Thermal Tensor Network Approach for Quantum Many-Body systems

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Oct. 19, 2022

Outline

1. Finite-T tensor network methods

- 1.1 Tensor network basis
- 1.2 Series-expansion thermal tensor network
- 1.3 Exponential tensor renormalization group
- 1.4 Differentiable tensor renormalization group

2. Application 1

- 2.1 Square-lattice Hubbard model
- 2.2 Triangular-lattice Hubbard model
- 2.3 Magic-angle twisted bilayer graphene model

3. Application 2

- 3.1 Finite-temperature entanglement spectrum
- 3.2 disorder operator

1.1 Motivation

❑Strong Correlated systems:

- High-T superconductivity in cuprate
- Quantum spin liquid
- Magic-angle twisted bilayer graphene
- …

"Exponential wall"

"Wheat and chessboard" problem

- **Quantum Monte Carlo (QMC)**

  Negative sign problem

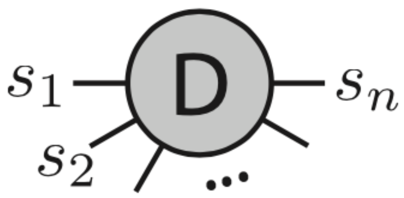
- **Tensor Network (TN)**

  capture the entanglement structure

➢ 1.1 Tensor network basis

❑ Basic terminology

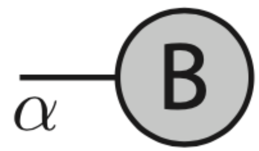
- Rank-n Tensor



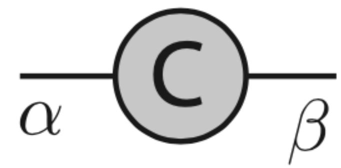
$$D_{s_1,\ s_2,\dots,\ s_n}$$

[special cases]

scalar

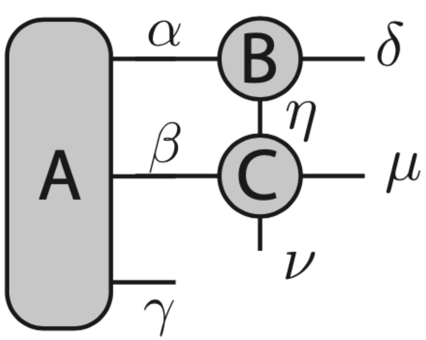


vector



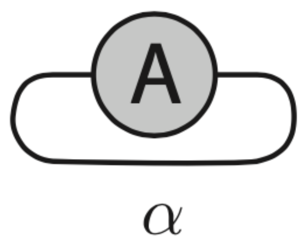
matrix

- Contraction

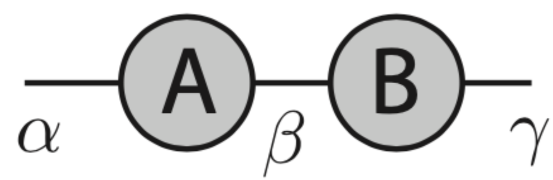


$$\sum_{\alpha,\beta,\eta} A_{\alpha,\beta,\gamma} B_{\alpha,\delta,\eta} C_{\beta,\eta,\mu,\nu}$$

[special cases]



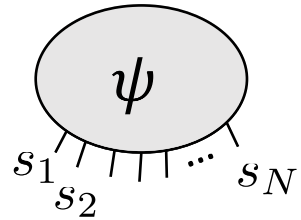
trace



matrix product

1.1 Tensor network basis

- Manybody wavefunction

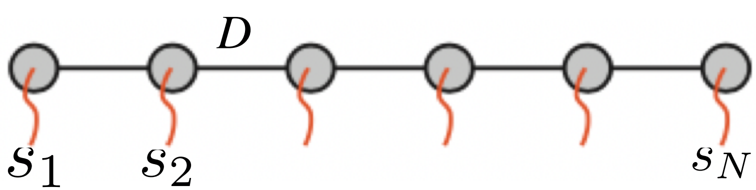


# of parameters: d^N

Exponential wall!

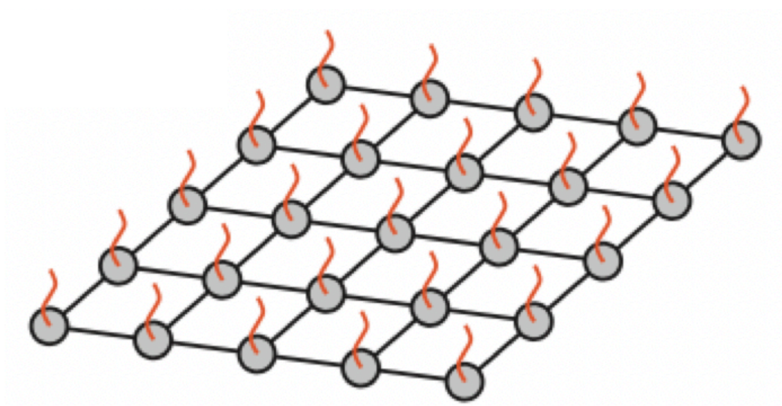
- Typical Tensor Network

✓ Matrix Product State (MPS)



$$\sim N \times (dD^2)$$

✓ Projected Entangled-Pair State (PEPS)

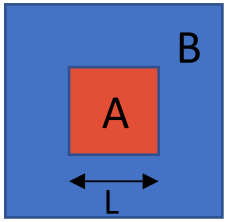


$$\sim N \times (dD^4)$$

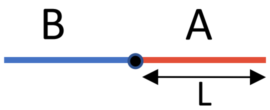
1.1 Tensor network basis

✓ Remarkable fact: For Hamiltonians with local interactions, the ground state entanglement entropy is governed by an “area law”(Eisert2010).

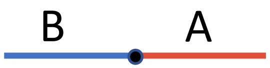
E.g., for 2D gapped systems, $S_E \sim L$



E.g., for 1D gapped systems, $S_E \sim \text{const.}$



E.g., for 1D gapless systems, $S_E \sim \ln L$



For a bond with dimension D, entanglement entropy $S_E = -\mathrm{Tr}\rho_A \ln \rho_A \leq \ln D$

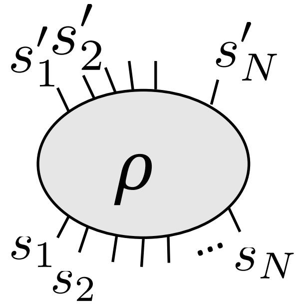
Then, for 2D gapped systems, $D \geq e^{S_E} \sim e^L$

for 1D gapped systems, $D \geq e^{S_E} \sim \text{const.}$ (independent of system size)

for 1D gapless systems, $D \geq e^{S_E} \sim L^\alpha$ (polynomial resources)

➢ 1.1 Tensor network basis

- ❑ Density operator

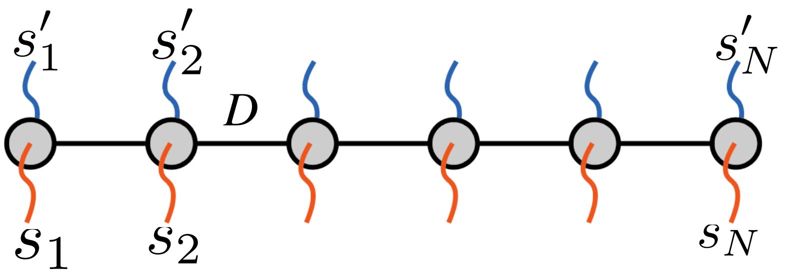


\# of parameters: d^{2N}

Exponential wall!

