計算科学・量子計算における情報圧縮

Data compression in computational science and quantum computing

2022.11.24

＃6:行列積表現の固有値問題への応用

Application of MPS to eigenvalue problems

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Today's topic

1. Computational science, quantum computing, and data compression
2. Review of linear algebra
3. Singular value decomposition
4. Application of SVD and generalization to tensors
5. Entanglement of information and matrix product states
6. Application of MPS to eigenvalue problems
7. Tensor network representation
8. Data compression in tensor network
9. Tensor network renormalization
10. Quantum mechanics and quantum computation
11. Simulation of quantum computers
12. Quantum-classical hybrid algorithms and tensor network
13. Quantum error correction and tensor network

Outline

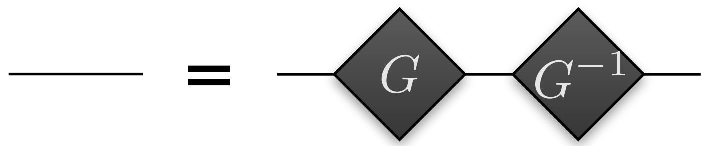
- Matrix product states
  - Canonical form
  - Infinite MPS
- Application to eigenvalue problem (Ground state of quantum many-body systems)
  - Variational algorithm
- Application to the time evolution of a quantum system
  - Time evolution using tensor network representations
  - TEBD algorithm
  - iTEBD and (i)TEBD for eigenvalue problems

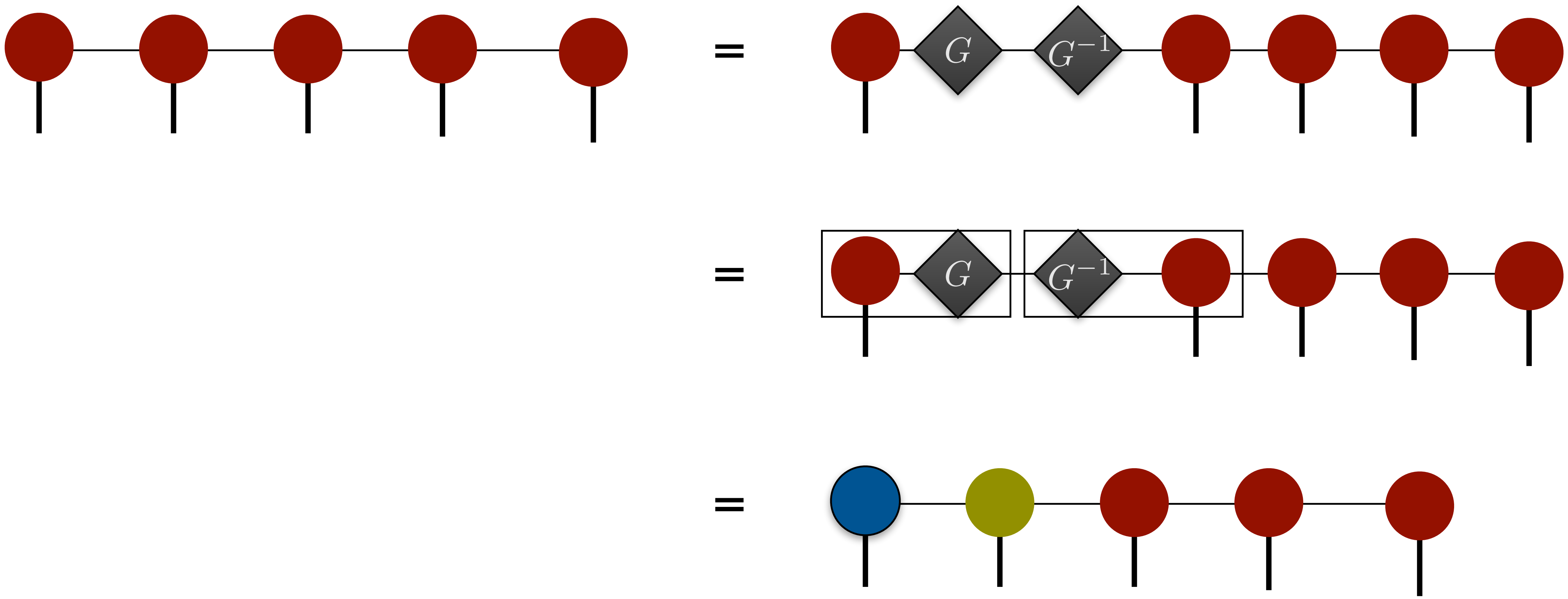
Matrix product states:
Canonical form

Gauge redundancy of MPS

- MPS is not unique
  - gauge degree of freedom
  - we can insert a pair of matrices GG^{-1} to MPS without changing the result of contraction

