Tensor Product States for 2D Spin Models

The 4^{th} Workshop on QST

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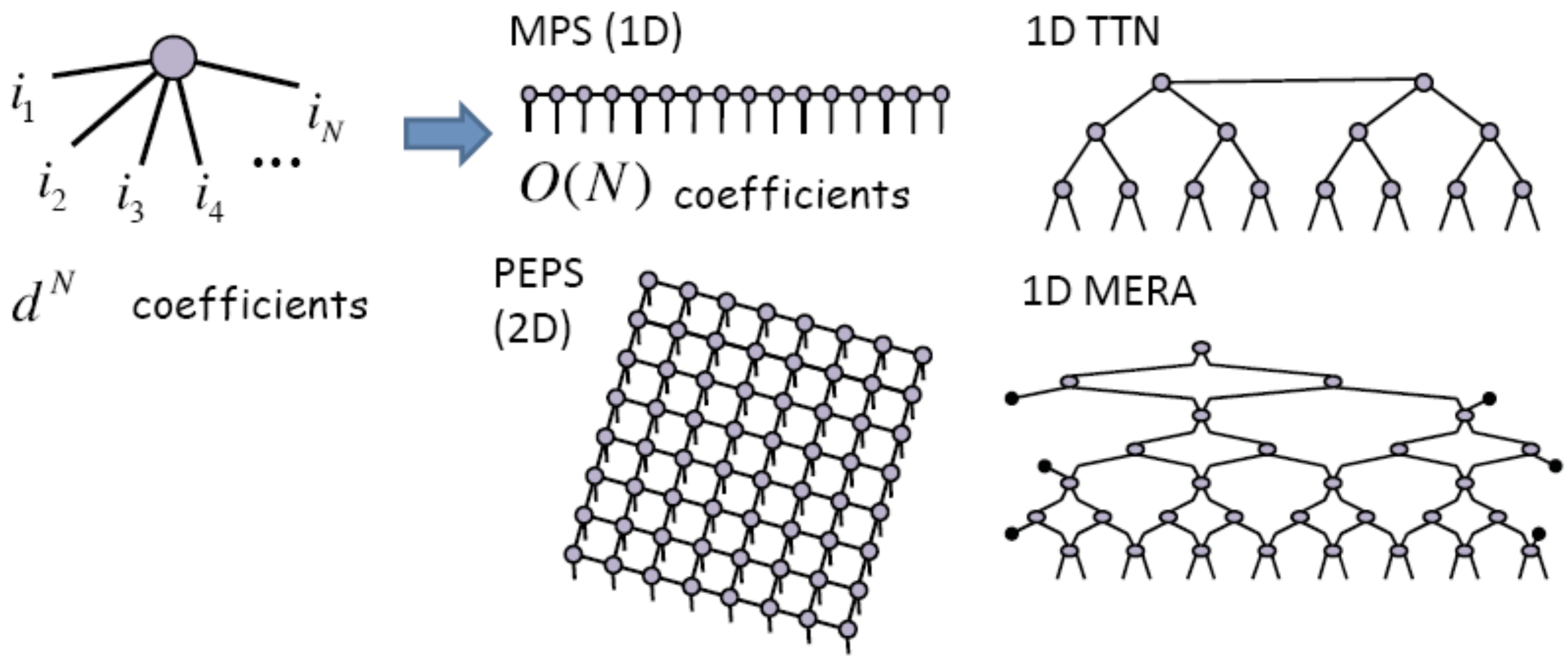
Use finite to capture the infinite

Tensor Network State

Tensor network state representation of a many-body state

$$|\psi\rangle = \sum_{i_1\cdots i_N} \psi_{i_1\cdots i_N} |i_1\cdots i_N\rangle \quad \Longrightarrow \quad |\psi\rangle = \sum_{i_1\cdots i_N} \mathbf{TN}(i_1\cdots i_N)|i_1\cdots i_N\rangle$$

$$|\Psi\rangle = \sum_{s_1 s_2\cdots s_N} \mathrm{Tr}\left[\mathrm{T}(s_1)\cdots \mathrm{T}(s_N)\right]|s_1 s_2\cdots s_N\rangle$$



Schmidt Decomposition

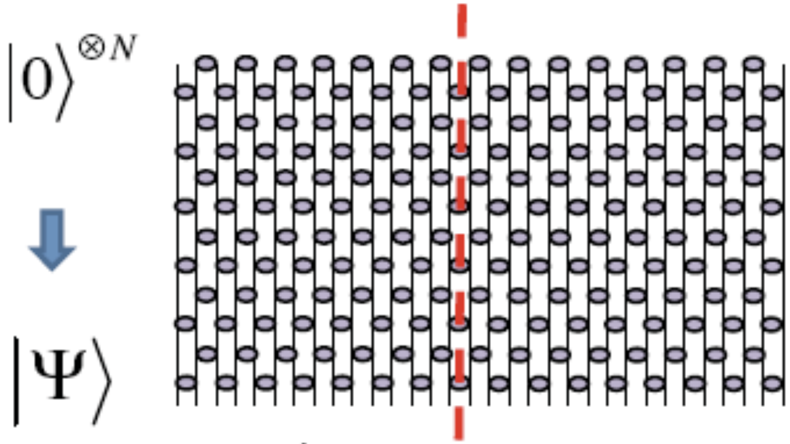
- Let H_1 and H_2 be Hilbert space of dim *n,m*
- Consider a state in the product space |ψ>

$$\left|\Psi\right\rangle = \sum_{i=1}^{\chi=\min(n,m)} \lambda_i \left|\alpha_i\right\rangle \left|\beta_i\right\rangle \approx \sum_{i=1}^{D<\chi} \lambda_i \left|\alpha_i\right\rangle \left|\beta_i\right\rangle$$

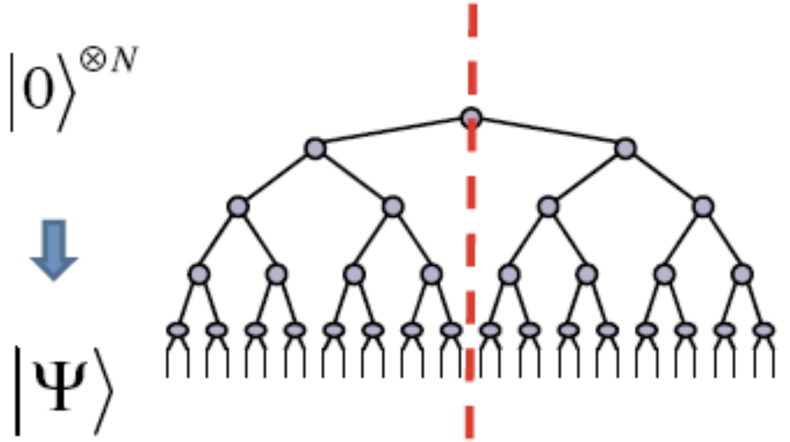
- Von Neumann entropy (Entanglement)

$$S\left(\rho_a\right) = S\left(\rho_b\right) = -\sum_{i=1}^{\chi} \lambda_i \log \lambda_i$$