- ❑ Typical Tensor Network

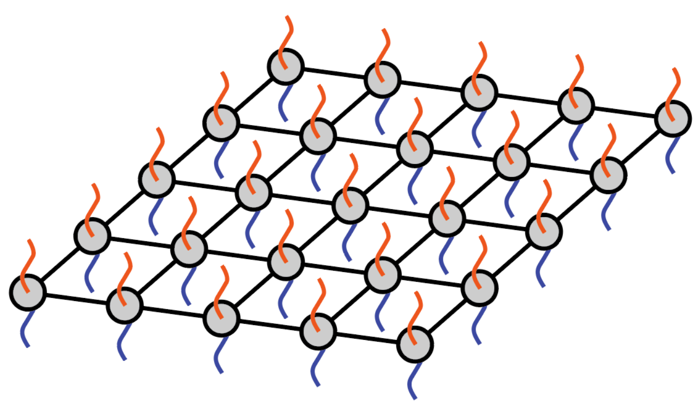
✓ Matrix Product Operator (MPO)



$\sim N \times (d^2 D^2)$

W. Li, et al. 2011; Dong, et al. 2017

✓ Projected Entangled-Pair Operator (PEPO)



$\sim N \times (d^2 D^4)$

Czarnik, et al. 2017

➢ 1.1 Path-Integral Thermal Tensor Network

Partition function for Hamiltonian with local interactions $H = \sum_i h_{i,i+1} = \sum_i S_i \cdot S_{i+1}$

$$Z = \mathrm{Tr}\ e^{-\beta H} = \mathrm{Tr}\ e^{-\beta \sum_i h_{i,i+1}}$$

$$= \sum_{\vec{\sigma}^1} \langle \vec{\sigma}^1 | e^{-\beta \sum_i h_{i,i+1}} | \vec{\sigma}^1 \rangle \qquad |\vec{\sigma}\rangle := |\sigma_1, \sigma_2, \cdots, \sigma_N\rangle$$

$$= \sum_{\vec{\sigma}^1, \vec{\sigma}^2, \cdots, \vec{\sigma}^M} \langle \vec{\sigma}^1 | e^{-\frac{\beta}{M} \sum_i h_{i,i+1}} | \vec{\sigma}^M \rangle \cdots \langle \vec{\sigma}^3 | e^{-\frac{\beta}{M} \sum_i h_{i,i+1}} | \vec{\sigma}^2 \rangle \langle \vec{\sigma}^2 | e^{-\frac{\beta}{M} \sum_i h_{i,i+1}} | \vec{\sigma}^1 \rangle$$

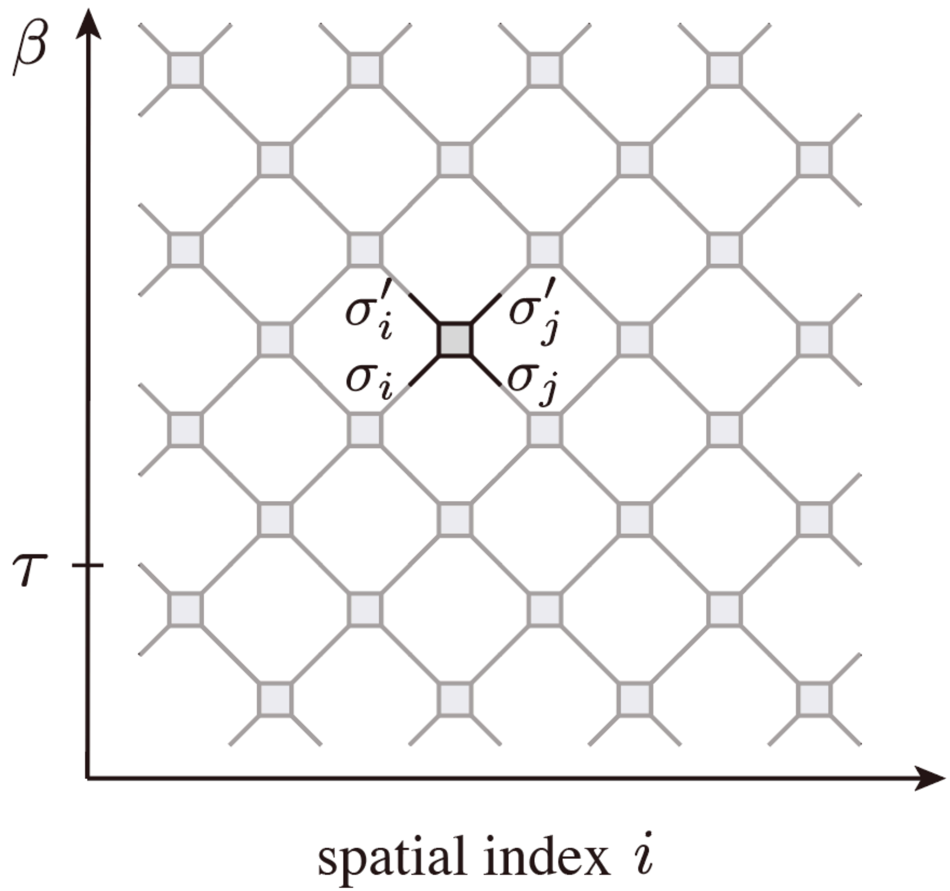
$$= \sum_{\vec{\sigma}^j} \prod_{j=1}^{M} \langle \vec{\sigma}^{j+1} | e^{-\tau \sum_i h_{i,i+1}} | \vec{\sigma}^j \rangle$$

$$= \sum_{\{\sigma_i^j\}} \prod_{i=1}^{N} \prod_{j=1}^{M} \langle \sigma_i^{j+1} \sigma_{i+1}^{j+1} | e^{-\tau h_{i,i+1}} | \sigma_i^j \sigma_{i+1}^j \rangle + O(\tau^2)$$

1.1 Path-Integral Thermal Tensor Network

$$Z = Tr(e^{-\beta H}) \xrightarrow{\text{Trotter}} Z \approx \sum_{\{\sigma_i^j\}} \prod_{i=1}^{N} \prod_{j=1}^{M} \langle \sigma_i^{j+1} \sigma_{i+1}^{j+1} | e^{-\tau h_{i,i+1}} | \sigma_i^j \sigma_{i+1}^j \rangle$$

- 1+1D Tensor Network



- Efficient contraction

Transfer Matrix RG

Wang and Xiang, 1997

Linearized Tensor RG

Li, et al. 2011

Dong, et al. 2017

Series-Expansion Thermal Tensor Network (SETTN)

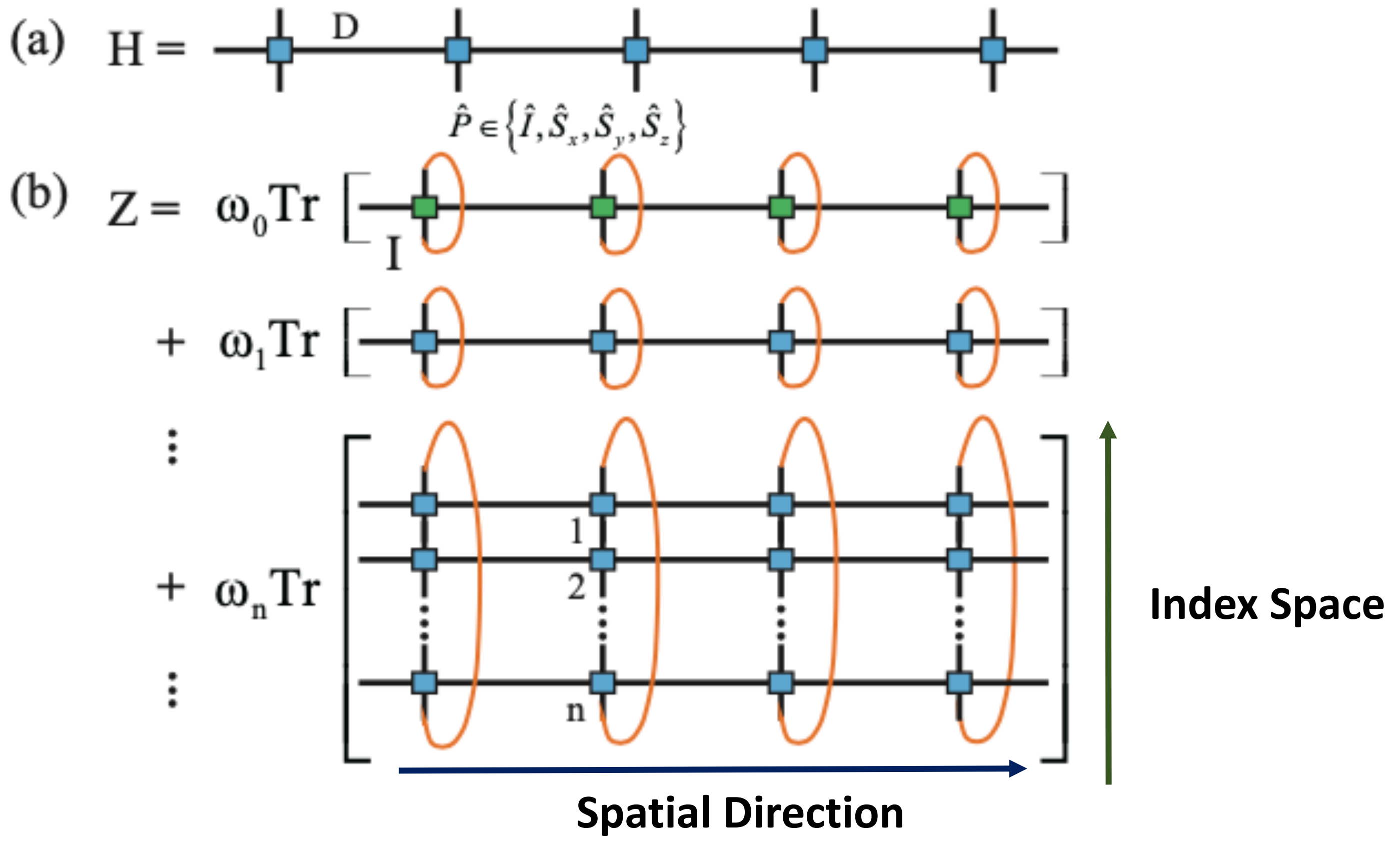
BC, Yun-Jing Liu, Ziyu Chen, Wei Li, ***PRB(R)*** 95, 161104