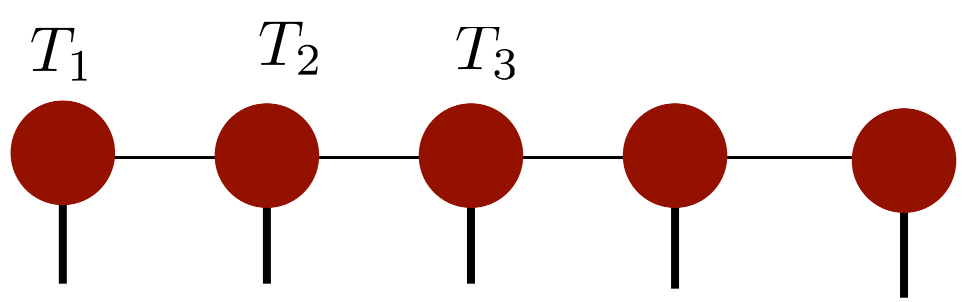
$$I = GG^{-1}$$

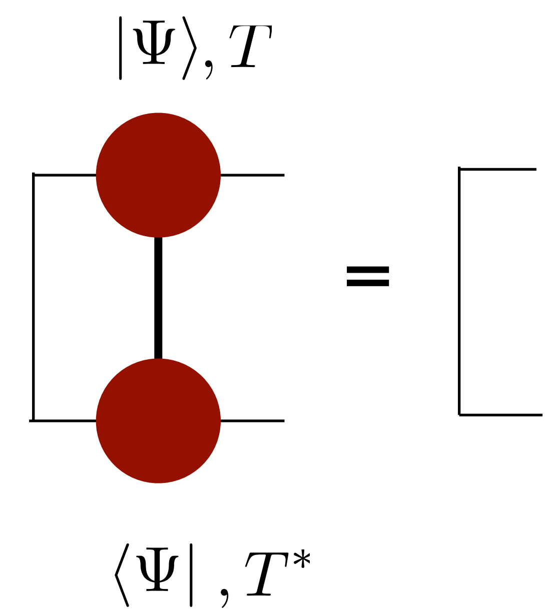




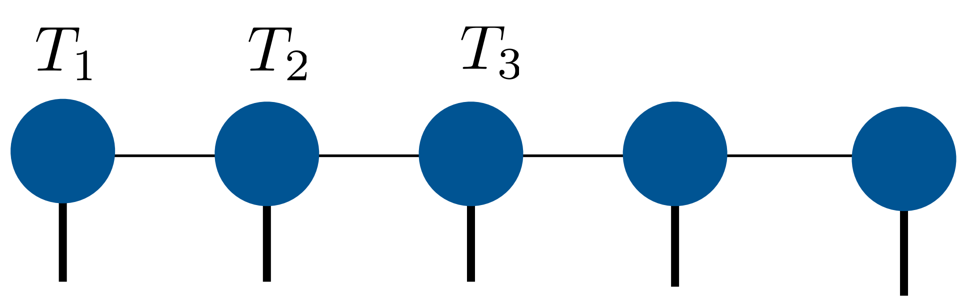
Canonical forms of MPS

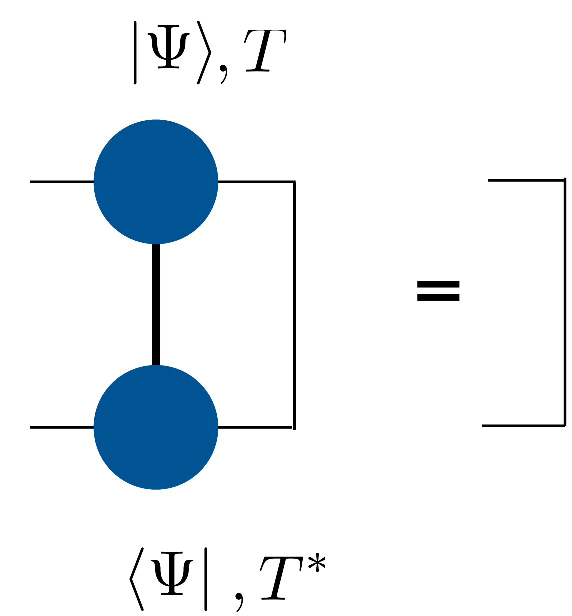
- We can use the gauge degrees of freedom to "canonicalize" MPS
  - left canonical form (left canonical condition)





  - right canonical form (right canonical condition)





  - one can find G by using SVD (or diagonalization)

Review: U. Schollwöck, Annals. of Physics 326, 96 (2011)

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Singular value decomposition (SVD)

Singular value decomposition (特異値分解)

$$A = \underbrace{U}_{}\Sigma\underbrace{V}_{}^\dagger$$

$$A : M \times N$$

$$A_{ij} \in \mathbb{C}$$

$U : M \times M$ **Unitary**

$V : N \times N$ **Unitary**

$$\Sigma = \begin{pmatrix} \underline{\Sigma_{r\times r}} & 0_{r\times(N-r)} \\ 0_{(M-r)\times r} & 0_{(M-r)\times N-r} \end{pmatrix}$$

$$\Sigma_{r\times r} = \begin{pmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_r \end{pmatrix}$$

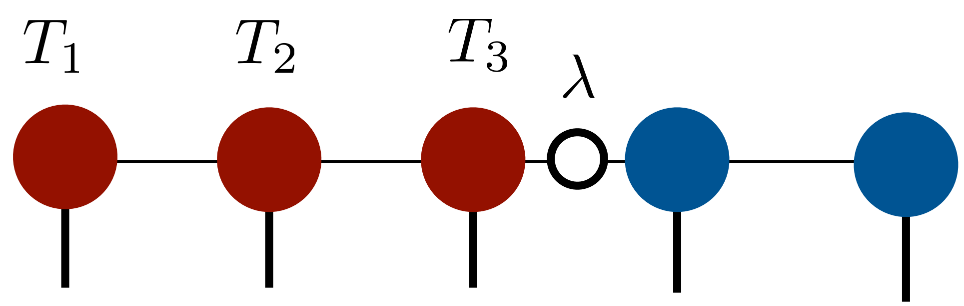
Diagonal matrix with non-negative real elements