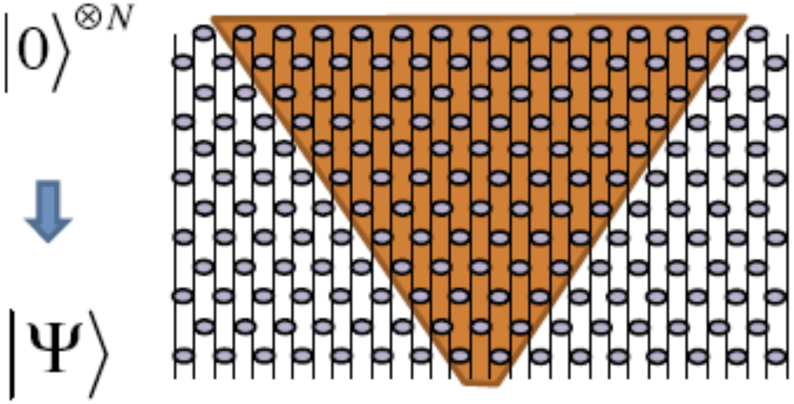
Entanglement v.s. Casual Cone



entanglement entropy $S_{N/2} \sim N/2$

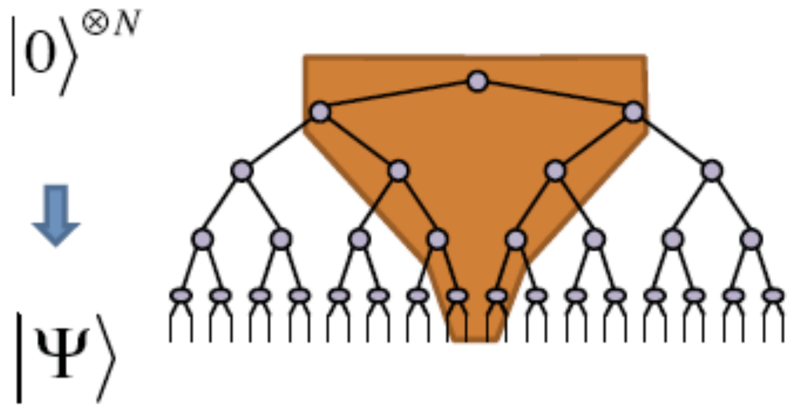


entanglement entropy $S_{N/2} \sim O(1)$



width ~ $O(N)$

cost ~ $\exp(N)$

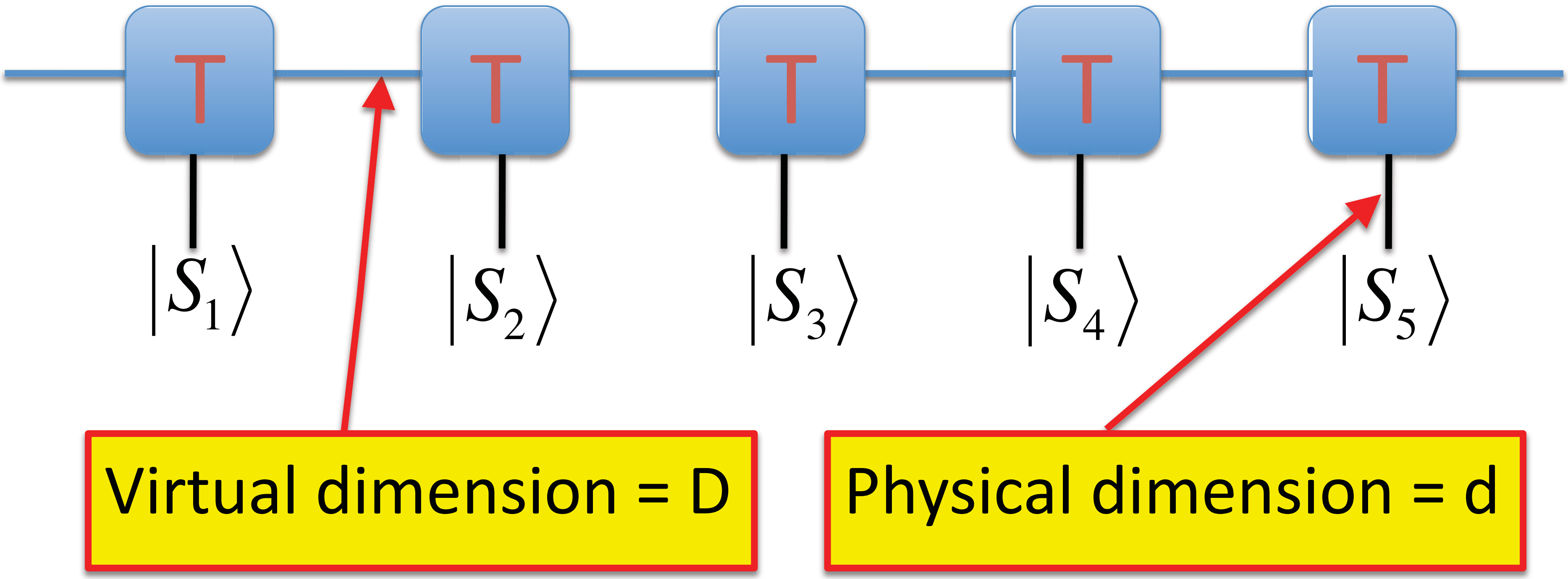


width ~ $O(1)$

cost ~ $O(\log N)$

1D Matrix Product State (1D-MPS)

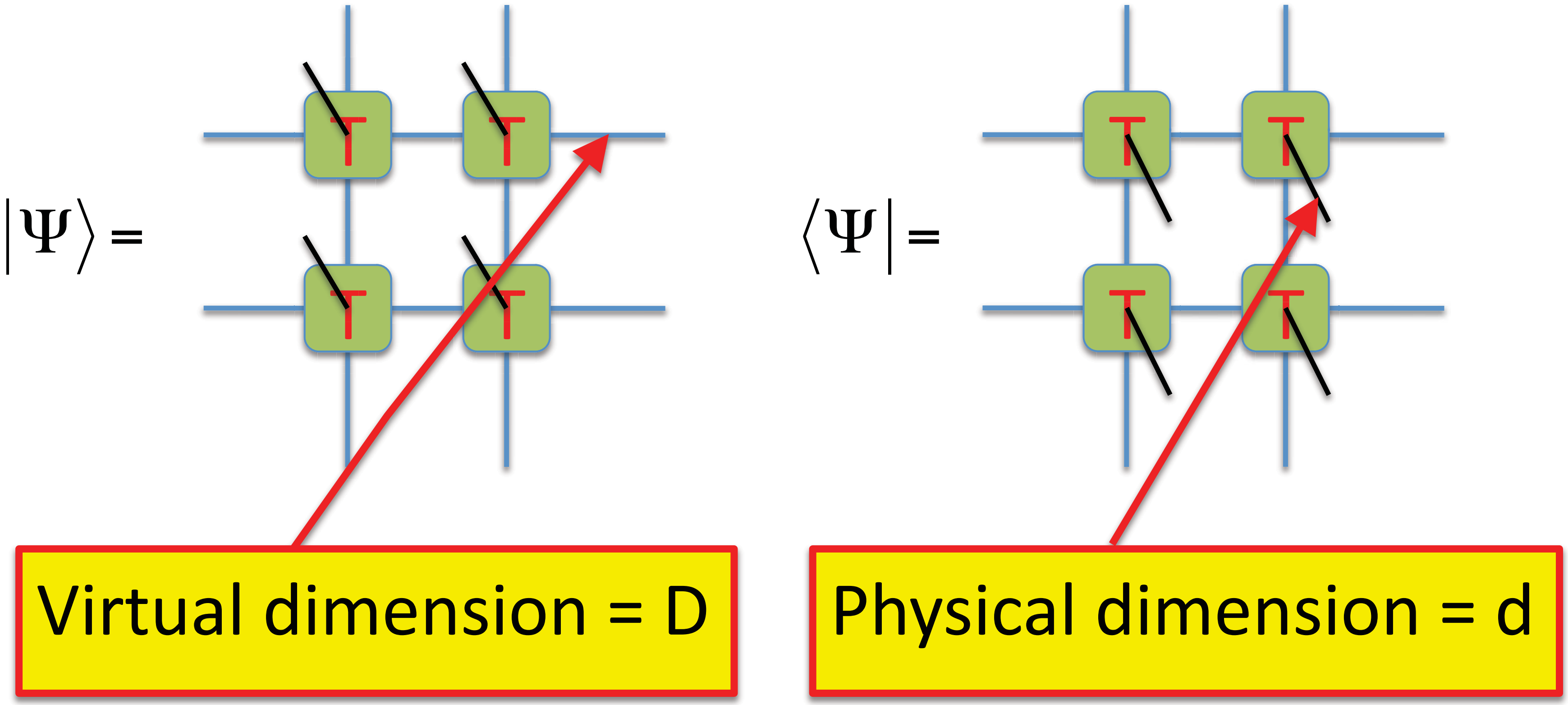
$$|\Psi\rangle = \sum_{s_1 s_2 \cdots s_N} \mathrm{Tr}[\mathrm{T}(s_1)][\mathrm{T}(s_2)]\cdots[\mathrm{T}(s_N)]|s_1 s_2 \cdots s_N\rangle$$



2D Tensor-Product State (TPS)

Represent wave-function by the tensor network of *T* tensors

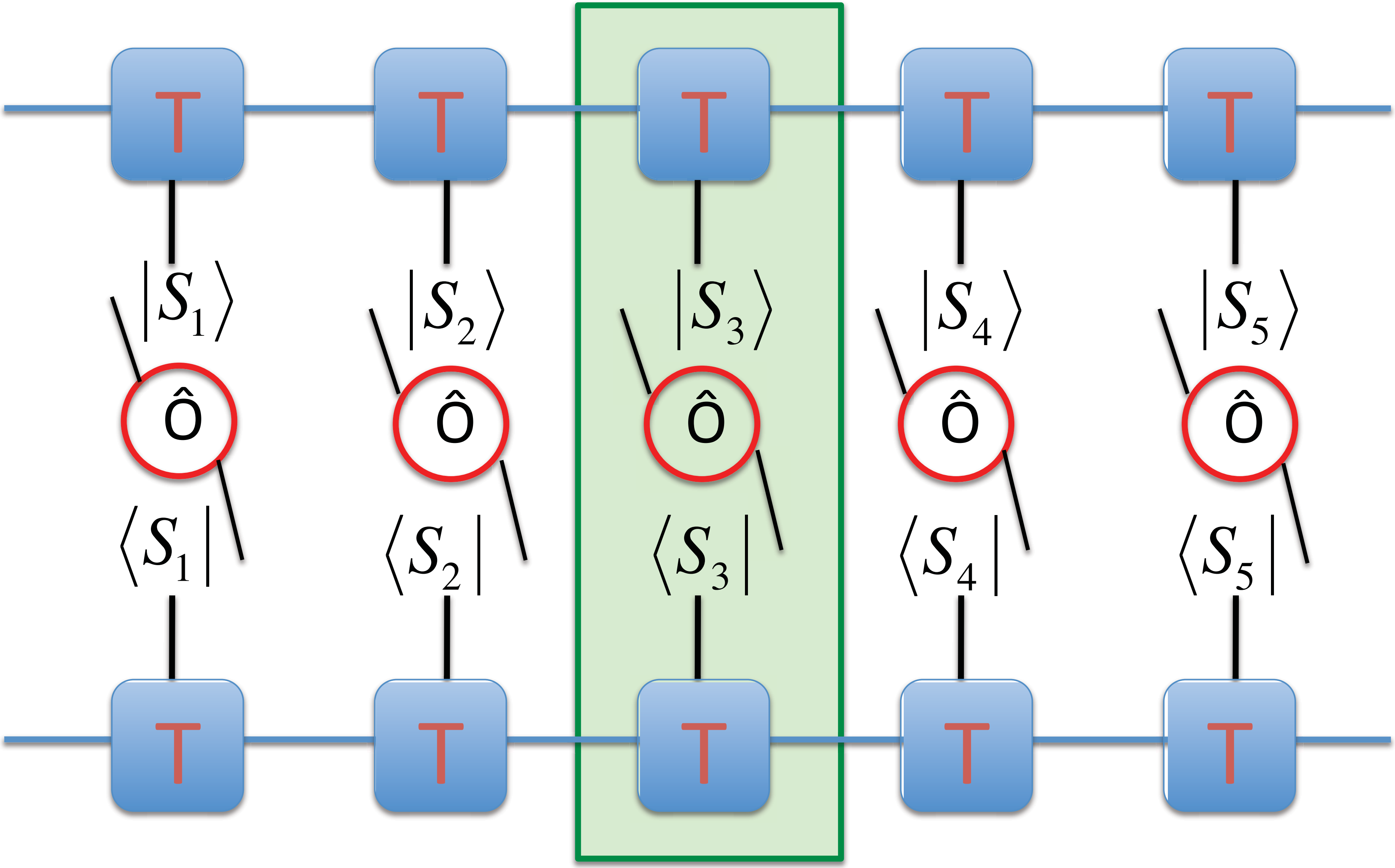
$$|\Psi\rangle = \sum_{S_i S_j \cdots} \mathrm{Tr}\left[T^{S_i}_{u_i l_i d_i r_i} T^{S_j}_{u_j l_j d_j r_j} \cdots\right] |S_i S_j \cdots\rangle$$



