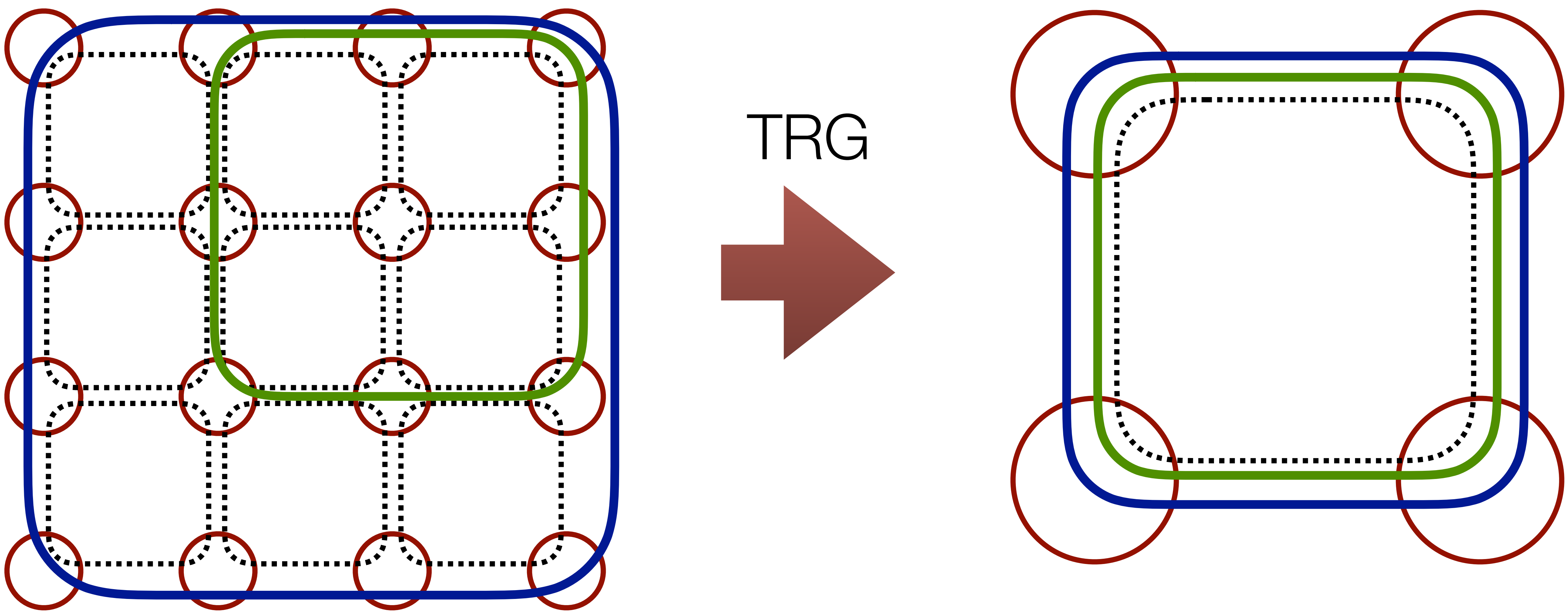
CDL tensor is a fixed point of TRG (and also HOTRG).

CDL tensor remains as CDL tensor along TRG.

Problems in TRG: accumulation of correlations

Correlation in several scales

Correlations remains after TRG.