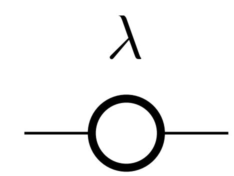
$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$$

Singular values

Mixed canonical form

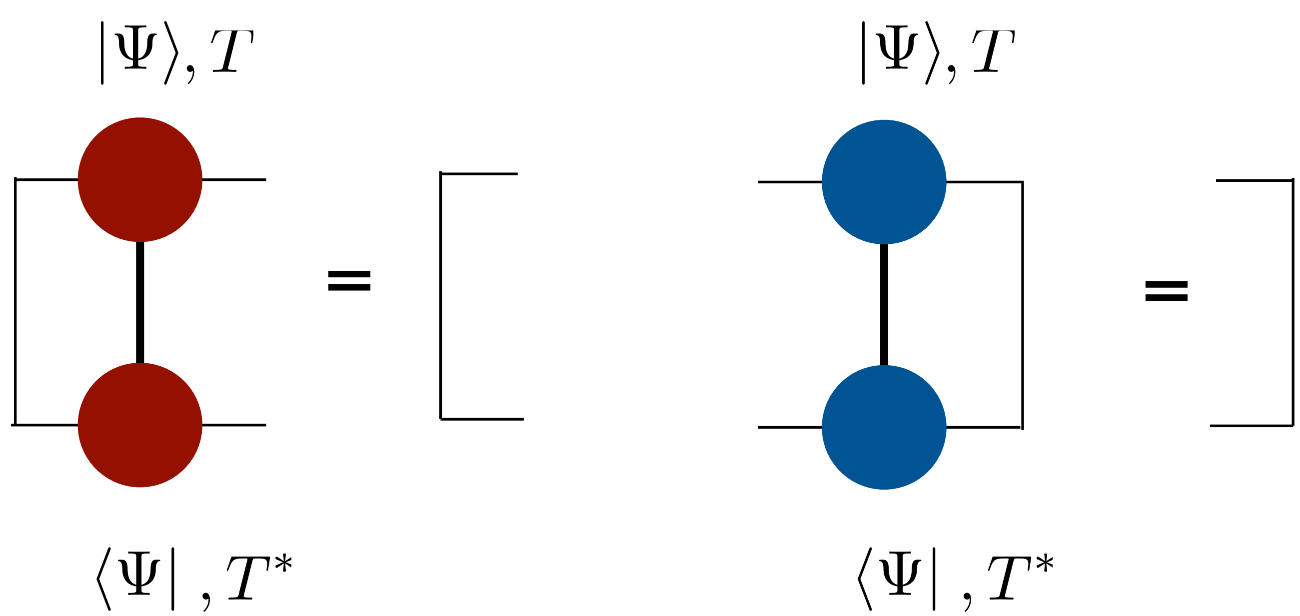
- Mixed canonical form





diagonal matrix
corresponding to
Schmidt coefficient

- Left / right canonical conditions

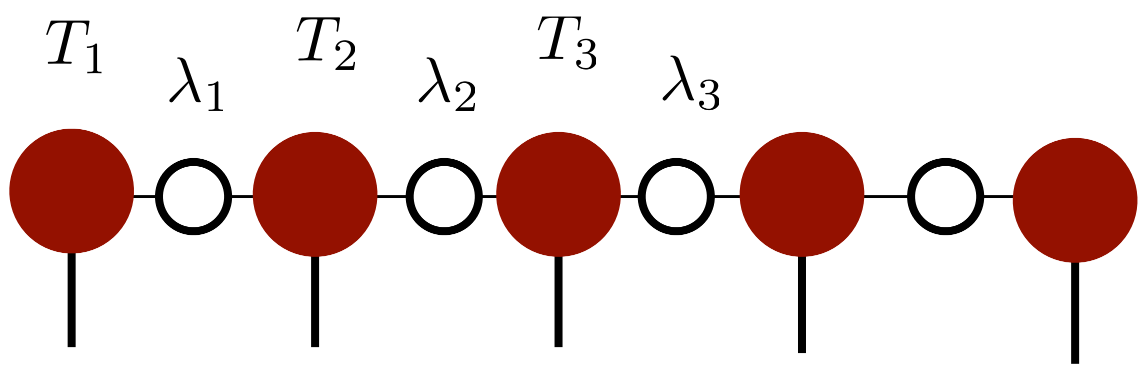


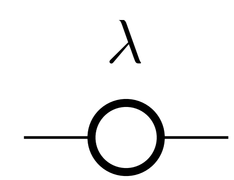
- boundary between left and right can be moved by using SVD

Review: U. Schollwöck, Annals. of Physics 326, 96 (2011)

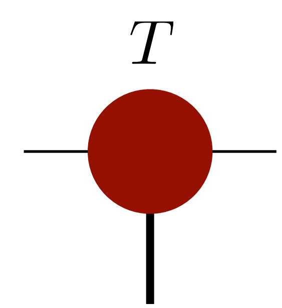
Vidal canonical form

- Another canonical form of MPS (Vidal canonical form)