Remarks

- Tensor network state as an ansatz
  - The quality of the ansatz depends on the virtual dimension D and the entanglement of the true ground state.
- Optimization of the ansatz
  - Direct optimization
  - Imaginary time evolution
- Expectation values
  - Energy, order parameters, and correlations

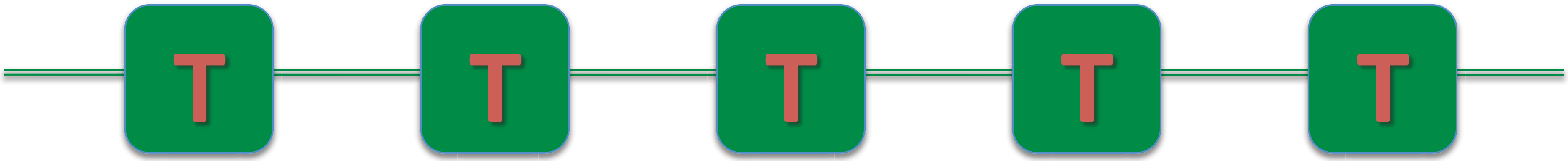
Expectation Value of 1D-MPS



Contraction of Double Tensor

$$\left[\mathbf{T}_N\right]_{(\tilde{\alpha}\alpha),(\tilde{\beta}\beta)} \equiv \sum_{\tilde{S}S} T^{*\tilde{S}}_{\tilde{\alpha}\tilde{\beta}} \langle \tilde{s} | O | s \rangle T^{S}_{\alpha\beta}$$

$$\langle \Psi | O_1 O_2 \cdots O_N | \Psi \rangle = \mathrm{Tr}\left[\mathbf{T}_1 \mathbf{T}_2 \cdots \mathbf{T}_N\right]$$

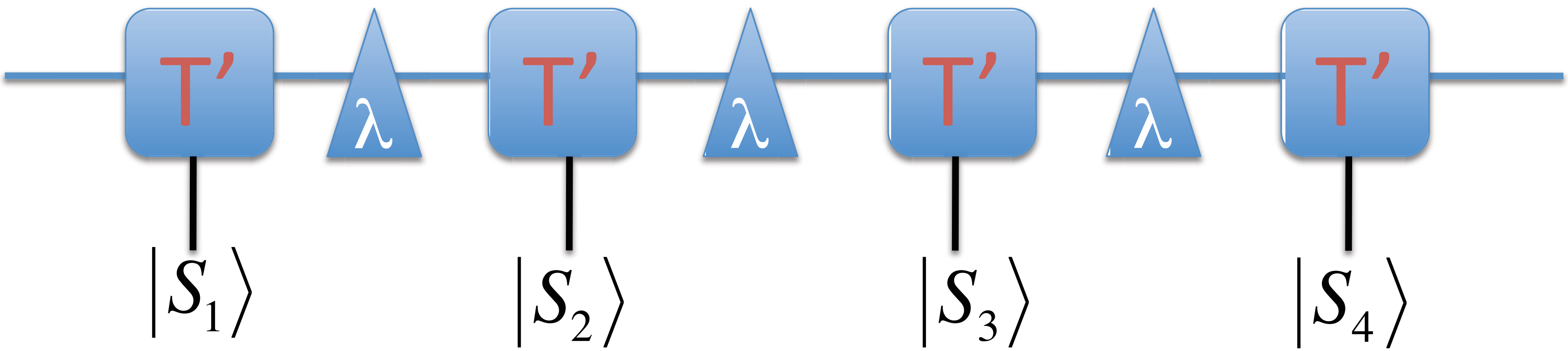


Expectation value = Contraction of double tensor **T**

Alternative Form of 1D-MPS

Introduce diagonal matrix (vector) λ

$$T = \sqrt{\lambda_L} T' \sqrt{\lambda_R}$$



Easier to simulate evolution using alternative form

Imaginary Time Evolution

- Use imaginary time to reach the ground state
- Assume initial state has some overlap with GS

$$\left|\Psi(0)\right\rangle = A_0\left|G\right\rangle + A_1\left|E_1\right\rangle + A_2\left|E_2\right\rangle + \cdots$$

- Imaginary time evolution single out the GS

$$\left|\Psi(t)\right\rangle = A_0\left|G\right\rangle + A_1 e^{-E_1}\left|E_1\right\rangle + A_2 e^{-E_2}\left|E_2\right\rangle + \cdots$$

- Obtain ground state by

$$\left|G\right\rangle = \lim_{N\to\infty} \frac{\left(e^{-\tau H}\right)^N \left|\Psi(0)\right\rangle}{\left\|\left(e^{-\tau H}\right)^N \left|\Psi(0)\right\rangle\right\|}$$

Suzuki-Trotter Formula

- Consider Hamiltonian with NN terms

$$H = \sum_{\langle ij \rangle} H_{ij} = H_{12} + H_{34} + \cdots + H_{23} + H_{45} + \cdots = H_{even} + H_{odd}$$

- Suzuki-Trotter Formula $e^{\tau(A+B)} \approx e^{\tau A} e^{\tau B} + O\left(\tau^2\right)$