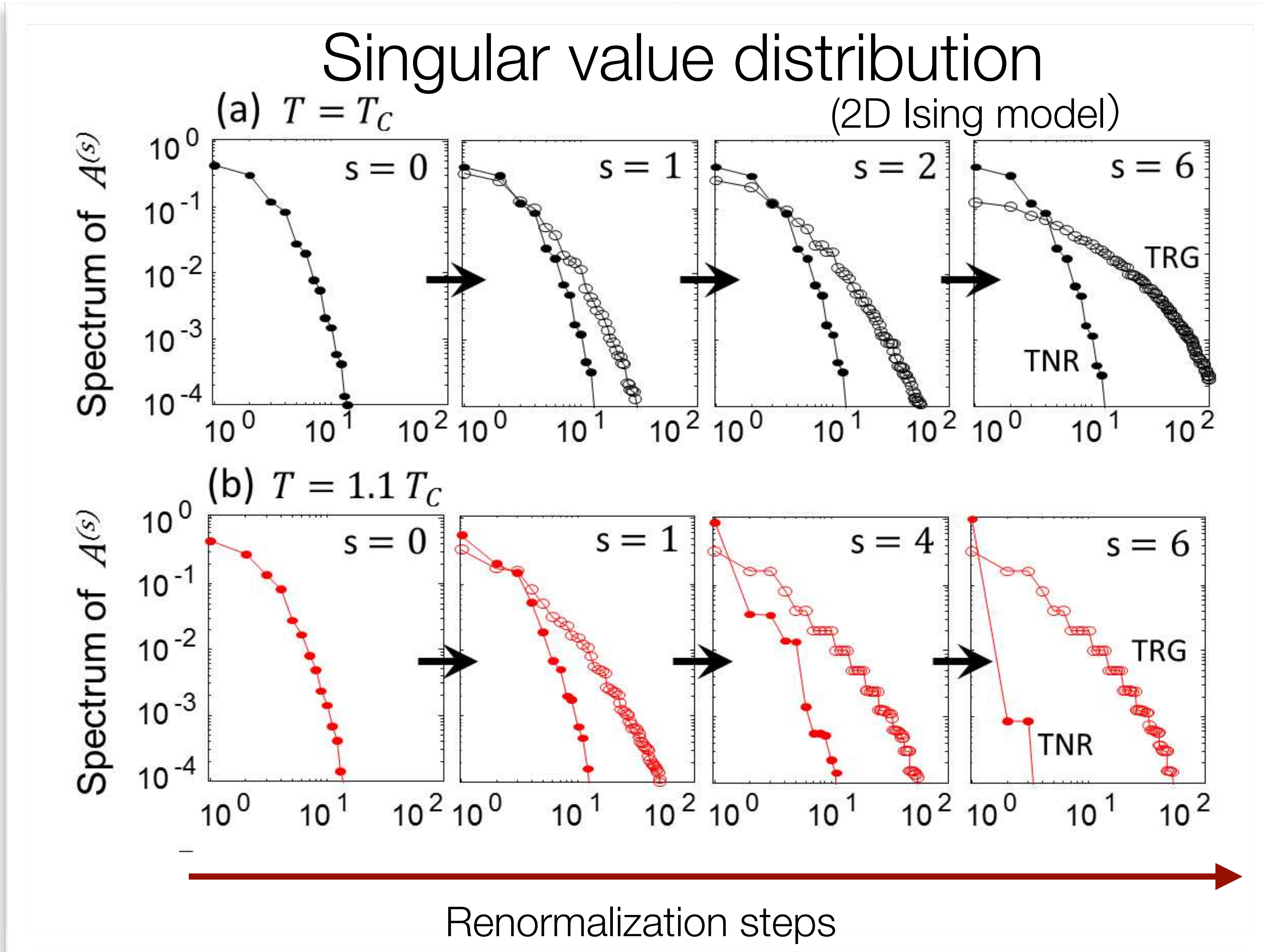
Ideal renormalization:

Correlation in shorter scales should be removed.
Only the correlation in the present scale exists.

TRG :

Correlations in all scales remain.

Problem in TRG: increase of truncation error



G. Evenbly and G. Vidal
Phys. Rev. Lett. **115**, 180405 (2015)

In TRG, the width of the singular value distribution increases along renormalization.

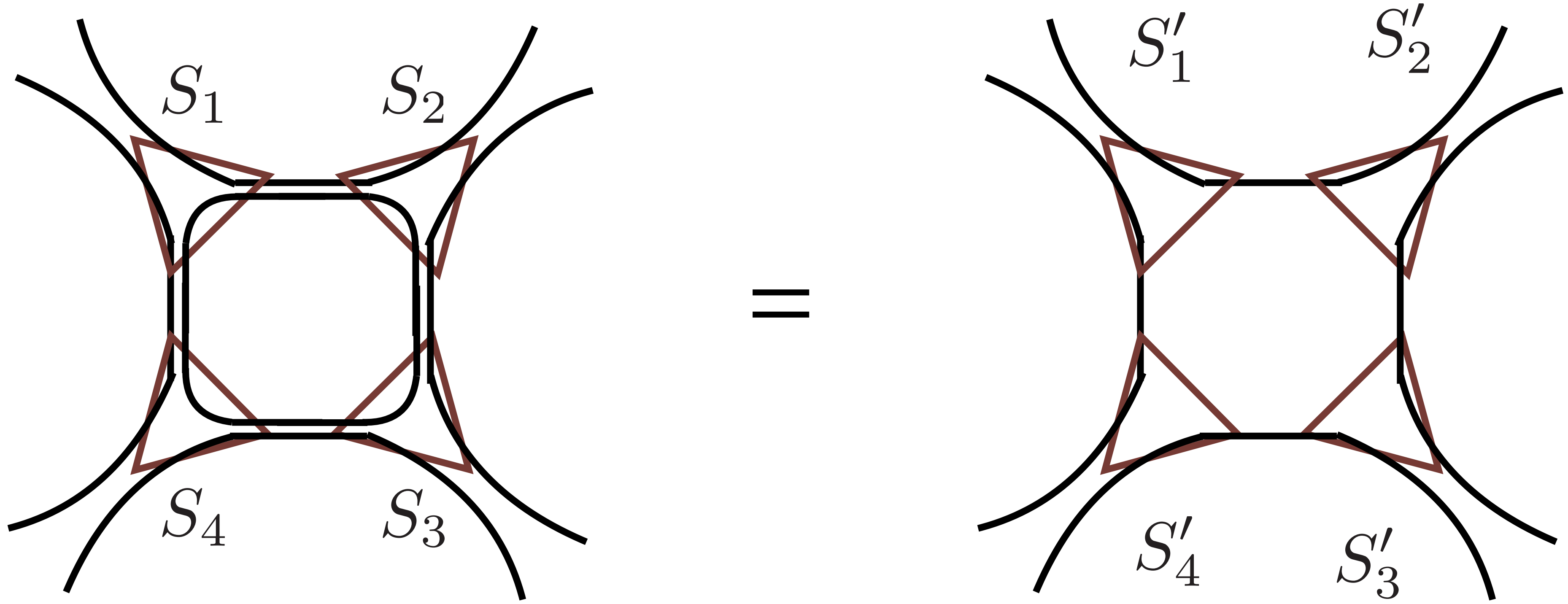
Increase of truncation error (decrease of accuracy)

Improvement of TRG：Entanglement Filtering

Try to remove CDL structure at renormalization steps.