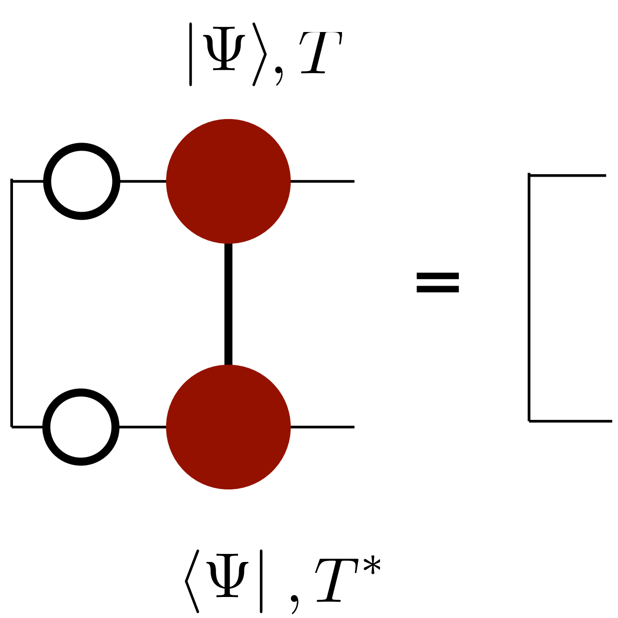


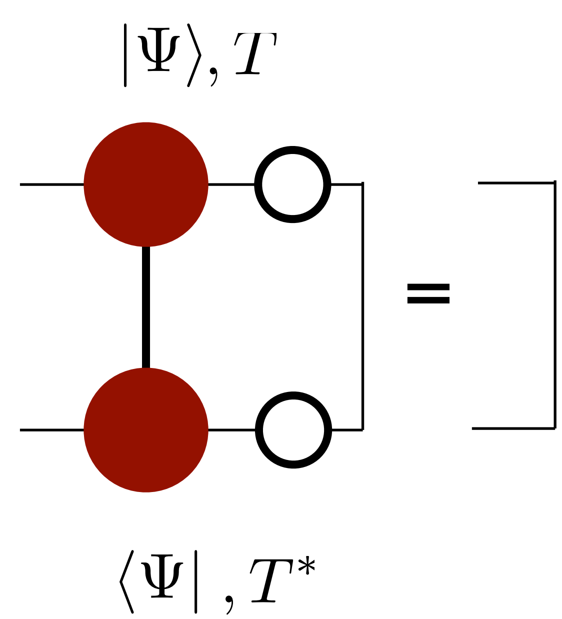
diagonal matrix corresponding to Schmidt coefficient