1.2 Basic Idea of SETTN

❑ Taylor Expansion of Partition Function:

$$Z(\beta) = \mathrm{Tr}(e^{-\beta H}) \simeq \sum_{n=0}^{N_c} \frac{(-\beta)^n}{n!} \mathrm{Tr}(H^n)$$

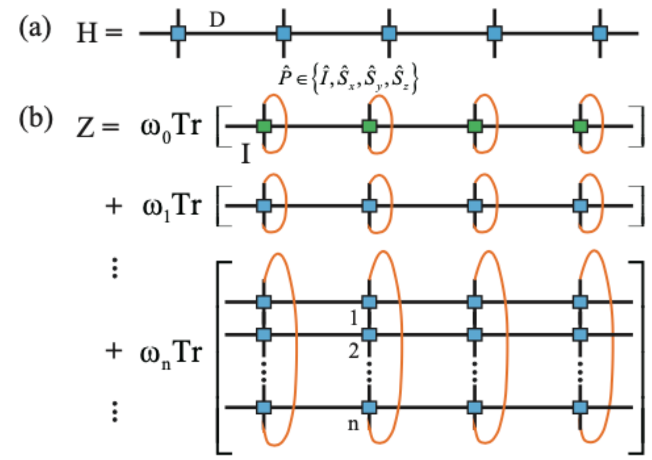
❑ Main Procedure:



➢ 1.2 Basic Idea of SETTN

❑ Taylor Expansion of Partition Function:

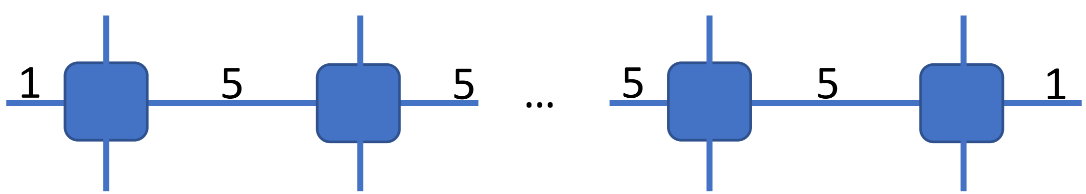
$$Z(\beta) = \mathrm{Tr}(e^{-\beta H}) \simeq \sum_{n=0}^{N_c} \frac{(-\beta)^n}{n!} \mathrm{Tr}(H^n)$$



❑ MPO of Hamiltonian: (e.g Heisenberg chain)

$$H = \sum_{i=1}^{N-1} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z)$$

$$= \begin{bmatrix} I & S^x & S^y & S^z & 0 \end{bmatrix} \underbrace{\begin{bmatrix} I & S^x & S^y & S^z & 0 \\ 0 & 0 & 0 & 0 & S^x \\ 0 & 0 & 0 & 0 & S^y \\ 0 & 0 & 0 & 0 & S^z \\ 0 & 0 & 0 & 0 & I \end{bmatrix} \cdots \begin{bmatrix} I & S^x & S^y & S^z & 0 \\ 0 & 0 & 0 & 0 & S^x \\ 0 & 0 & 0 & 0 & S^y \\ 0 & 0 & 0 & 0 & S^z \\ 0 & 0 & 0 & 0 & I \end{bmatrix}}_{\text{N-2}} \begin{bmatrix} 0 \\ S^x \\ S^y \\ S^z \\ I \end{bmatrix}$$

$=$ 

1.2 Basic Idea of SETTN

E.g. N= 4 Heisenberg chain

$$\begin{bmatrix} I & S^x & S^y & S^z & 0 \end{bmatrix} \begin{bmatrix} I & S^x & S^y & S^z & 0 \\ 0 & 0 & 0 & 0 & S^x \\ 0 & 0 & 0 & 0 & S^y \\ 0 & 0 & 0 & 0 & S^z \\ 0 & 0 & 0 & 0 & I \end{bmatrix} \boxed{\begin{bmatrix} I & S^x & S^y & S^z & 0 \\ 0 & 0 & 0 & 0 & S^x \\ 0 & 0 & 0 & 0 & S^y \\ 0 & 0 & 0 & 0 & S^z \\ 0 & 0 & 0 & 0 & I \end{bmatrix} \begin{bmatrix} 0 \\ S^x \\ S^y \\ S^z \\ I \end{bmatrix}}$$

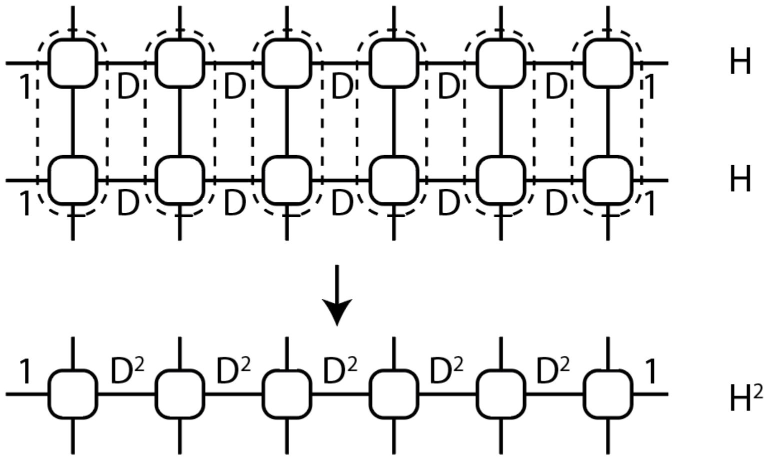
$$= \begin{bmatrix} I & S^x & S^y & S^z & 0 \end{bmatrix} \boxed{\begin{bmatrix} I & S^x & S^y & S^z & 0 \\ 0 & 0 & 0 & 0 & S^x \\ 0 & 0 & 0 & 0 & S^y \\ 0 & 0 & 0 & 0 & S^z \\ 0 & 0 & 0 & 0 & I \end{bmatrix} \begin{bmatrix} S^x S^x + S^y S^y + S^z S^z \\ S^x I \\ S^y I \\ S^z I \\ II \end{bmatrix}}$$

$$= \boxed{\begin{bmatrix} I & S^x & S^y & S^z & 0 \end{bmatrix} \begin{bmatrix} IS^x S^x + IS^y S^y + IS^z S^z + S^x S^x I + S^y S^y I + S^z S^z I \\ S^x II \\ S^y II \\ S^z II \\ II \end{bmatrix}}$$

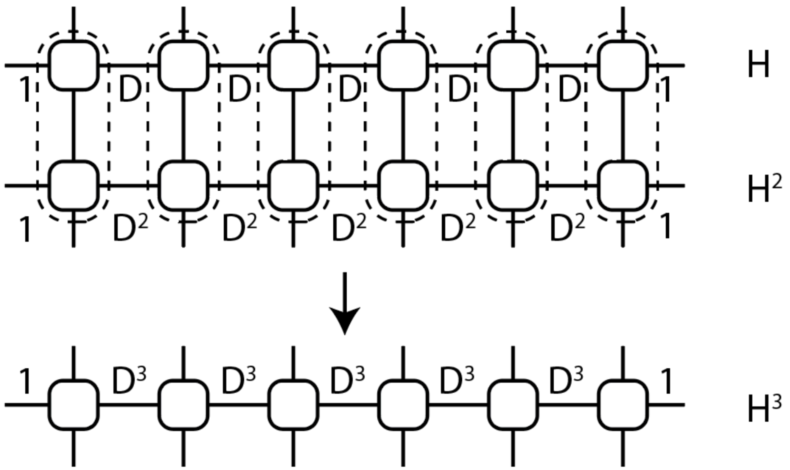
$$= \begin{array}{l} \quad IIS^x S^x + IIS^y S^y + IIS^z S^z \\ + IS^x S^x I + IS^y S^y I + IS^z S^z I \\ + S^x S^x II + S^y S^y II + S^z S^z II \end{array}$$