Z.-C. Gu and X.-G Wen, Phys. Rev. B 80, 155131 (2009)

Idea:



S: $D \times D \times D$

S': $D \times D' \times D'$

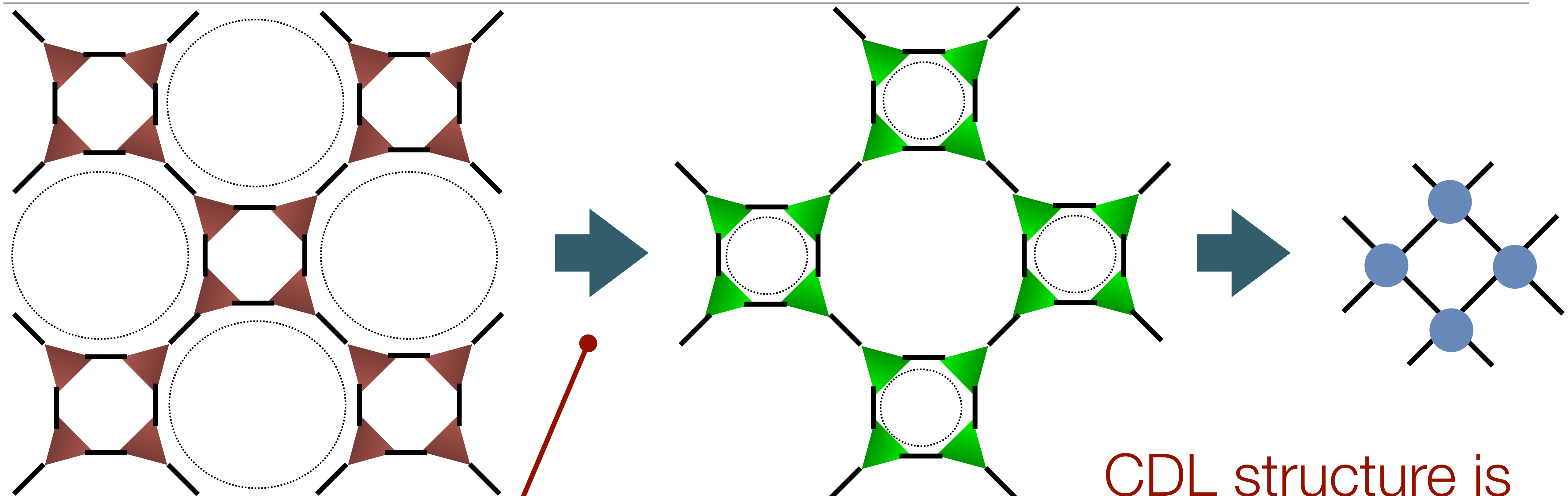
$$\mathbf{S'} = \square^{1/4}\,\mathbf{S}$$

$$D' \sim \sqrt{D}$$

Insert this "approximation" into the TRG algorithm.

Tensor Entanglement Filtering Renormalization

Z.-C. Gu and X.-G Wen, Phys. Rev. B 80, 155131 (2009)

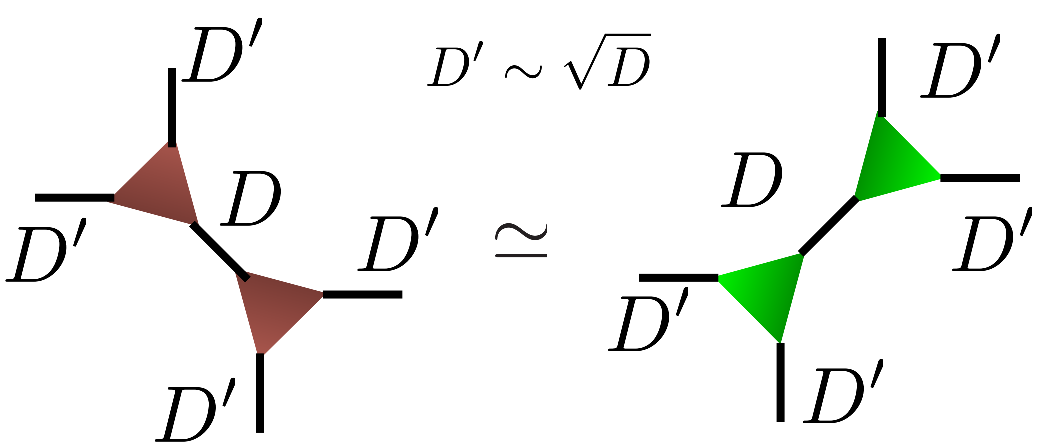


S' (after approximation)