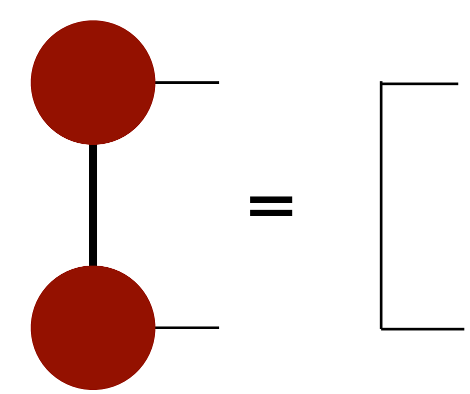


Virtual indices corresponding to Schmidt basis

- Left / right / boundary canonical conditions





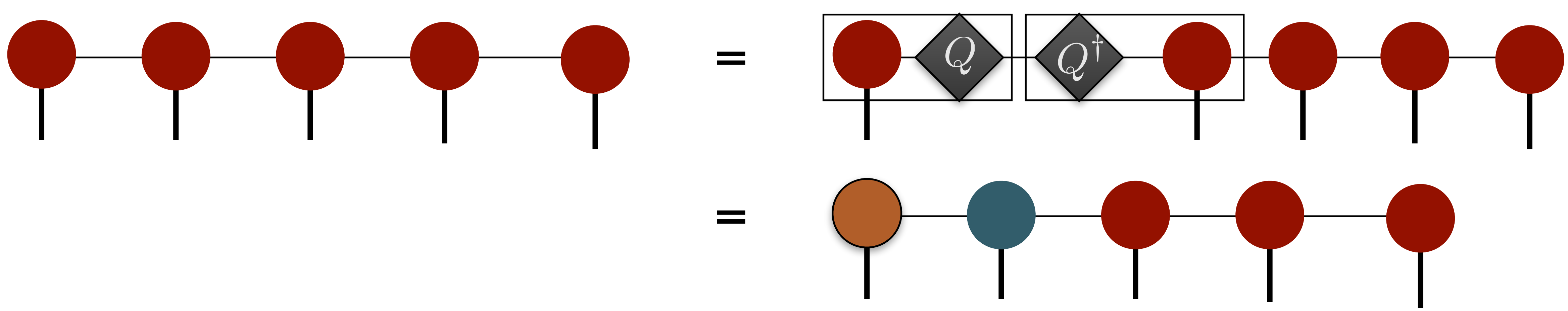


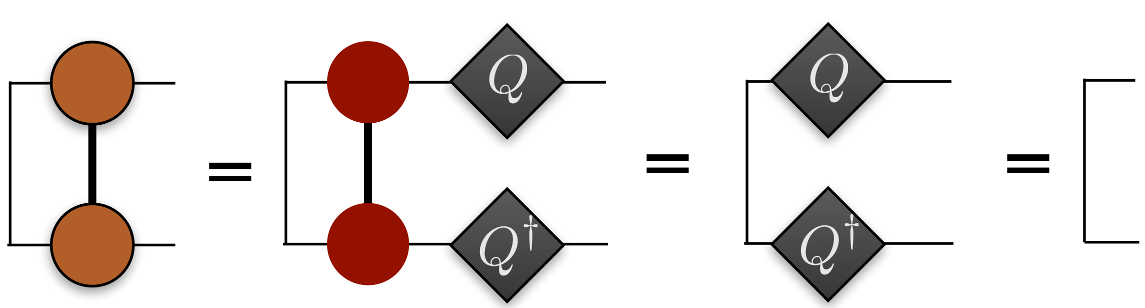
G. Vidal, Phys. Rev. Lett. 91, 147902 (2003)

Notes on canonical forms

- Vidal canonical form is unique
  - up to trivial unitary transformation to virtual indices which keep the same diagonal matrix structure (Schmidt coefficients).
- Left, right and mixed canonical forms are not unique
  - under general unitary transformation to virtual indices, they remains to satisfy the canonical condition

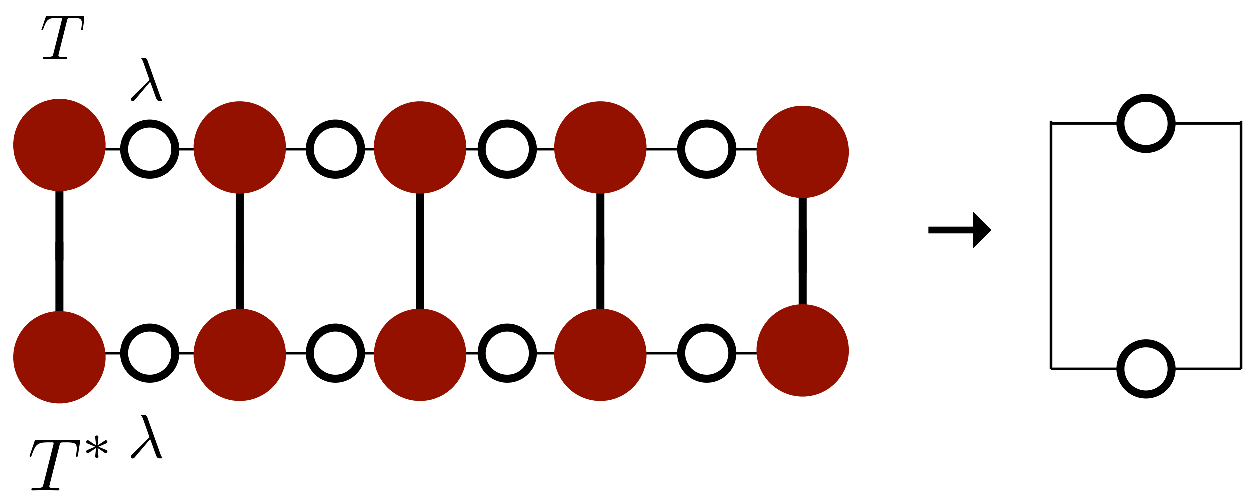
$$QQ^\dagger = Q^\dagger Q = I$$



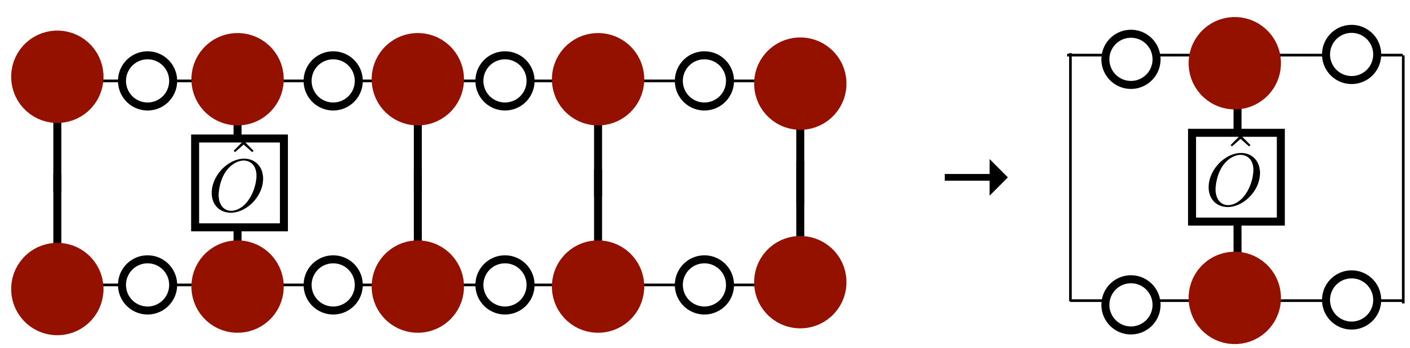


Expectation values of MPS with canonical form

- Evaluation of expectation values becomes extremely simple under canonical condition