➢ 1.2 Efficient contraction of H^n

Construction of H^2



Construction of H^3

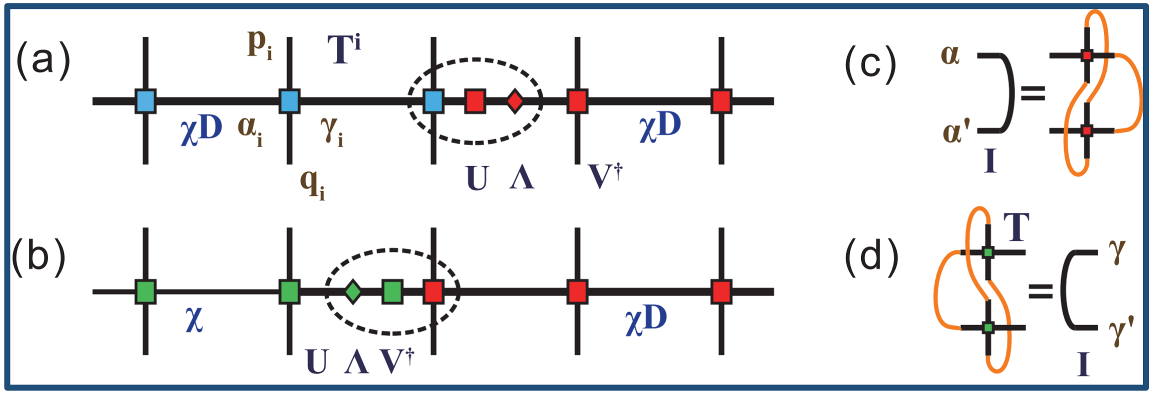


Similarly, H^n will have bond dimension D^n

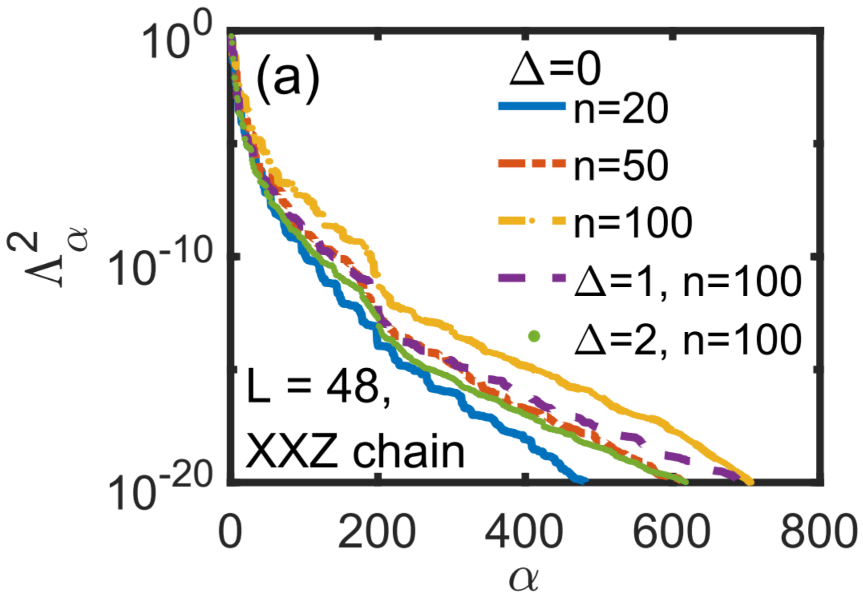
Bond dimension scales exponentially and will quickly become unaffordable.

1.2 Efficient contraction of H^n

❑ Canonical form:

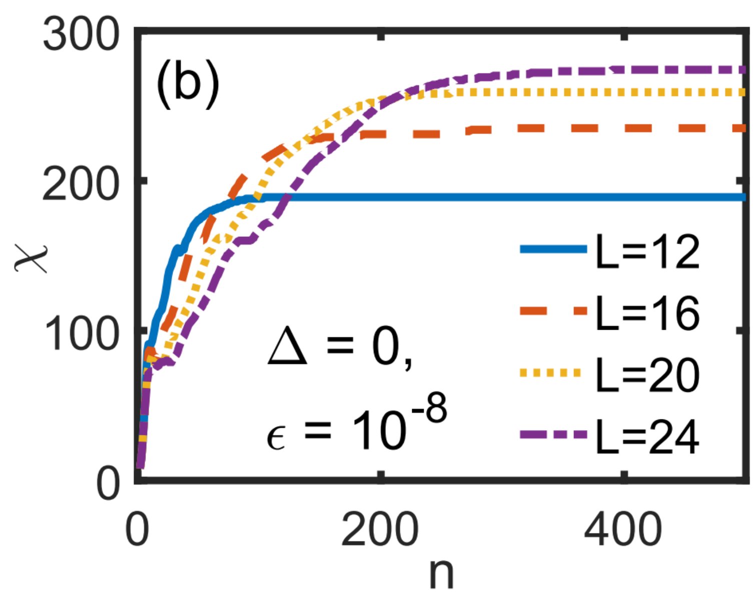


❑ "Entanglement" spectrum



Decay rapidly

❑ Required bond dimension



saturate with n

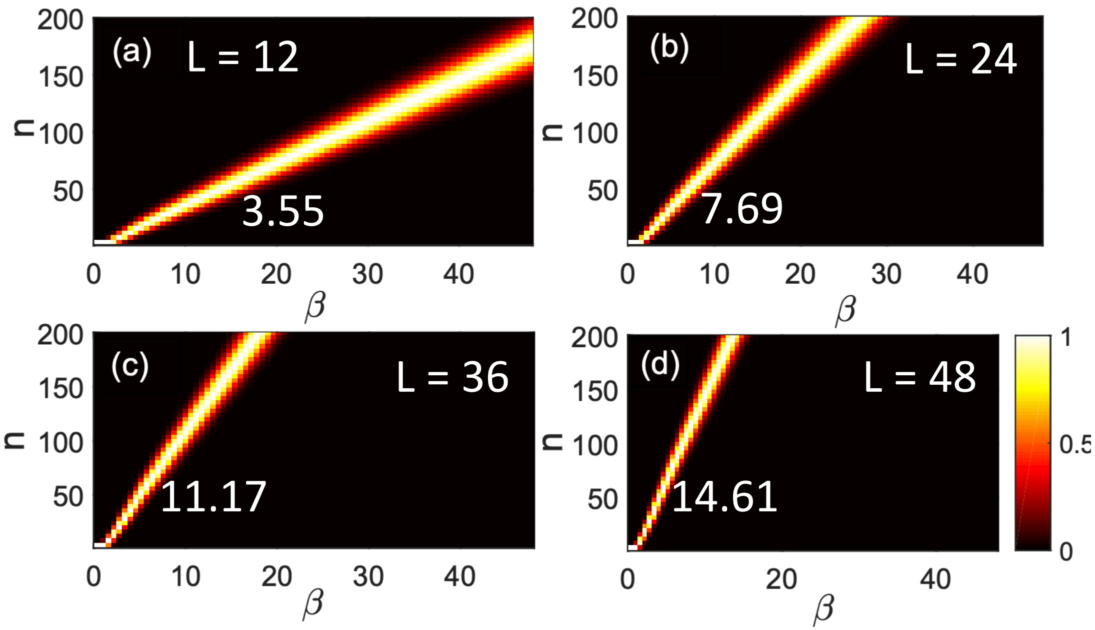
➢ 1.2 Expansion cutoff

$$Z(\beta) = \mathrm{Tr}(e^{-\beta H}) \simeq \sum_{n=0}^{N_c} \frac{(-\beta)^n}{n!} \mathrm{Tr}(H^n)$$

For large n, we have $\mathrm{Tr}(H^n) \propto (E_{\mathrm{ln}})^n = (e_{\mathrm{ln}} L)^n$