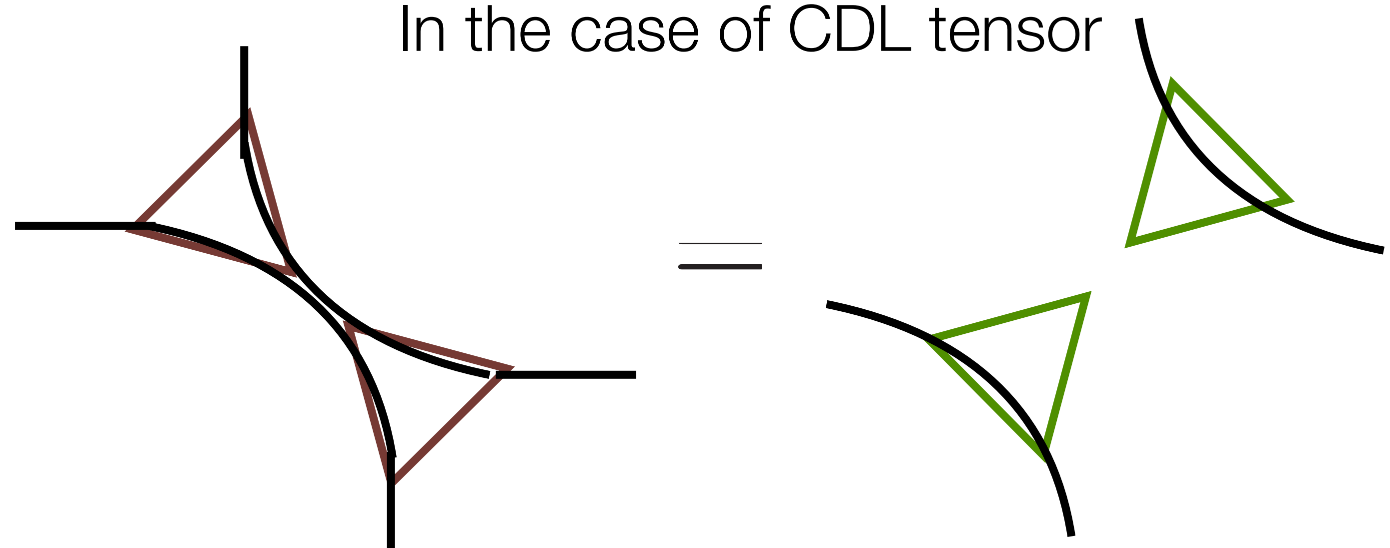
CDL structure is perfectly removed!