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

$= \sum_i \lambda_i^2 = 1$

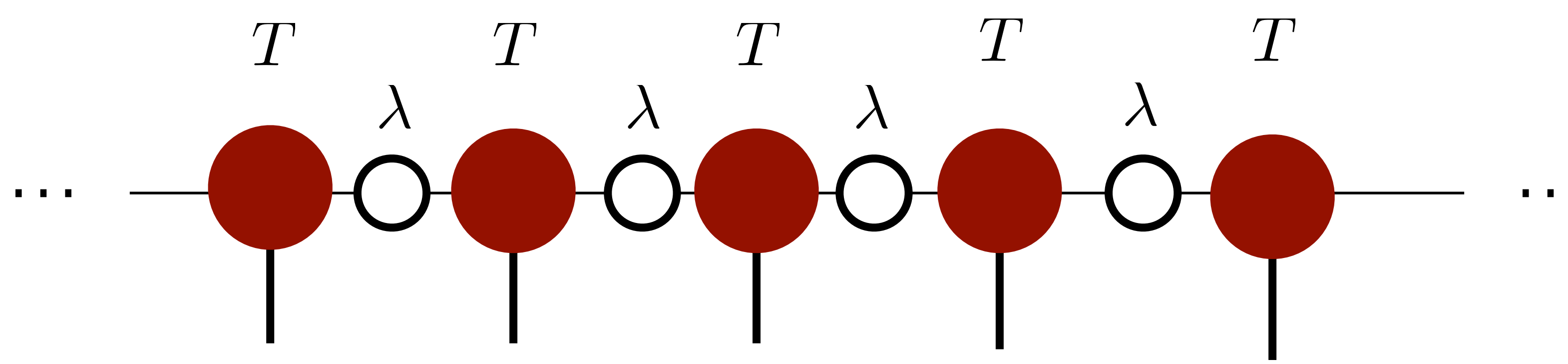
$\langle \Psi | \hat{O} | \Psi \rangle =$ 

- similar simple diagram can also be obtained with mixed canonical form

Matrix product states:
Infinite MPS

MPS for infinite chains

- By using MPS, we can write the wave function of a translationally invariant infinite chain
  - infinite MPS (iMPS) is made by repeating T and λ infinitely

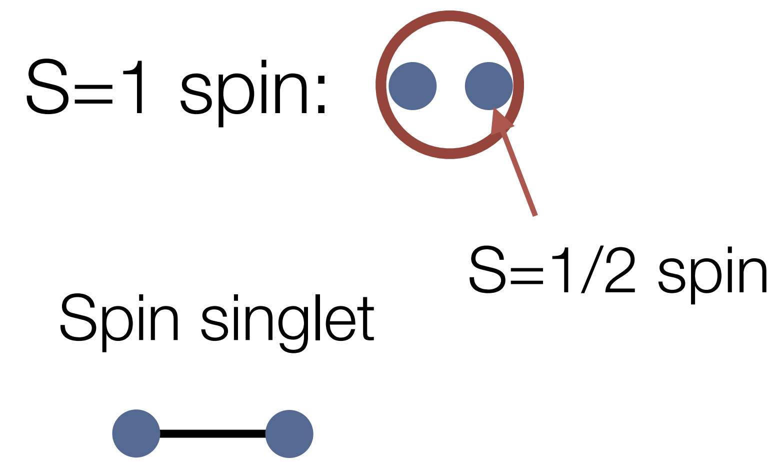


  - translationally invariant system → T and λ are independent of positions
- Infinite MPS can be accurate only when EE satisfies the 1d area low $(S \sim O(1))$
  - if the EE increases as increase the system size, we may need infinitely large χ for infinite system
  - In practice, we can obtain a reasonable approximation with finite χ

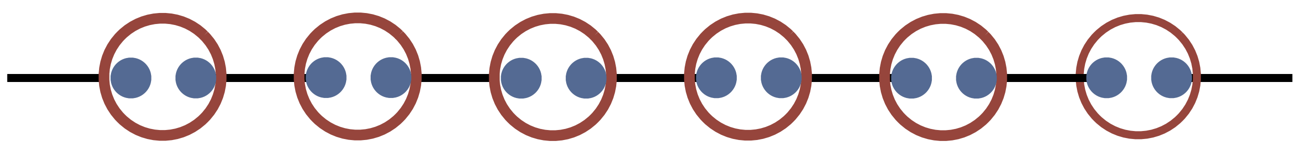
Example of iMPS: AKLT state

- S=1 Affleck-Kennedy-Lieb-Tasaki (AKLT) Hamiltonian

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + \frac{J}{3} \sum_{\langle i,j \rangle} \left(\vec{S}_i \cdot \vec{S}_j \right)^2 \qquad (J > 0)$$



- ground state of AKLT model

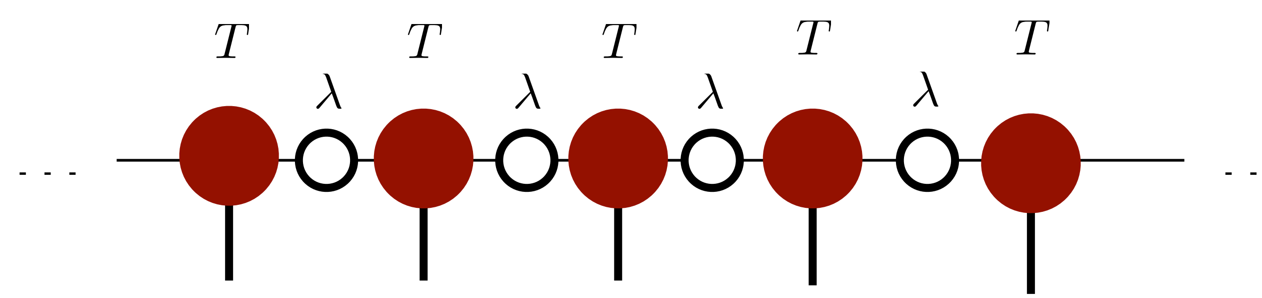


- iMPS representation of AKLT state (χ =2)

$$T[S_z = 1] = \sqrt{\frac{4}{3}} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$T[S_z = 0] = \sqrt{\frac{2}{3}} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$T[S_z = -1] = \sqrt{\frac{4}{3}} \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}$$



$$\lambda = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Application to eigenvalue problem: Variational algorithm