Partition function is sum of $\kappa(n) = \frac{(-\beta L e_{\mathrm{ln}})^n}{n!} = \frac{(\beta L |e_{\mathrm{g}}|)^n}{n!}$

which is most prominent around $n = \beta L |e_{\mathrm{g}}|$



E.g., XY chain: $e_{\mathrm{g}} = -1/\pi$

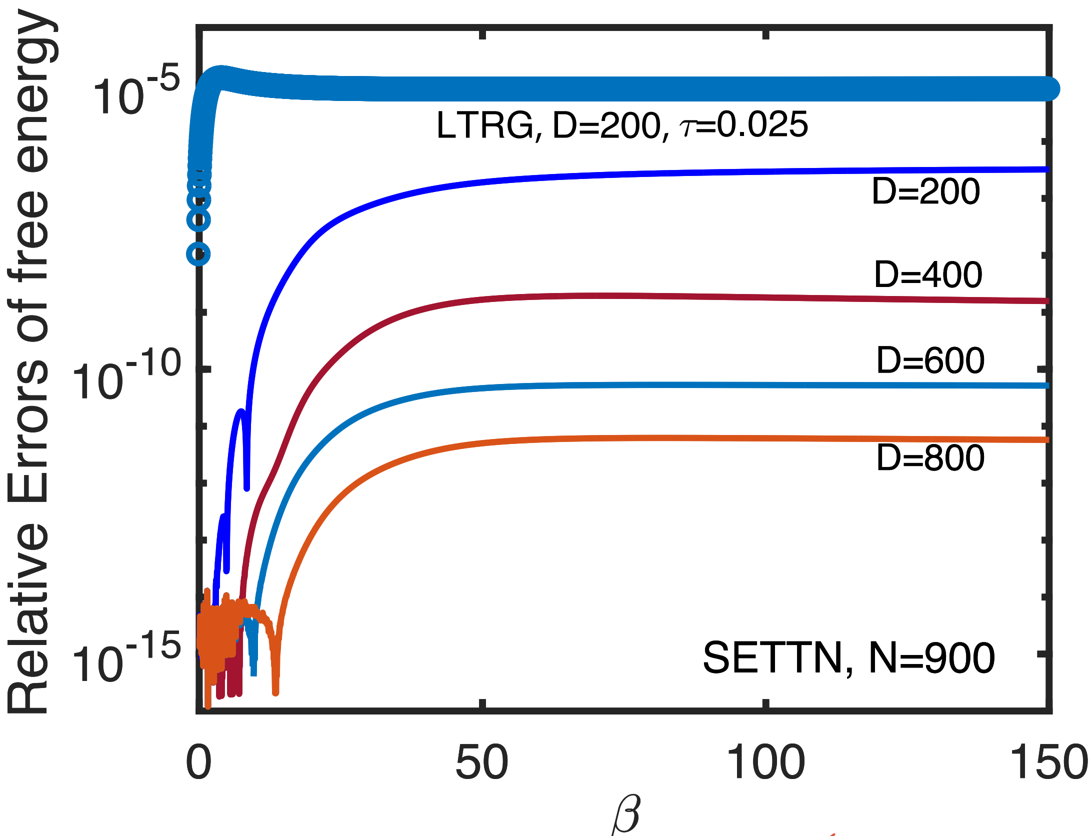
Then partition function is dominant by weight around

$$n = \beta L/\pi$$

➢ 1.2 Performance of SETTN

- L=14 XY chain

$$H = J \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y)$$



✓ Extremely accurate at high-T

✓ SETTN outperform Trotter

1.2 Summary of SETTN

- Trotter-error free ✅
- Continuous Time ✅
- Long-Range Couplings ✅

The problem is still very challenging for 2D system at Low *T*.

10-min break; coming back at 10:50 am

Exponential Tensor Renormalization Group (XTRG)

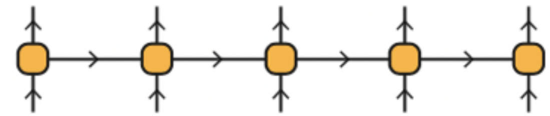
[1] **BC**, L. Chen, Z. Chen, W. Li, A. Weichselbaum. ***PRX*** *8, 031082*

[2] L. Chen, D.-W. Qu, H. Li, **BC**, S.-S. Gong, J. von Delft, A. Weichselbaum, W. Li. ***PRB(R)*** *99, 140404*

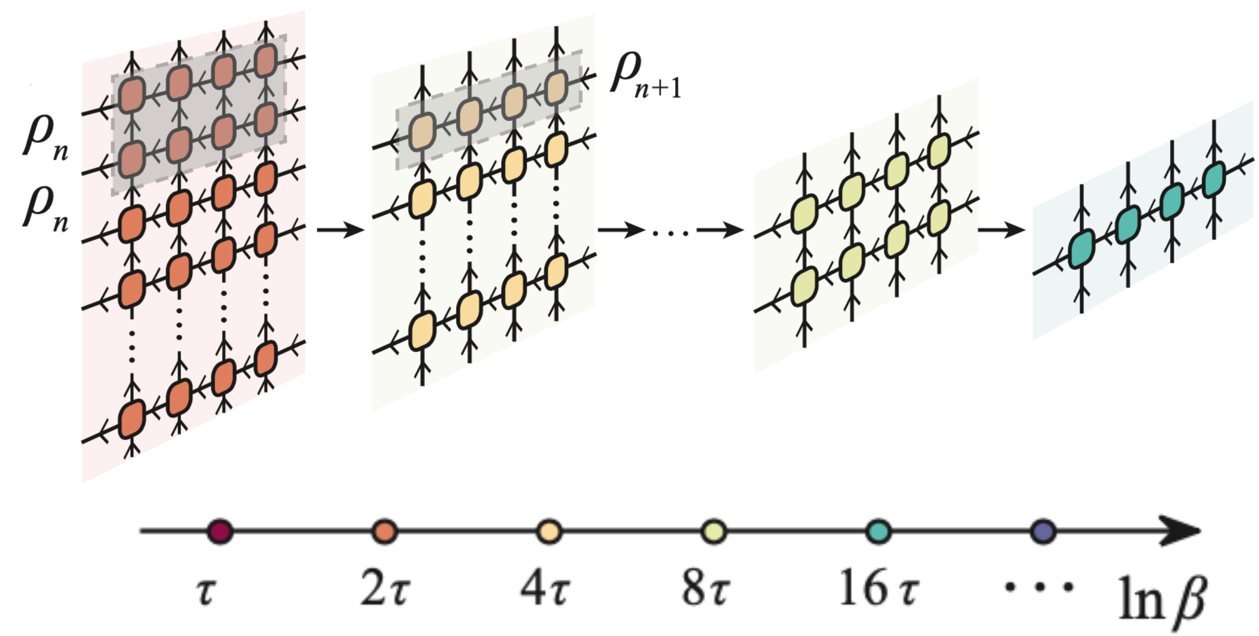
[3] H. Li, **BC**, Z. Chen, J. von Delft, A. Weichselbaum, W. Li. ***PRB(R)*** *100, 045110*

➢ 1.3 Basic Idea of XTRG

1) SETTN initialization at high Temperature

$\rho_0 \equiv \rho(\tau)$ 

2) Exponential evolution $\rho_n \cdot \rho_n \rightarrow \rho_{n+1}$

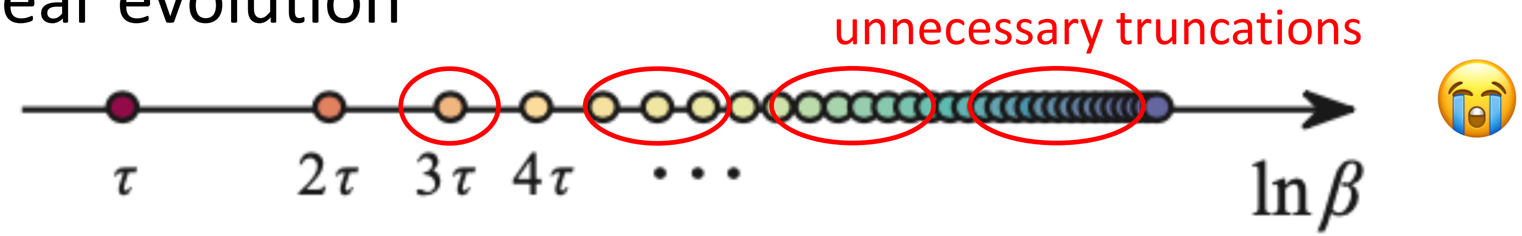


1.3 Reduce numbers of truncation steps

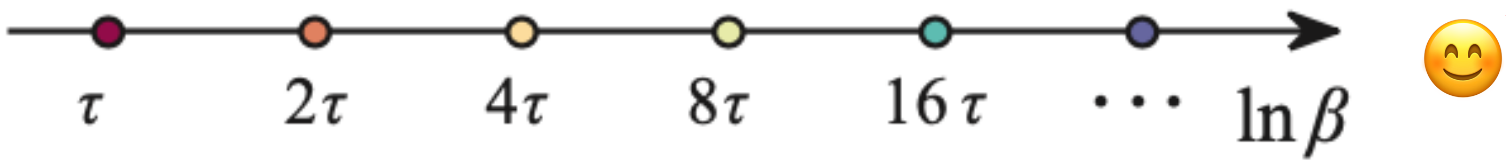
- logarithmic scaling of entanglement entropy