Change of SVD: $D' < D$

$D' \sim \sqrt{D}$



In the case of CDL tensor

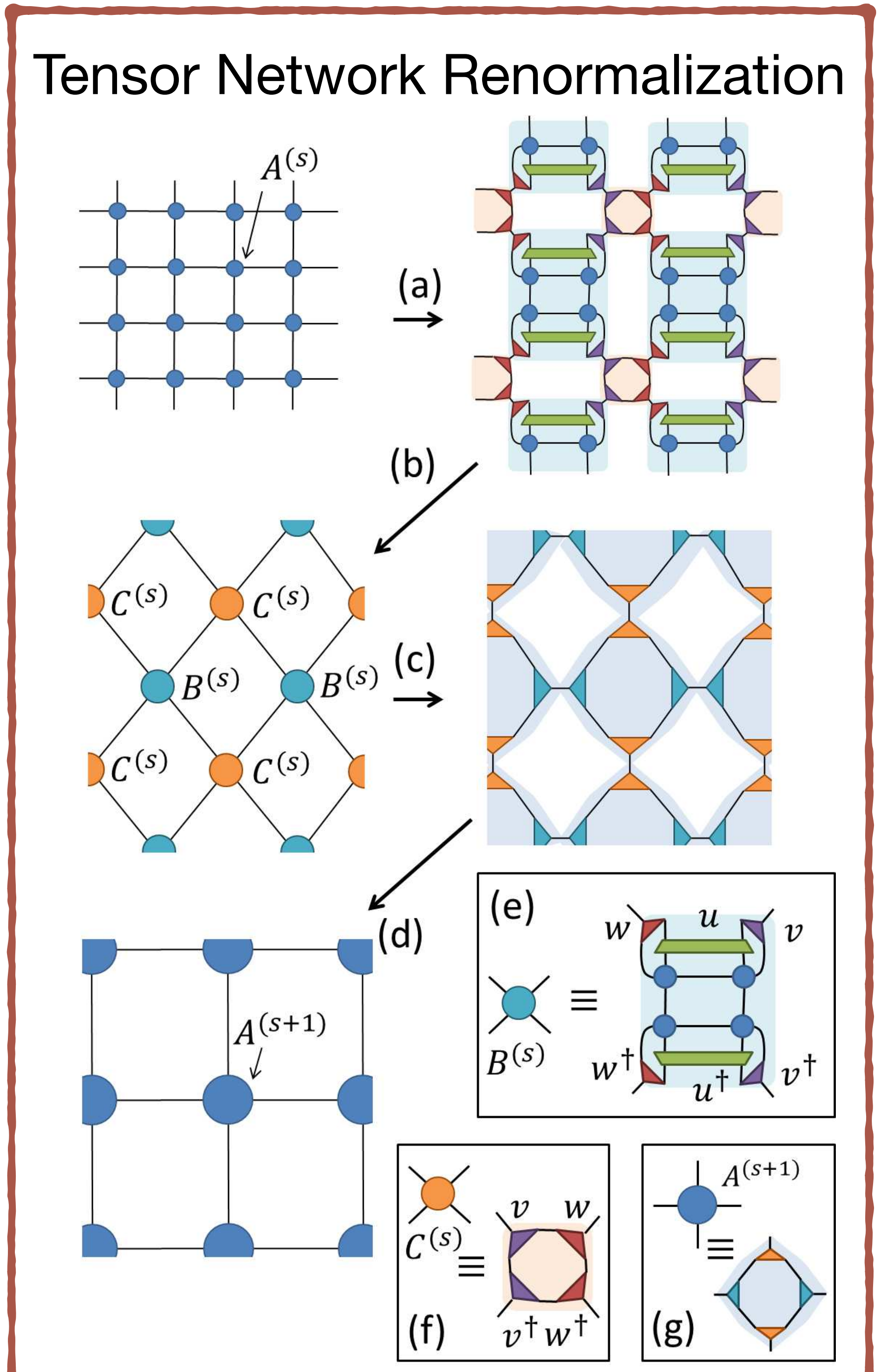


Remaining problem in TEFR

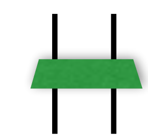
- TEFR works well far from the critical point.
  - Because it can remove CDL structure.
- In the vicinity of the critical point, the accuracy is still poor.
  - Because the actual entanglement is not necessarily perfect CDL structure.
- In order to improve further, we need to consider the entanglement structure beyond CDL tensor.

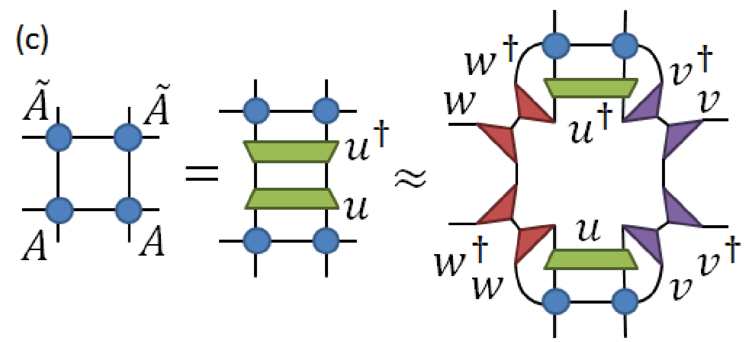
Recent progress: Tensor Network Renormalization

G. Evenbly and G. Vidal, Phys. Rev. Lett. **115**, 180405(2015).
arXiv:1412.0732.



Point of TNR

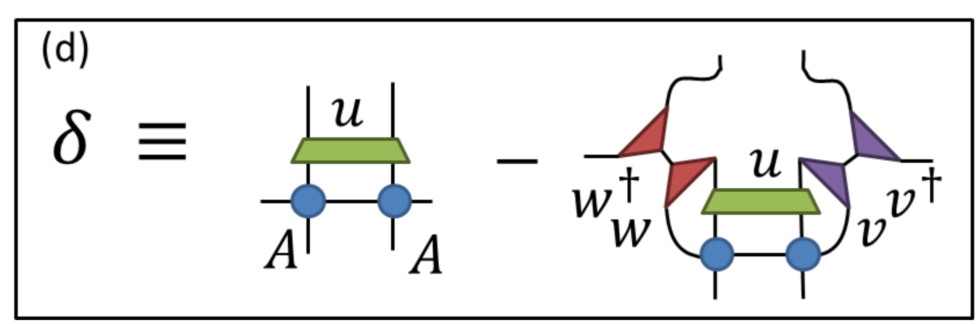
Use of a disentangler(Unitary tensor) 



It can remove short range entanglement efficiently.