Eigenvalue problem

- Target vector space
  - exponentially large Hilbert space

$$\vec{v} \in \mathbb{C}^M \text{ with } M \sim a^N$$

  - total Hilbert space is decomposed as a product of "local" Hilbert space

$$\mathbb{C}^M = \mathbb{C}^a \otimes \mathbb{C}^a \otimes \cdots \mathbb{C}^a$$

- Target matrix
  - $\mathcal{H}$: Hermitian and sparse
  - (typically, only $O(M)$ ($= O(a^N)$) elements are finite)

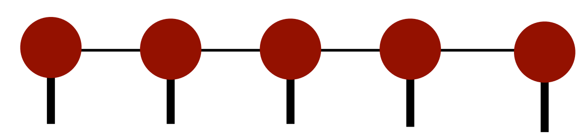
- We consider the situation where vector of length $O(M)$ can not be stored in the memory.

Problem

- Find (approximately) the smallest eigenvalue and its eigenvector

$$\mathcal{H}\vec{v}_0 = E_0\vec{v}_0 \quad \Longrightarrow \quad \min_{\vec{\psi}\in\mathbb{C}^M} \frac{\vec{\psi}^\dagger(\mathcal{H}\vec{\psi})}{\vec{\psi}^\dagger\vec{\psi}} \left(= \min_{|\psi\rangle} \frac{\langle\psi|\mathcal{H}|\psi\rangle}{\langle\psi|\psi\rangle} \right)$$

- Variational approach using MPS

$\vec{\psi} =$ 

  - cost function

$$F = \frac{\vec{\psi}^\dagger(\mathcal{H}\vec{\psi})}{\vec{\psi}^\dagger\vec{\psi}}$$

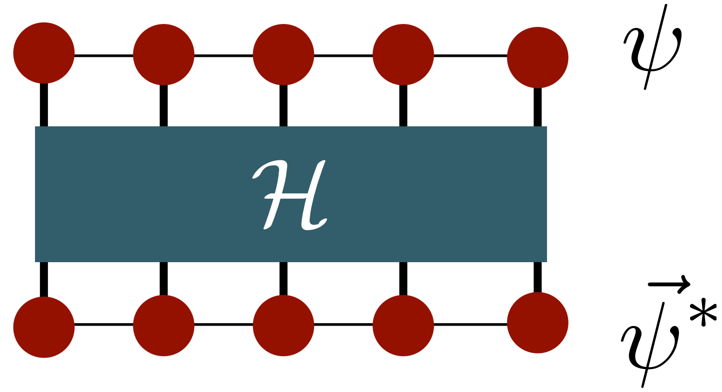
  - find a MPS that minimizes F by optimizing matrices in MPS

Graphical representation

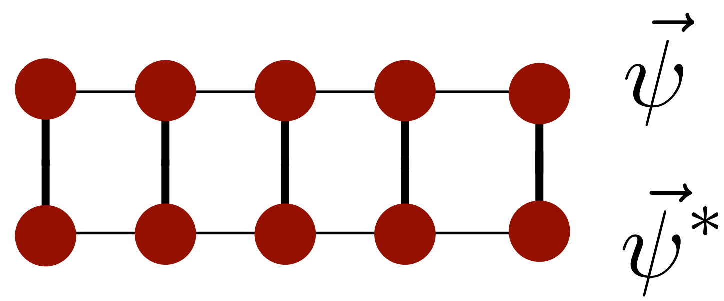
- Cost function

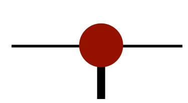
$$F = \frac{\vec{\psi}^\dagger(\mathcal{H}\vec{\psi})}{\vec{\psi}^\dagger\vec{\psi}}$$