$$S_E \sim (c/3)\ln\beta$$

- Linear evolution



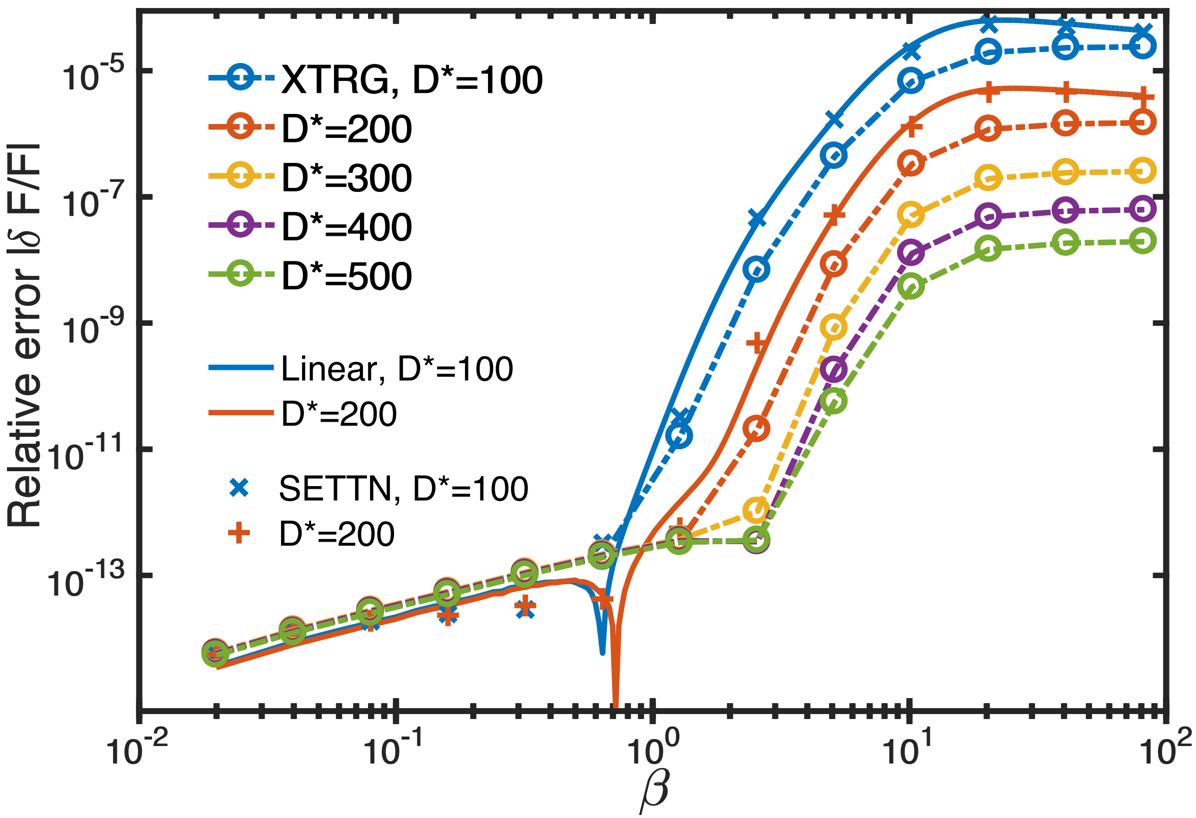
- Exponential evolution



➢ 1.3 Performance of XTRG

❑ *L*=18 Heisenberg chain

$$H = J\sum_{i,j}(S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z)$$

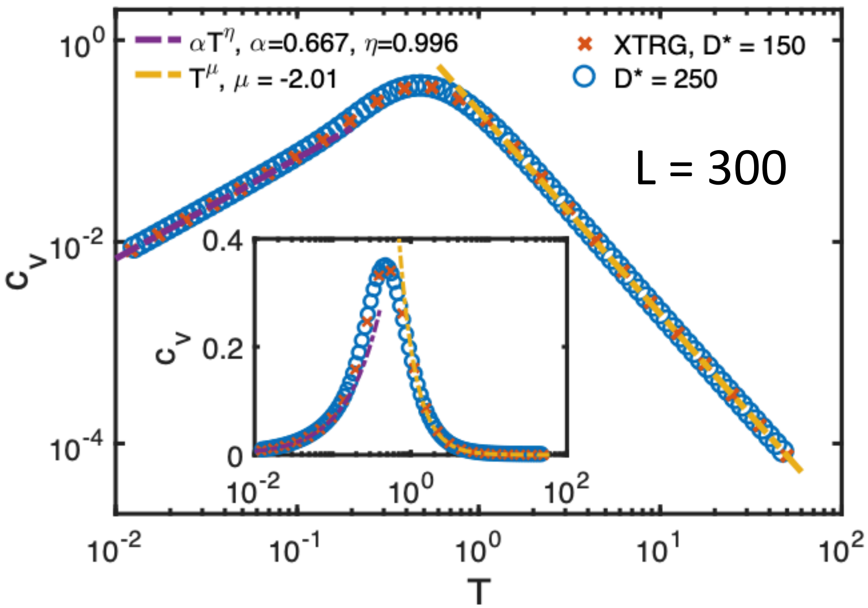


1 order of magnitude better than Linear scheme and also SETTN

➢ 1.3 More data of XTRG

✓ Long Heisenberg chain

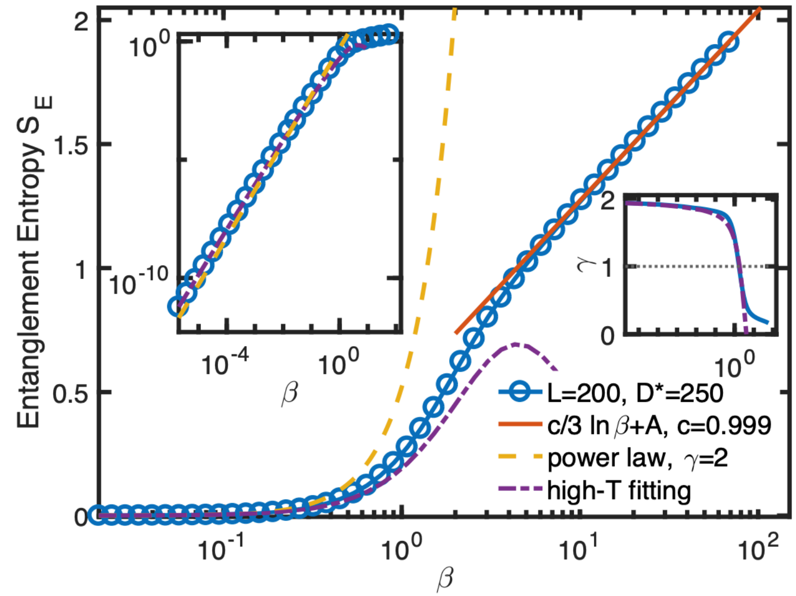
Extraction of central charge



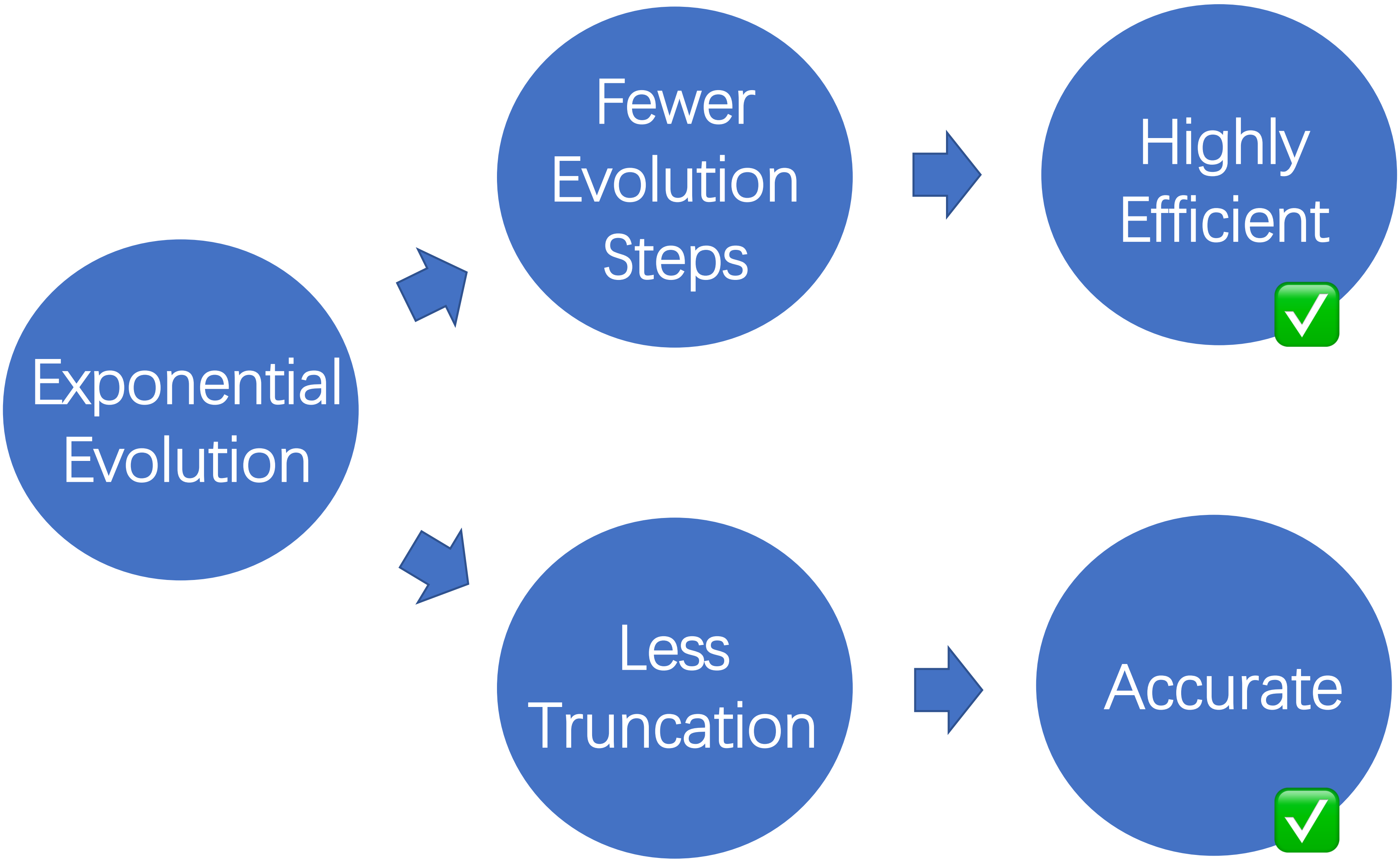
$$c_V = \alpha T^{\eta} \qquad \alpha = \frac{\pi c}{3v}$$