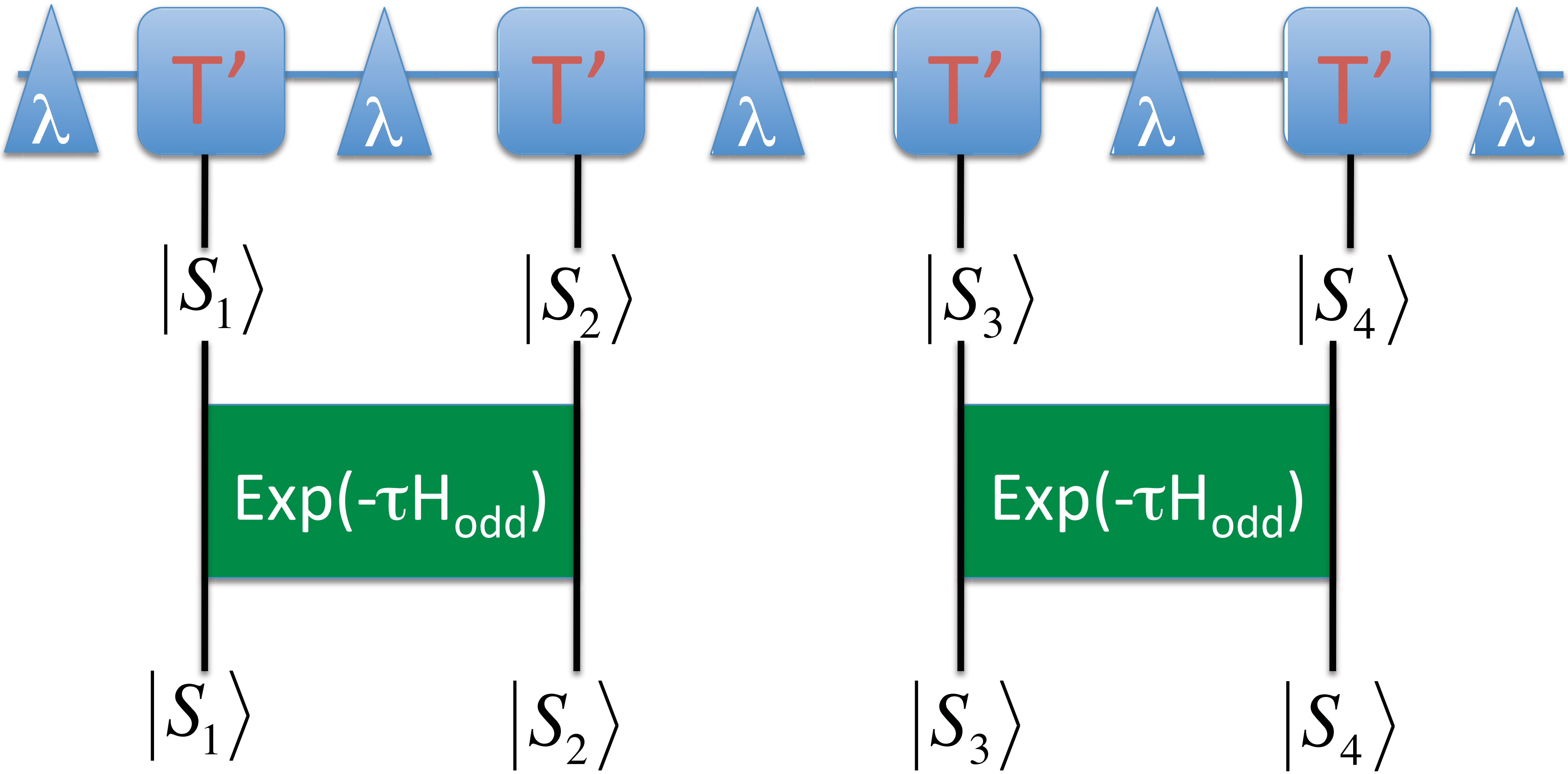
- Applied to imaginary time evolution

$$e^{\tau H} \approx e^{\tau H_{even}} e^{\tau H_{odd}}$$

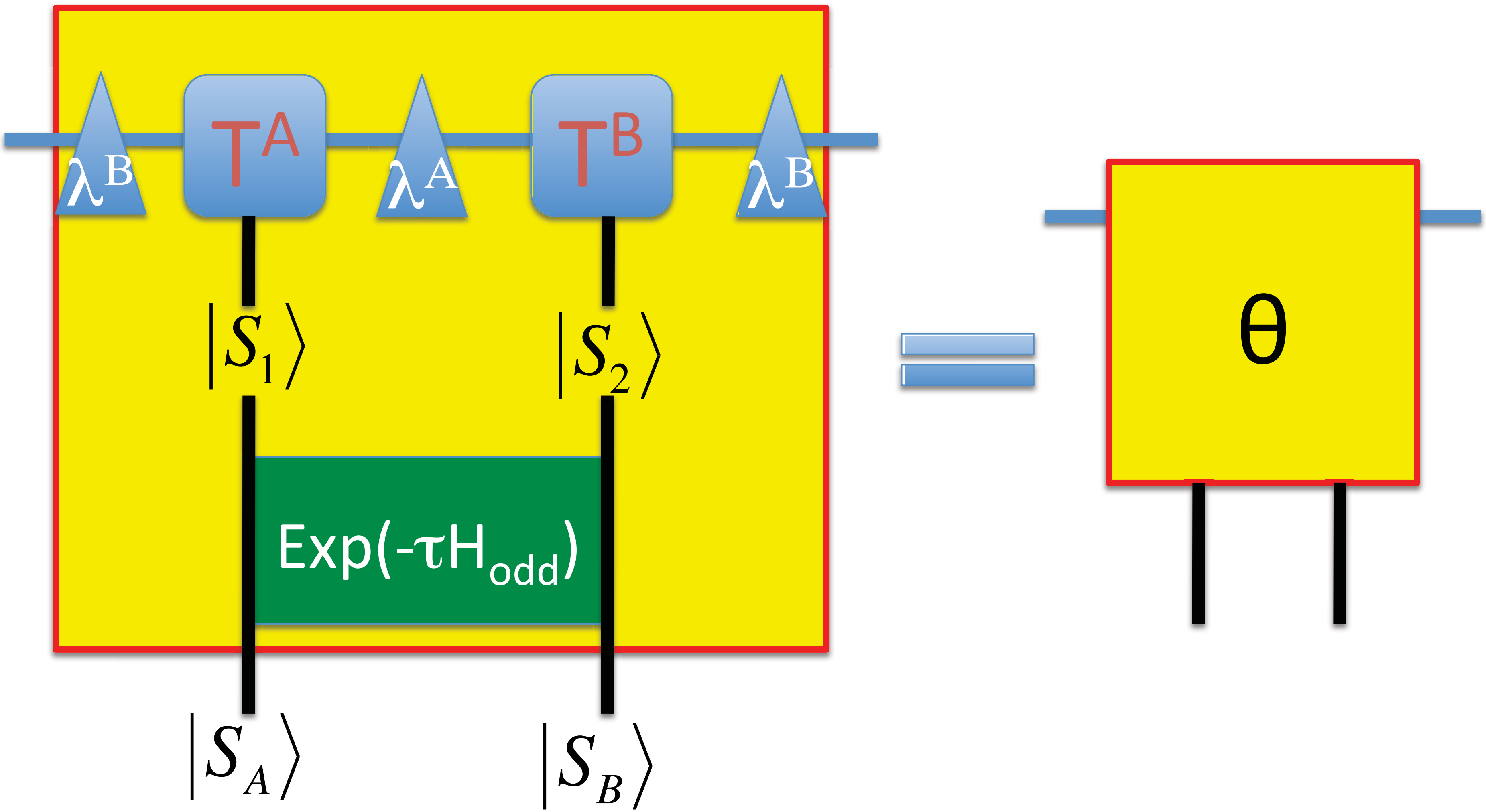
- Translational invariant → Simplification

Applying Exp(-τH_{odd}) or Exp(-τH_{even})

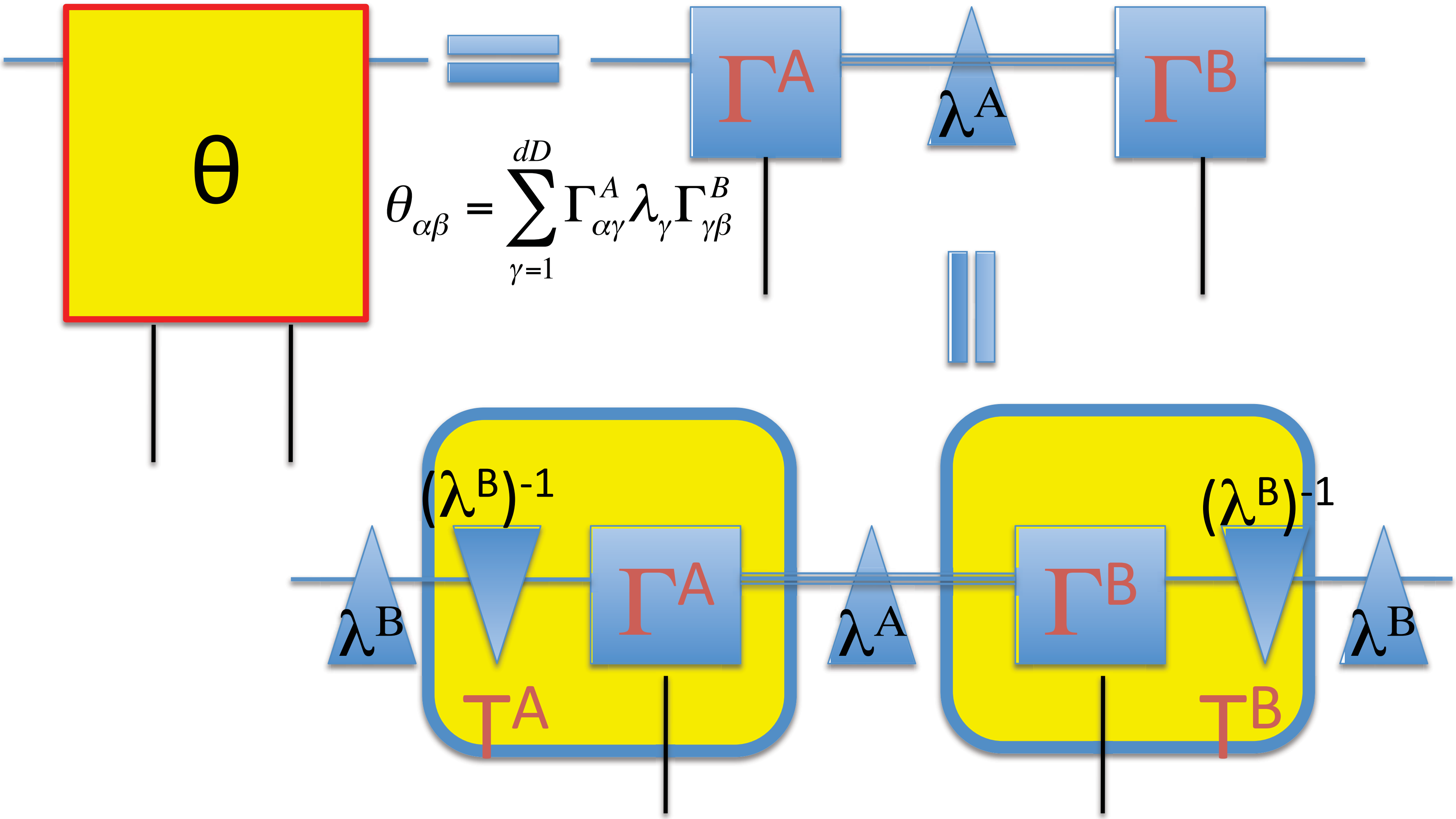
$$|\Psi'\rangle = e^{-\tau H_{odd}}|\Psi\rangle$$



Time-Evolving Block Decimation (TEBD)



Singular Value Decomposition (SVD)



$$\theta_{\alpha\beta} = \sum_{\gamma=1}^{dD} \Gamma^{A}_{\alpha\gamma} \lambda_{\gamma} \Gamma^{B}_{\gamma\beta}$$

Generalization to 2D Problems

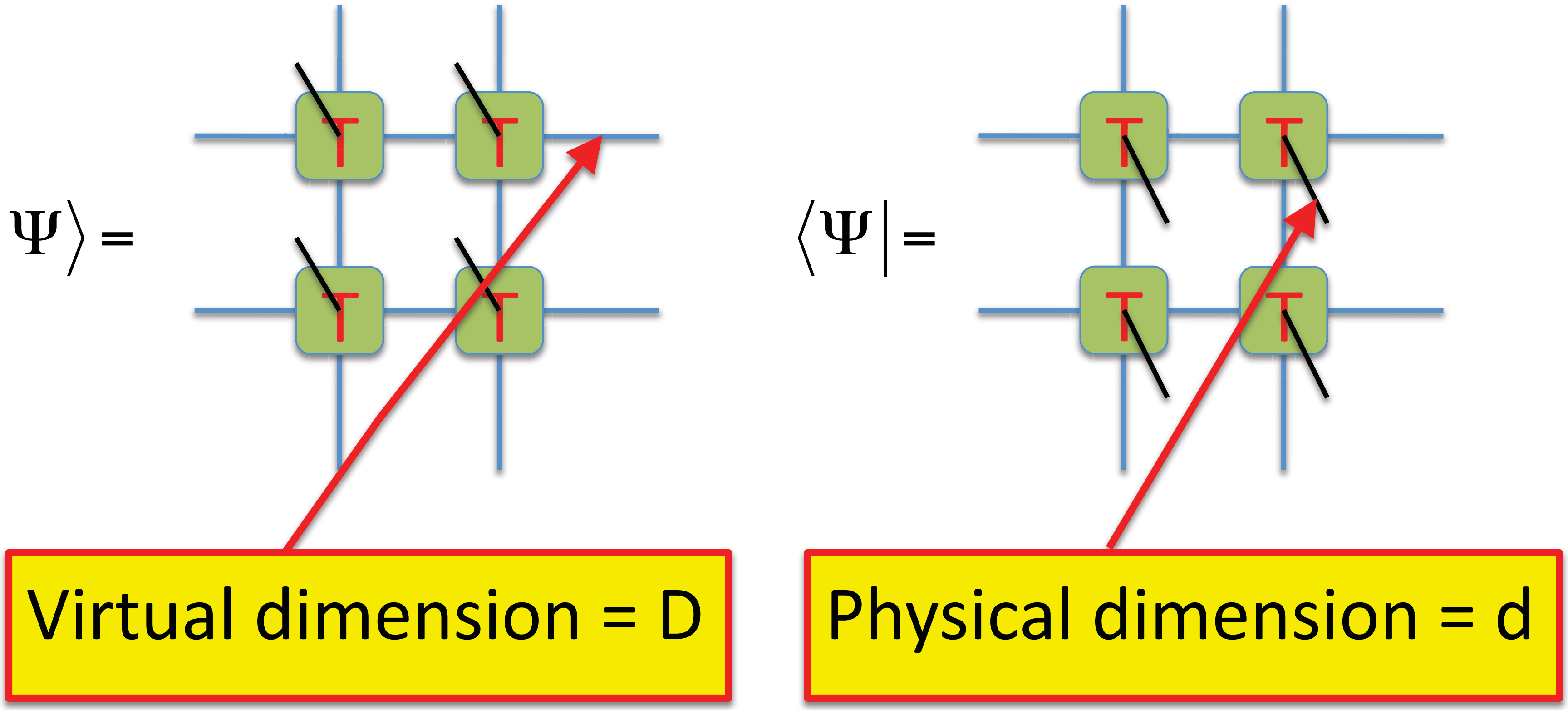
- The easy part
  - Promote 1D MPS to 2D Tensor Product State (TPS)
- The difficult part
  - How to efficiently calculate expectation value
  - How to perform imaginary time evolution