(Not only CDL)

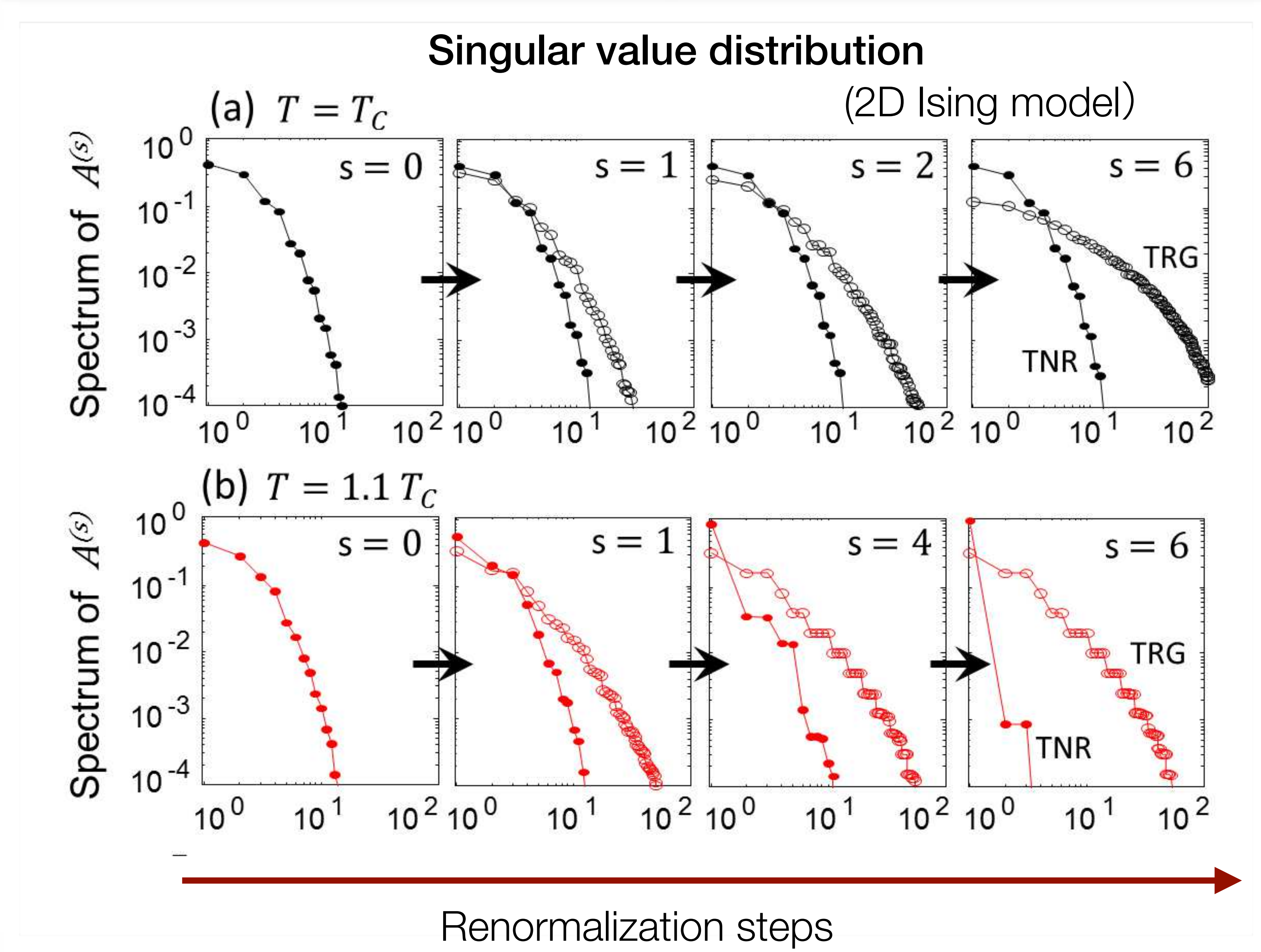
Approximation by using two-tensor cluster:

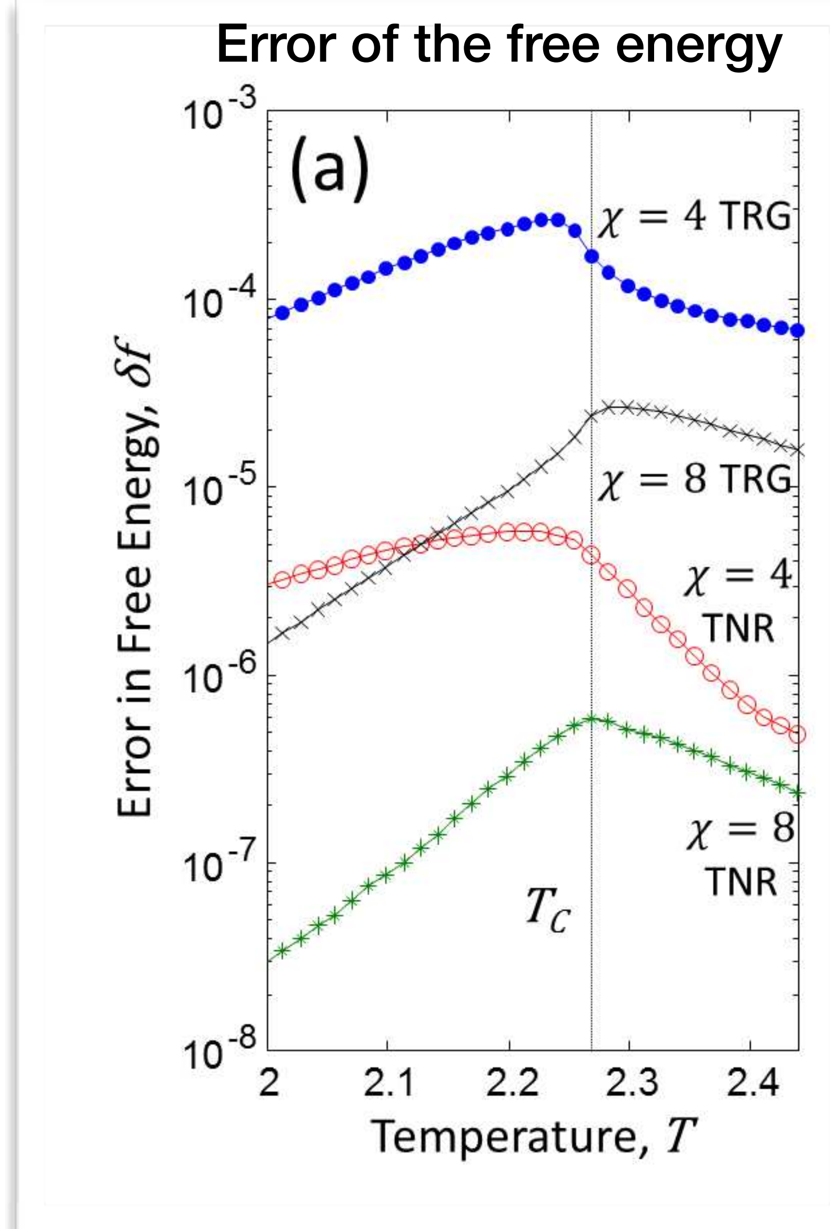


Better accuracy than the simple SVD of single tensor

Power of TNR

G. Evenbly and G. Vidal,Phys. Rev. Lett. **115**, 180405 (2015)
,arXiv: 1412.0732v2 (free energy).





In TNR:
- The singular value distribution is narrower than that of TRG.
- It is almost unchanged at Tc.
  - Indicating scale invariance of the critical system.

Interesting topics in tensor network renormalization

- Try to find efficient algorithm to remove "short range" entanglement
  - TNR, Loop-TNR, GILT

TNR: G. Evenbly and G. Vidal,Phys. Rev. Lett. **115**, 180405 (2015)
Loop-TNR: S. Yang, Z.-C. Gu and , X.-G. Wen, Phys. Rev. Lett. **118**, 110504 (2017)
GILT: M. Hauru, C. Delcamp. S. Mizera arXiv:1709.07460

- Application to lattice QCD
  - TRG with Grassmann algebra

Z.-C. Gu, F. Verstraete, and X.-G. Wen, arXiv:1004.2563
S. Takeda, and Y. Yoshimura PTEP **2015**, 043B1 (2015).

- Property at the criticality
  - Relation between TNR and MERA
  - Relation to Conformal invariance

G. Evenbly and G. Vidal,Phys. Rev. Lett. **115**, 200401 (2015)
G. Evenbly, Phys. Rev. B **95**, 045117 (2017)

Report problems

- Pleas solve both of the problems:
  1. Report problem (EE in TPS)
  2. Report problem (TRG)
- Please include your name and student id in your report.
- Please submit through ITC LMS
  (If you have any troubles, please send us email:
  t-okubo@phys.s.u-tokyo.ac.jp
- Deadline is 2018/1/31 (23:30)

Report problem (EE in TPS)

1. Explain the upper bound of entanglement entropy of MPS (compulsory)
    1. Consider enough large vector with dimension m^N and suppose it is represented by MPS with bond dimension χ.
       (The vector is normalized.)
    2. Divide the system into two part (for example at the center of MPS), and represent the reduced density matrix by matrices of MPS
    3. Show the rank of the reduced density matrix by using χ.
       (Please include "derivation" of the result.)
    4. Explain the upper bound of the entanglement entropy calculated from the reduced density matrix.

       You can use the following fact:

$$-\mathrm{Tr}\ \rho \log \rho \leq \mathrm{dim}\rho$$

ρ : (reduced) density matrix

Report problem (EE in TPS)

2.Explain the upper bound of entanglement entropy of TPS (optional)

1. By using similar argument to the case of MPS, explain the upper bound of EE of TPS (on d-dimensional cubic lattice).
2. Explain general relation between upper bound of EE and tensor network structure.