logarithmic scaling of entanglement entropy

$$S_E \sim (c/3) \ln \beta$$



1.3 Summary of XTRG

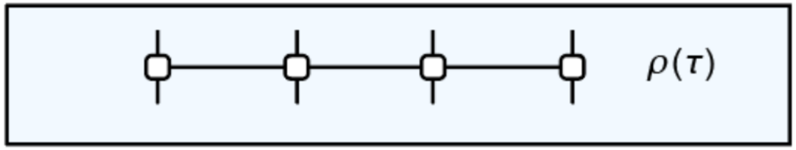


Differentiable Tensor Renormalization Group (∂TRG)

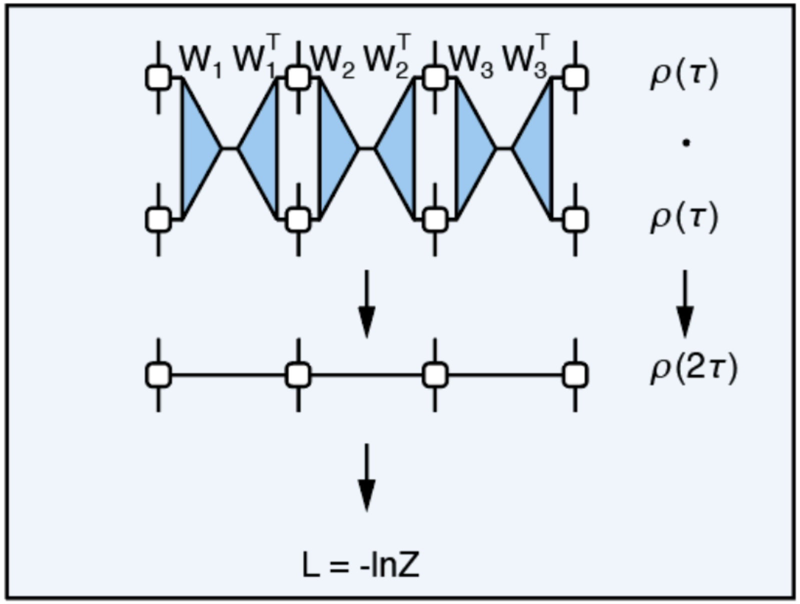
BC, Y. Gao, Y.-B. Guo, Y. Liu, H.-H. Zhao, H.-J. Liao, L. Wang, T. Xiang, W. Li, Z. Y. Xie. ***PRB(R)*** *101, 220409*

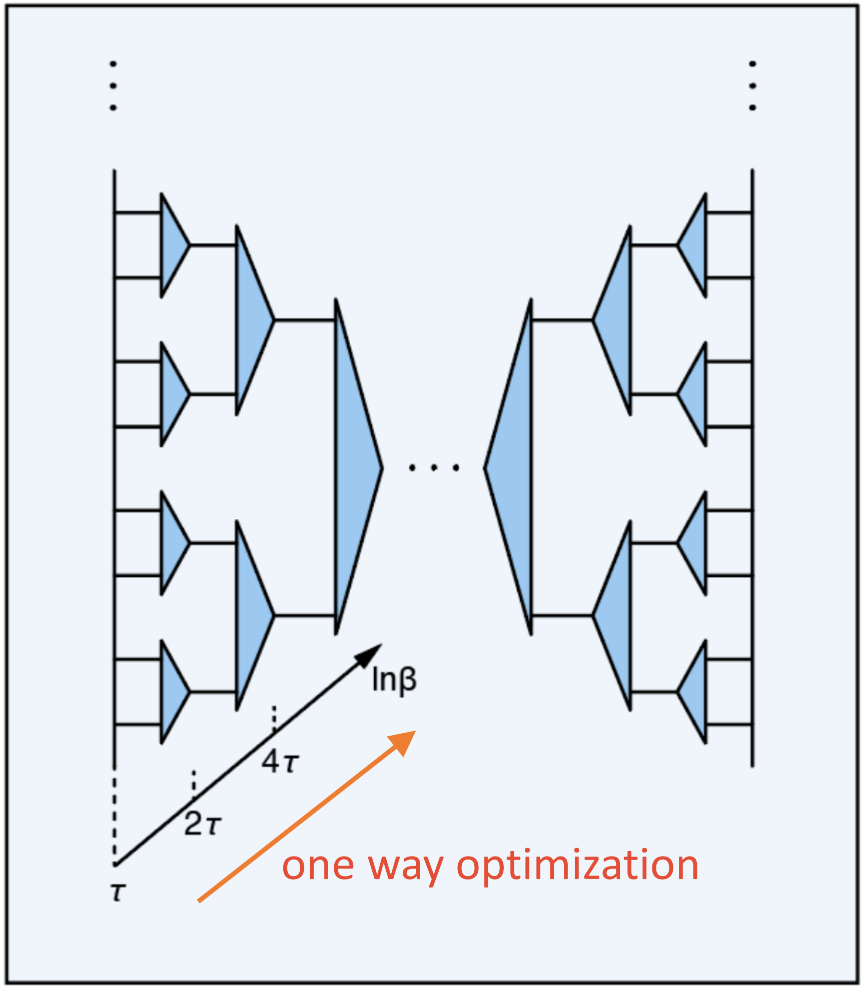
1.4 Basic Idea of ∂TRG

1) SETTN initialization at high temperature



2) Forward TRG





➢ 1.4 Basic Idea of ∂TRG

3) Backward optimization

By using Automatic Differentiation,
We can calculate environment

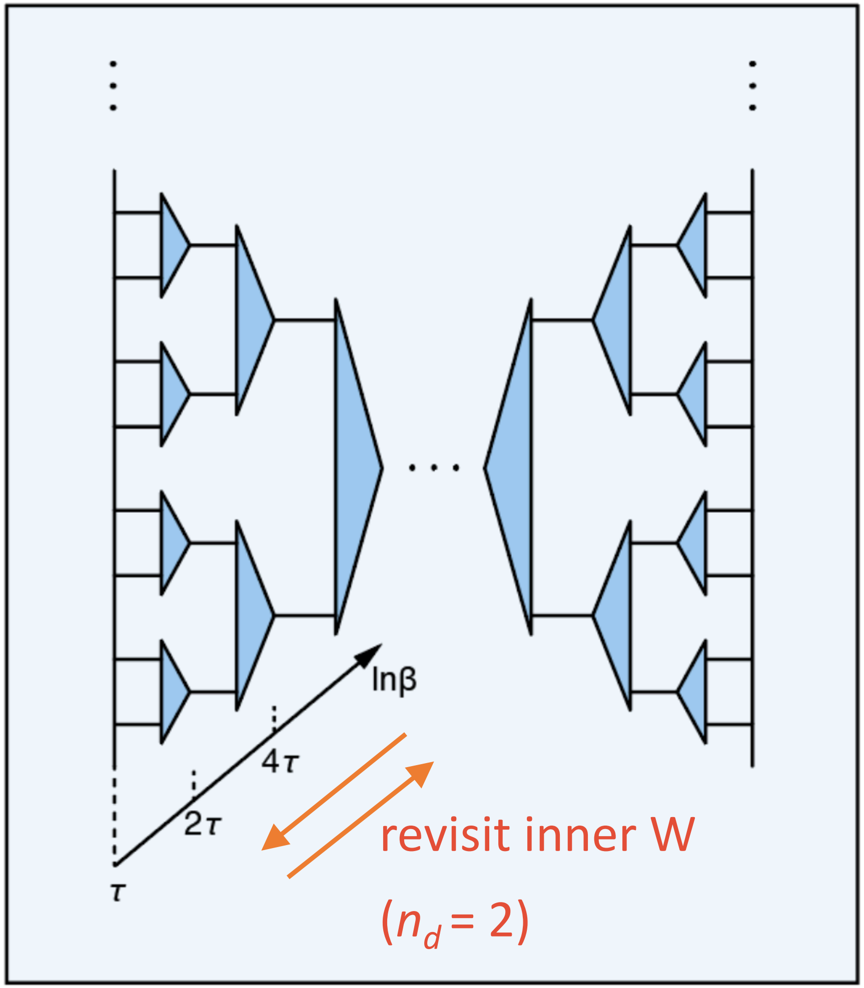
$$\frac{\partial \mathcal{L}}{\partial W_i}$$