2D Tensor-Product State (TPS)

Represent wave-function by the tensor network of *T* tensors

$$|\Psi\rangle = \sum_{S_i S_j \cdots} \mathrm{Tr}\left[T^{S_i}_{u_i l_i d_i r_i} T^{S_j}_{u_j l_j d_j r_j} \cdots \right] |S_i S_j \cdots \rangle$$

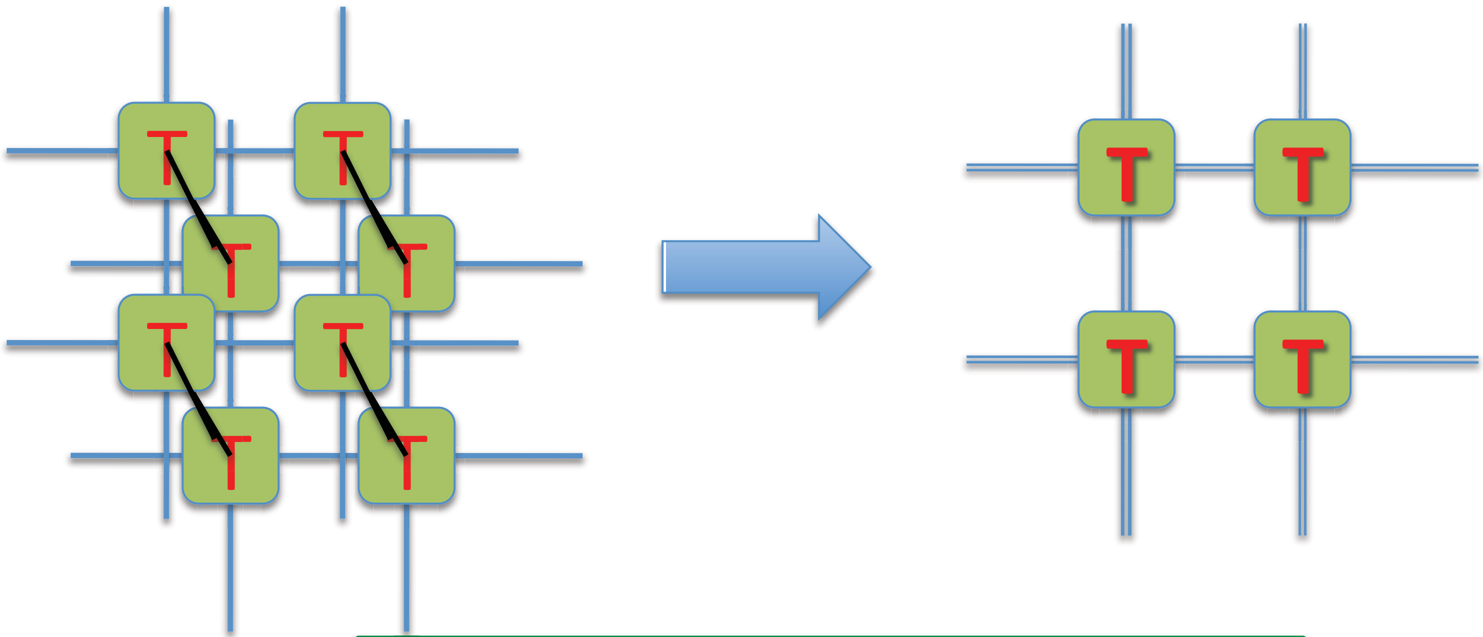
$|\Psi\rangle =$ $\langle \Psi | =$



Expectation Value of TPS

Represent expectation value by the tensor network of **T** tensors

$$\langle \Psi | \Psi \rangle =$$



Double tensor **T**

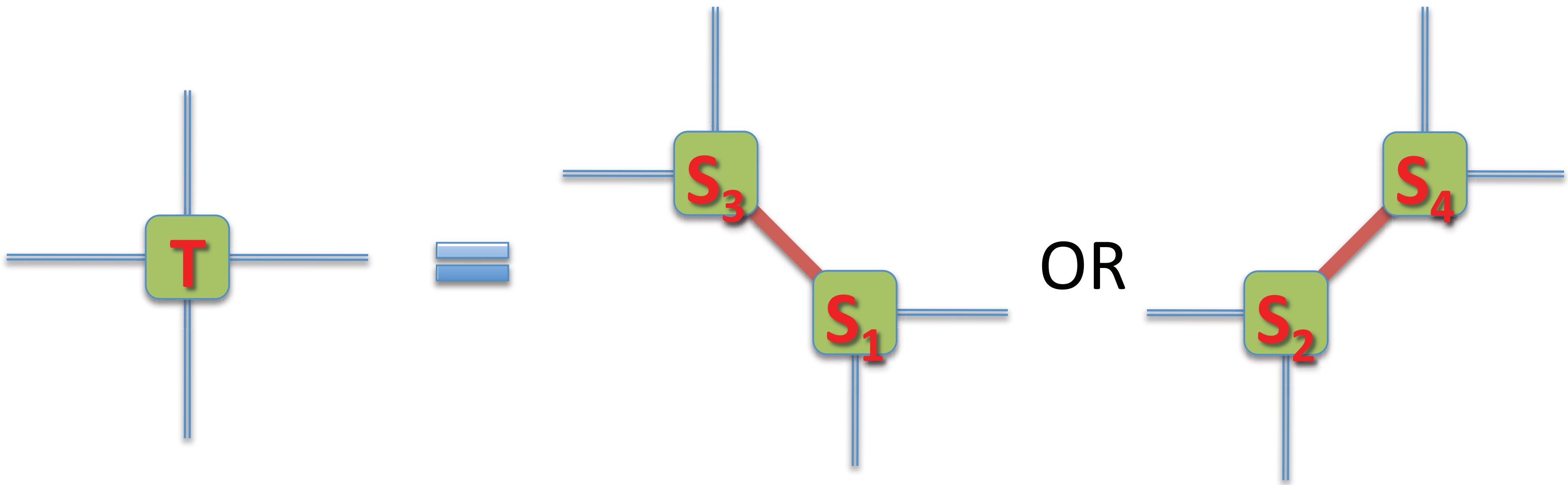
$$\mathbf{T}_{(\tilde{u}u,\tilde{l}l,\tilde{d}d,\tilde{r}r)} = \sum_{S} T^{*S}_{\tilde{u}\tilde{l}\tilde{d}\tilde{r}} T^{S}_{uldr}$$

$$\mathbf{T}^{A}_{(\tilde{u}u,\tilde{l}l,\tilde{d}d,\tilde{r}r)} = \sum_{\tilde{S}S} T^{*\tilde{S}}_{\tilde{u}\tilde{l}\tilde{d}\tilde{r}} \langle \tilde{S} | O^{A} | S \rangle T^{S}_{uldr}$$