Report problem (TRG)

1. Calculate the singular value spectrum obtained by TRG (compulsory)
    1. Consider classical Ising model on the square lattice.
    2. Perform TRG in several steps for a few temperature with bond dimension D.
    3. Plot singular values at the SVD (Please normalize it as $\sum_i \sigma_i = 1$.)
    4. By changing temperatures and the bond dimensions, discuss the shape of singular value distribution.
       (Recommendation: try around Tc and far from Tc)

This can be done by sample python code Report_TRG.py

Usage: python Report_TRG.py -D D -n n -T T

output:

```
okubo$ python Report_TRG.py -D 8 -n 4 -T 2.0
T=  2.0
L=  16
D=  8
free energy density=  -2.05699380572
```

Report problem (TRG)

1. Calculate the singular value spectrum obtained by TRG (compulsory)

Usage: python Report_TRG.py -D D -n n -T T

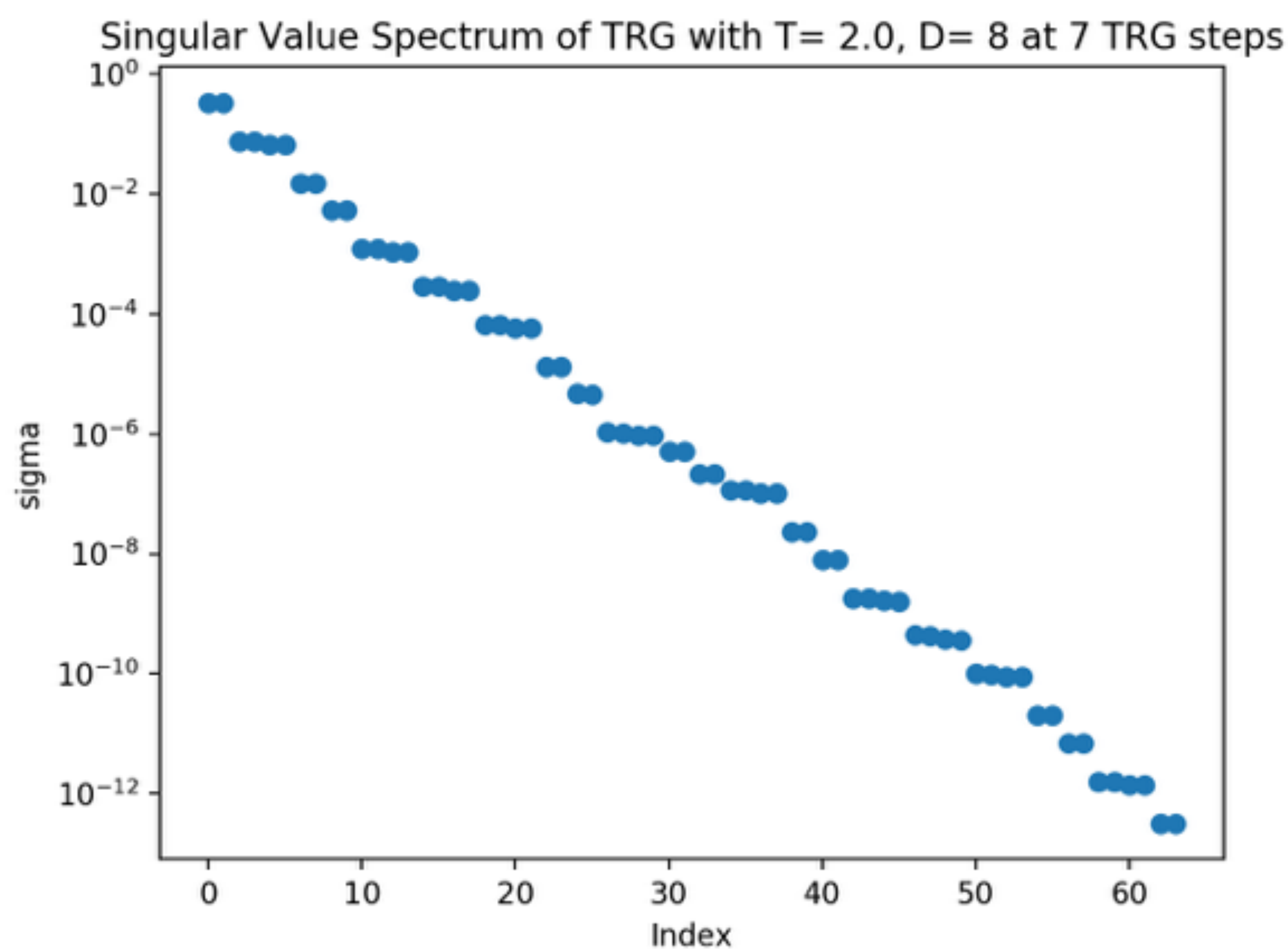
D: bond dimension

T: temperature

n: related to TRG steps through the relation

TRG step $=2n-1$

The standard output is free energy density of $L=2^n$ Ising model



Keywords

第１回：　現代物理学における巨大なデータ
第２回：　情報圧縮と繰り込み
第３回：　情報圧縮の数理１　(線形代数の復習)
第４回：　情報圧縮の数理２　(特異値分解と低ランク近似)
第５回：　情報圧縮の数理３　(スパース・モデリングの基礎)
第６回：　情報圧縮の数理４　(クリロフ部分空間法の基礎)
第７回：　物質科学における情報圧縮
第８回：　スパース・モデリングの物質科学への応用
第９回：　クリロフ部分空間法の物質科学への応用
第１０回：　行列積表現の基礎
第１１回：　行列積表現の応用
第１２回：　テンソルネットワーク表現への発展
第１３回：　テンソルネットワーク繰り込みと低ランク近似の応用