and update W_i

4) Repeat forward and backward for all

$$W_i$$

within optimization depth n_d



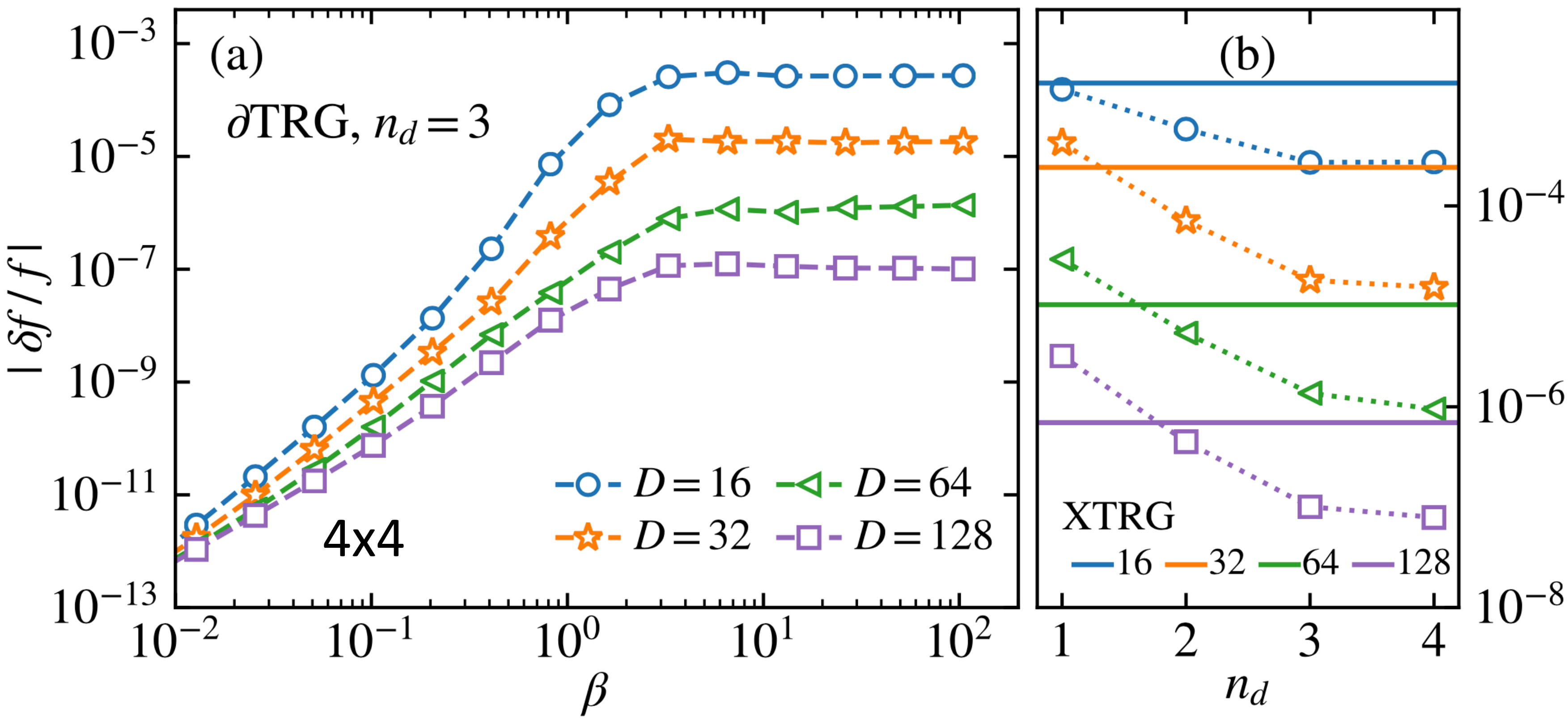
Deep optimization in thermal tensor network

1.4 2D transverse-field Ising model

$$H = J \sum_{i,j} S_i^z S_j^z + h \sum_i S_i^x$$

with J=-1, h = h_c = 1.522

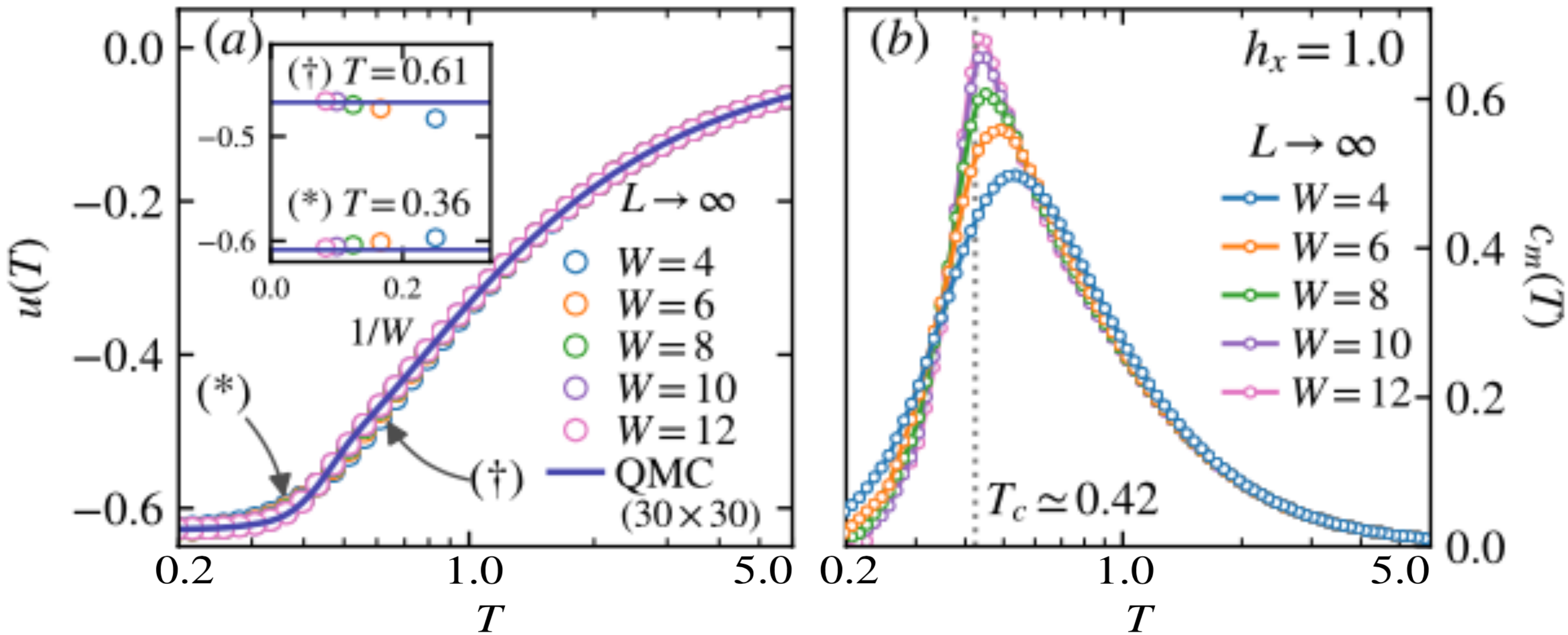
- relative error of free energy



➢ 1.4 transverse-field Ising model

$$H = J\sum_{i,j} S_i^z S_j^z + h\sum_i S_i^x$$ with *J*=-1, *h* = 1 T_c = 0.42

- internal energy
- specific heat



accurate estimate of transition temperature ~1%

Summary of ∂TRG

Deep optimization in TTN $\Rightarrow$ Higher accuracy