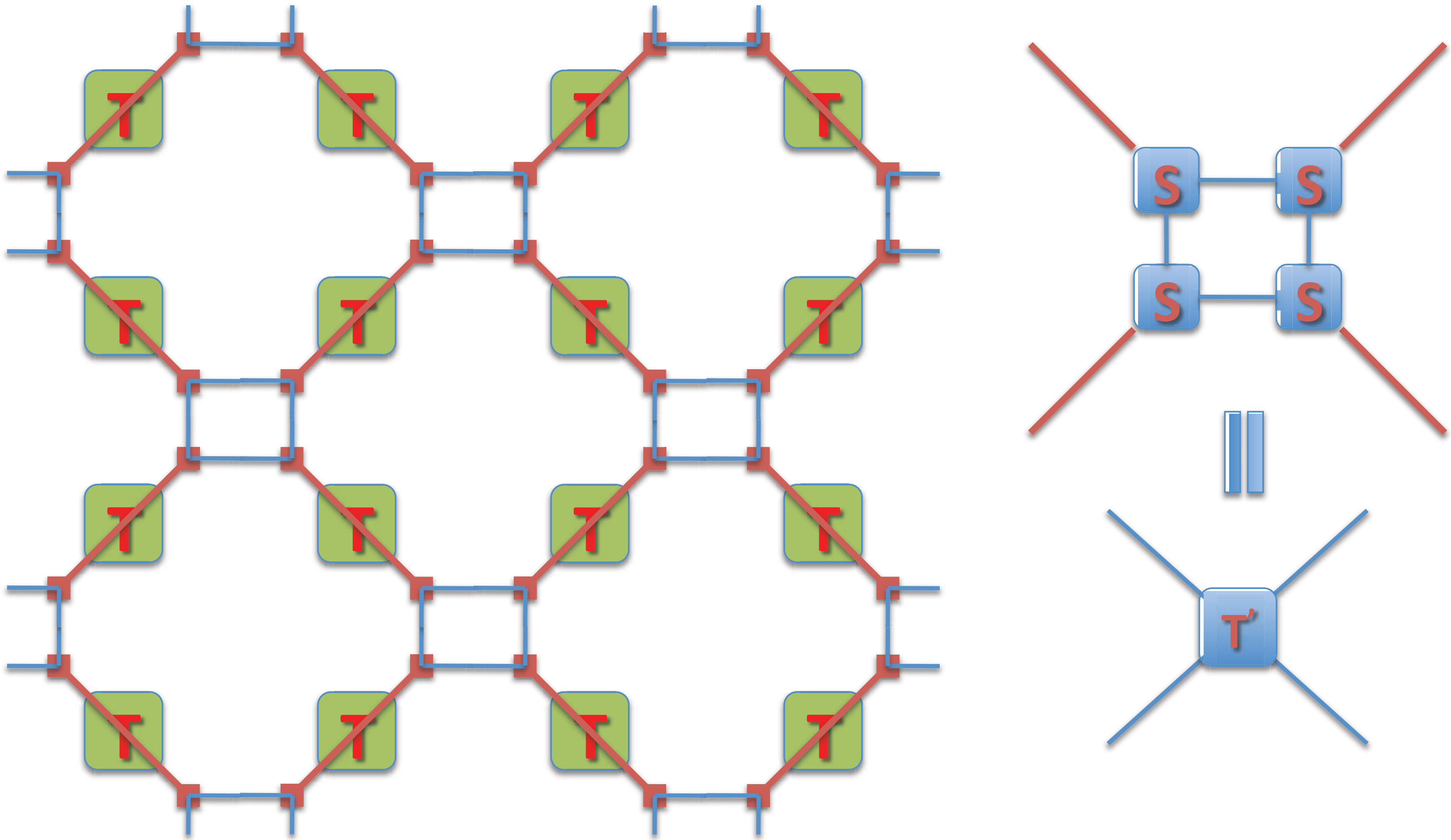
Contraction of Tensor Network

Rewrite rank 4 tensor **T** into product of two rank 3 tensor **S**

$$\mathbf{T}_{\alpha\beta\mu\nu} \cong \sum_{\gamma=1}^{D_{cut}} S_{3,\alpha\delta\gamma} S_{1,\mu\nu\gamma}$$

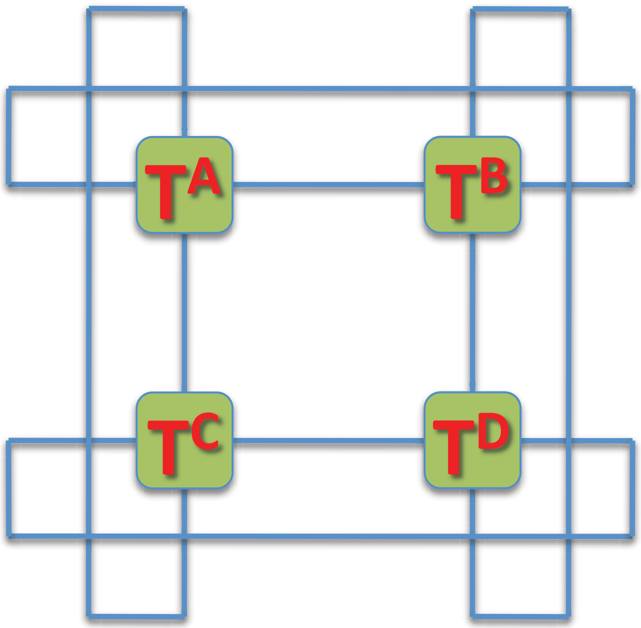


Coarse-Grained Tensor Network



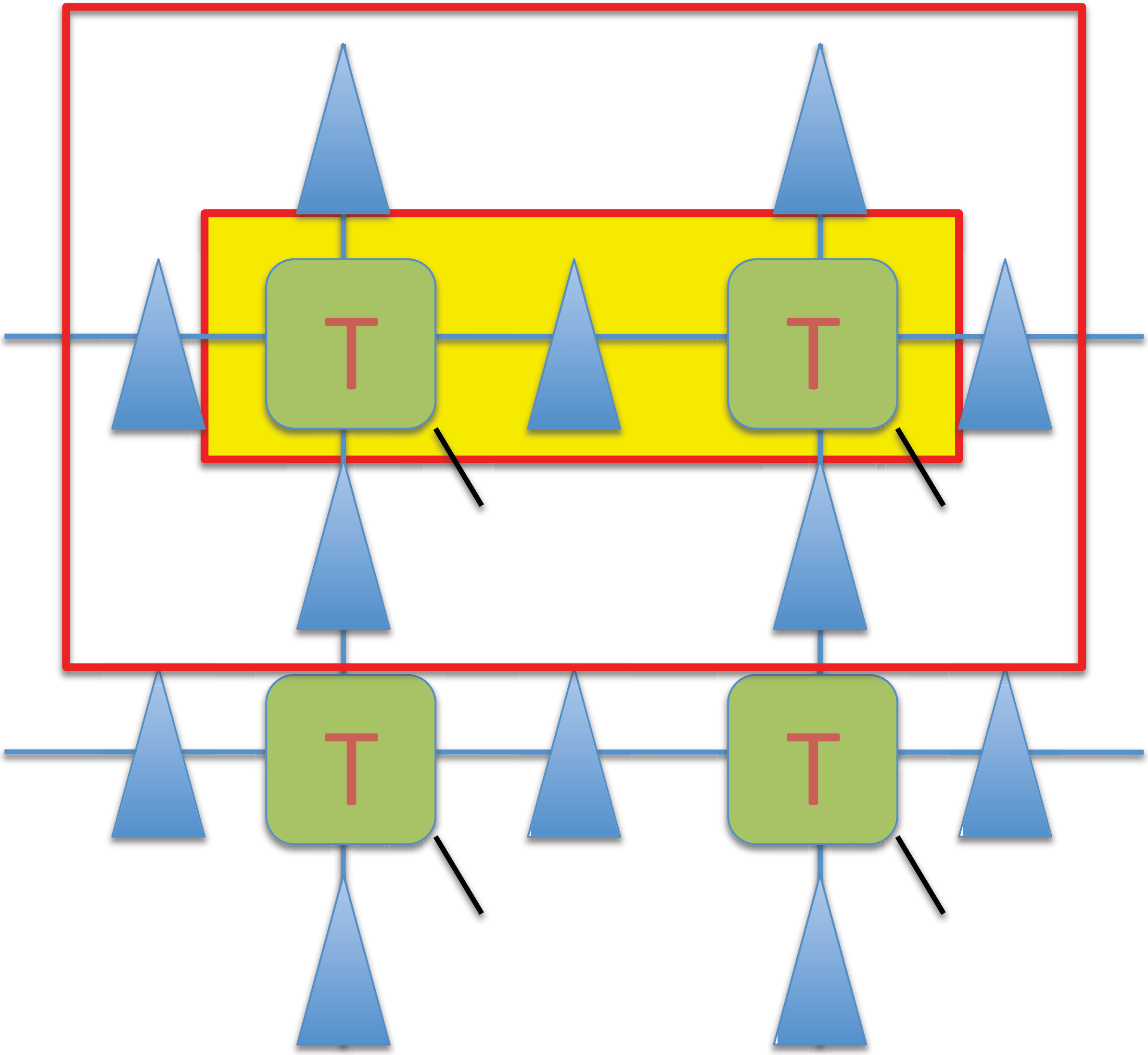
Final 2x2 Plaque

After N iteration of RG, 2x2 plaque effective represent $2^N x 2^N$ lattice
Tensor contract can be done exactly for the 2x2 plaque



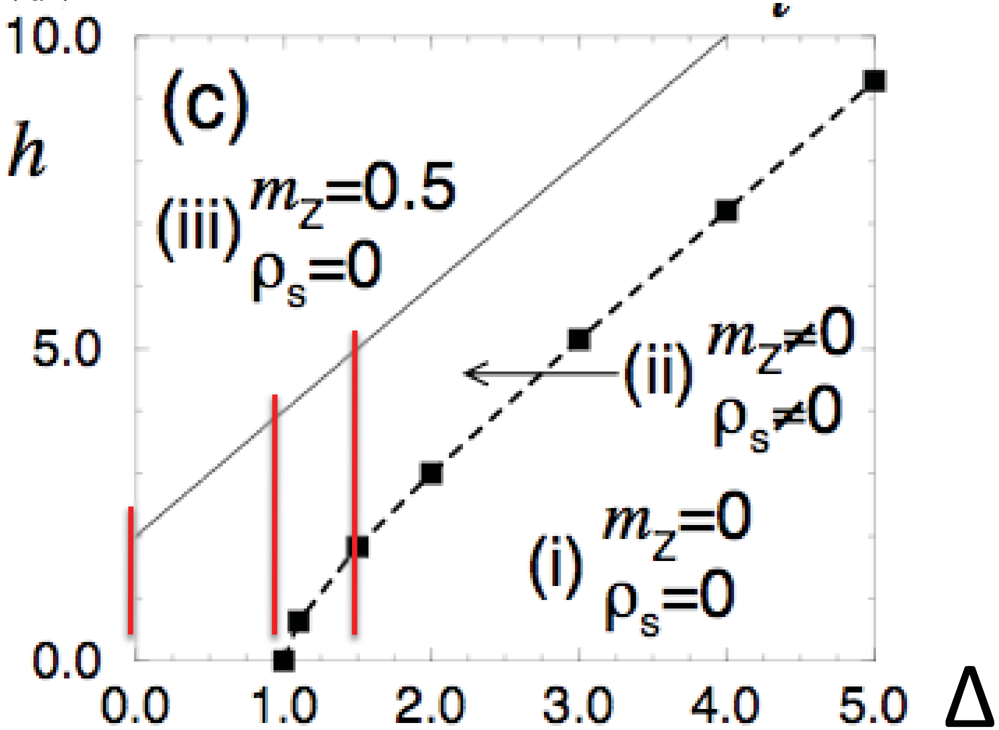
Expectation value of TPS can be approximately but efficiently calculated via TERG

Imaginary Time Evolution of TPS
2D TEBD



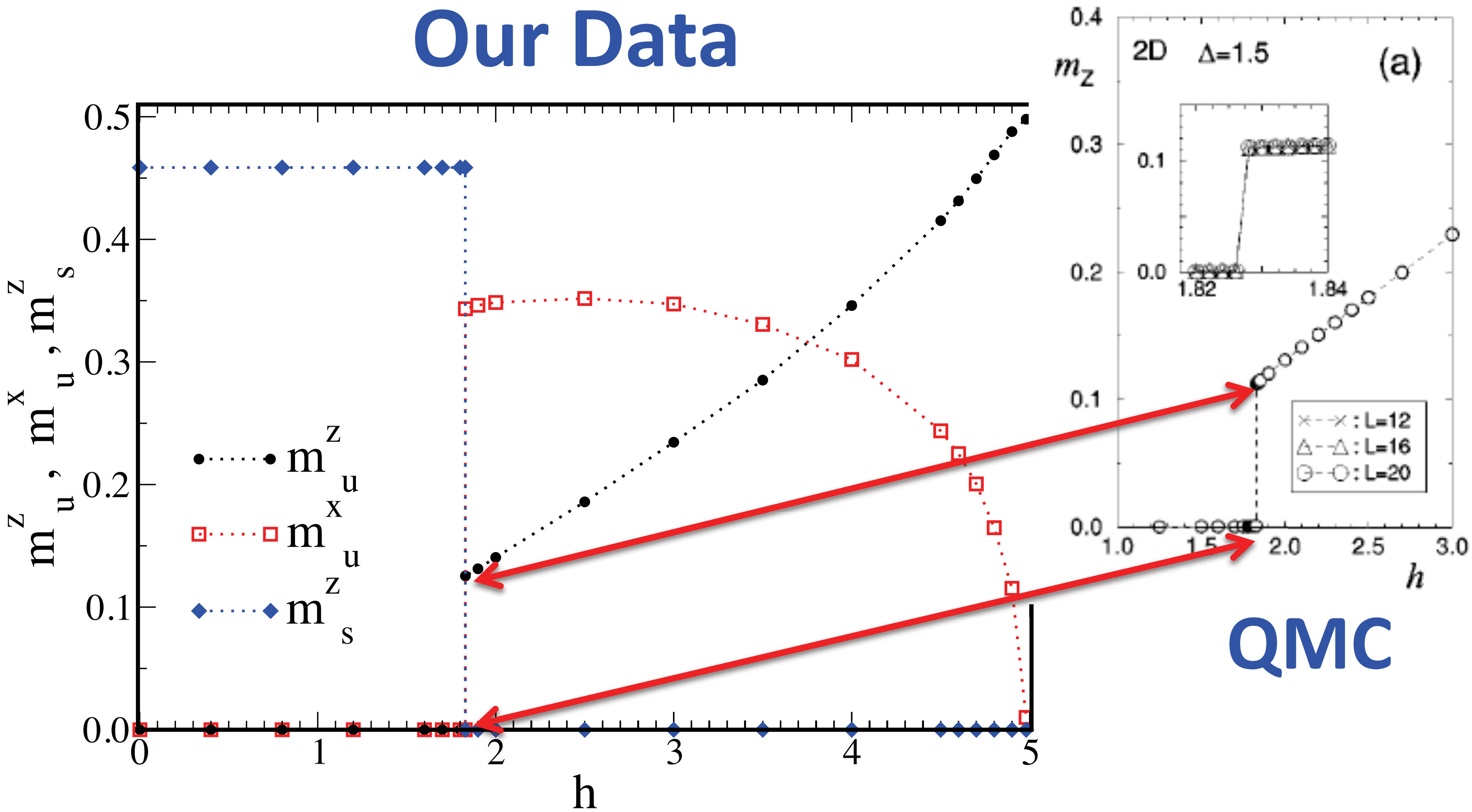
2D XXZ Model

$$H = J\sum_{\langle ij\rangle} -S_i^+ S_j^- - S_i^- S_j^+ + \Delta S_i^z S_j^z - h\sum_i S_i^z$$

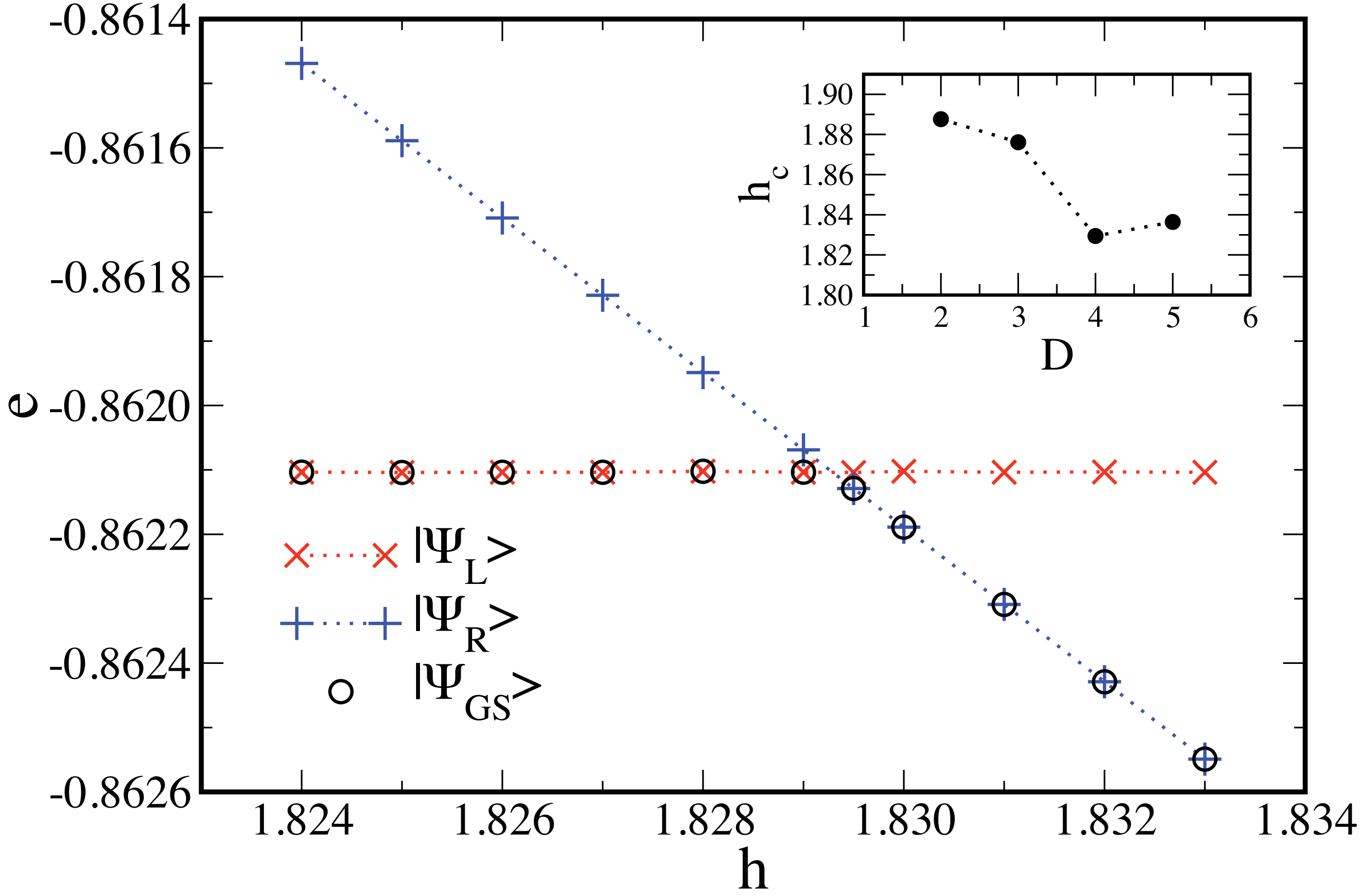


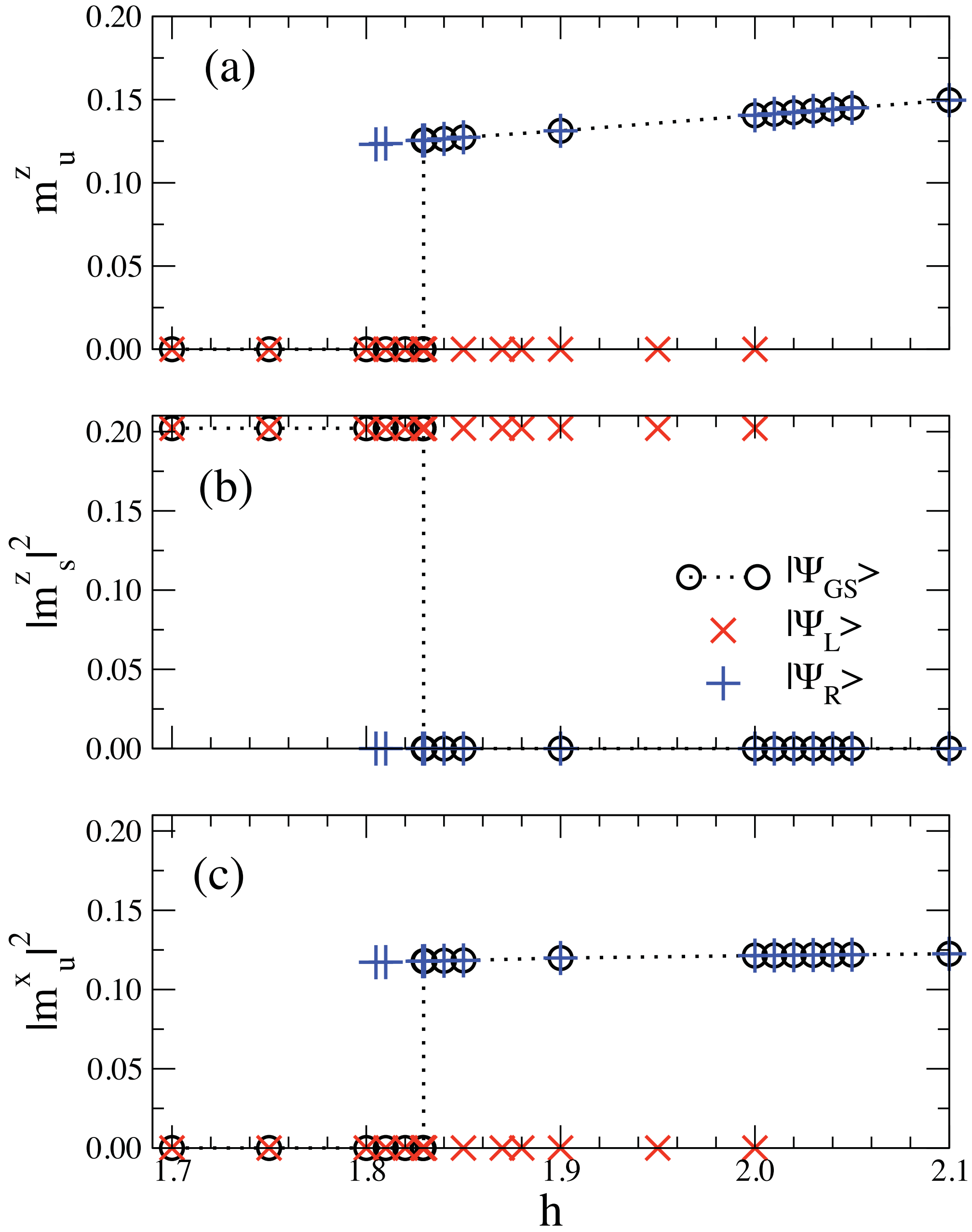
Pochung Chen, Chen-Yen Lai, Min-Fong Yang, arXiv:0905.4110

XXZ Model (Δ=1.5)



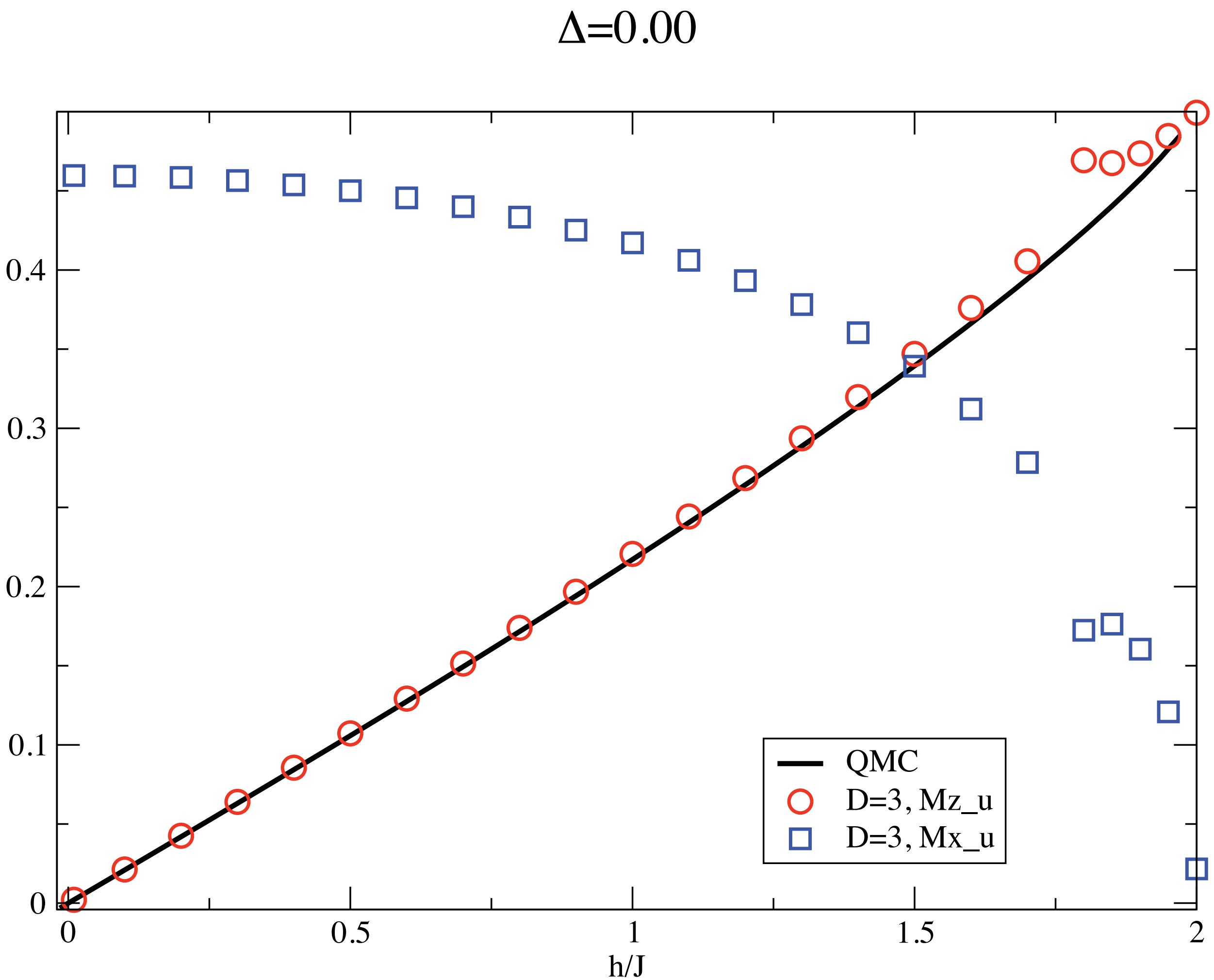
XXZ Model (Δ=1.5)



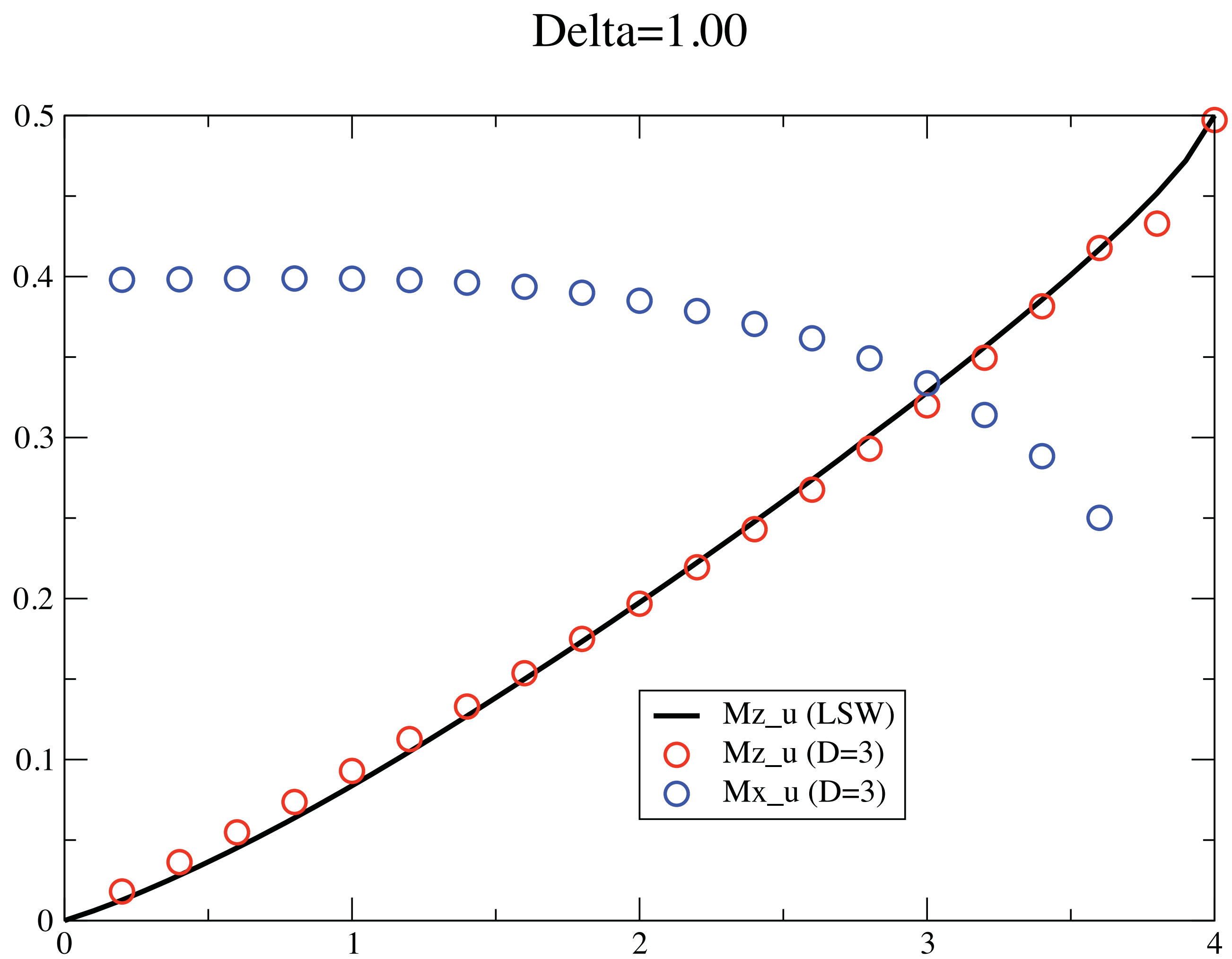


(a)
m^z_u
0.20
0.15
0.10
0.05
0.00
(b)
$|m^z_s|^2$
$|\Psi_{GS}>$
$|\Psi_L>$
$|\Psi_R>$
(c)
$|m^x_u|^2$
1.7
1.8
1.9
2.0
2.1
h

XY Model (Δ=0)



Heisenberg Model (Δ=1)



Summary

- Tensor network state ansatz
- Main ingredients
  - 2D Tensor Product States (TPS)
  - 2D Time-Evolving Block Decimation (TEBD)
  - Tensor Renormalization Group (TRG)
- Application to spin model without frustration
  - Accurate results are obtained
- Outlook
  - Spin model with frustration
  - The effect of the environment