$$\vec{\psi}^\dagger(\mathcal{H}\vec{\psi}) =$$



$$\vec{\psi}^\dagger\vec{\psi} =$$



- find $A_i[\sigma_i] =$  that minimizes F

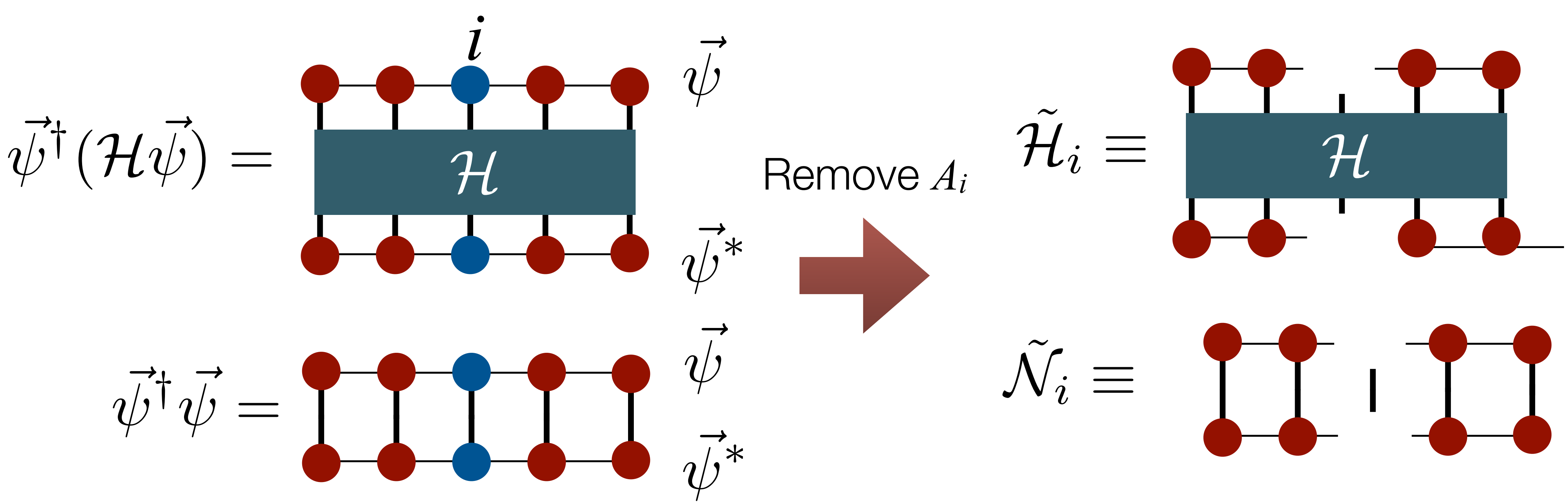
Iterative optimization

- Optimize one matrix at site "i" by fixing the other matrices

$$F = \frac{\vec{\psi}^\dagger(\mathcal{H}\vec{\psi})}{\vec{\psi}^\dagger\vec{\psi}} = \frac{A_i^\dagger(\tilde{\mathcal{H}}_i A_i)}{A_i^\dagger(\tilde{N}_i A_i)}$$

  - → lowest eigenvalue in generalized eigenvalue problem of $a\chi^2 \times a\chi^2$ matrix

$$\tilde{\mathcal{H}}_i A_i = \epsilon \tilde{\mathcal{N}}_i A_i$$

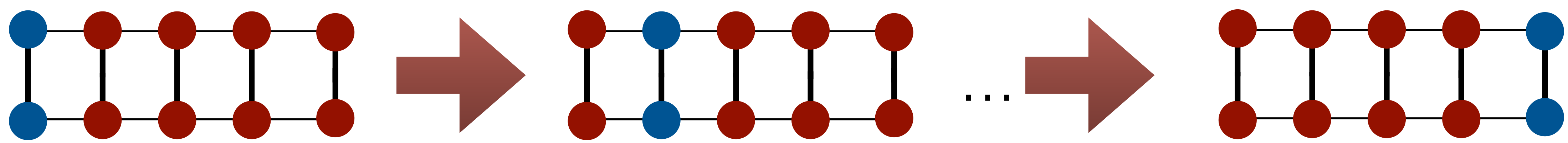


  - if we impose (mixed) canonical condition, $\tilde{N}$ becomes an identity

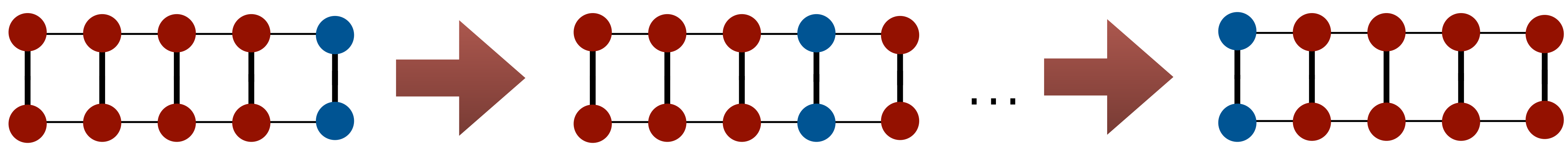
F. Verstraete, D. Porras, and J. I. Cirac, Phys. Rev. Lett. **93**, 227205 (2004)

Iterative optimization

- Update A_i's by "sweeping" sites from $i = 1$ to N



  - and sweeping sites backward from $i = N$ to 1

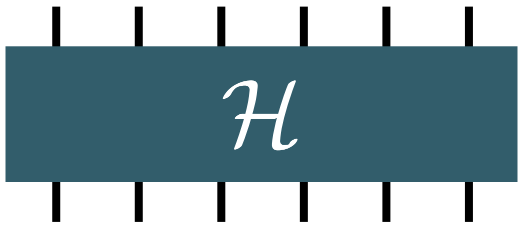


  - repeat sweeping until the matrices converge
- Variational MPS method is essentially the same with so-called "Density Matrix Renormalization Group (DMRG)" method
  - original DMRG did not use MPS explicitly, but MPS gives a theoretical explanation why DMRG works well

F. Verstraete, D. Porras, and J. I. Cirac, Phys. Rev. Lett. **93**, 227205 (2004)
S. R. White, Phys. Rev. Lett. **69**, 2863 (1992)

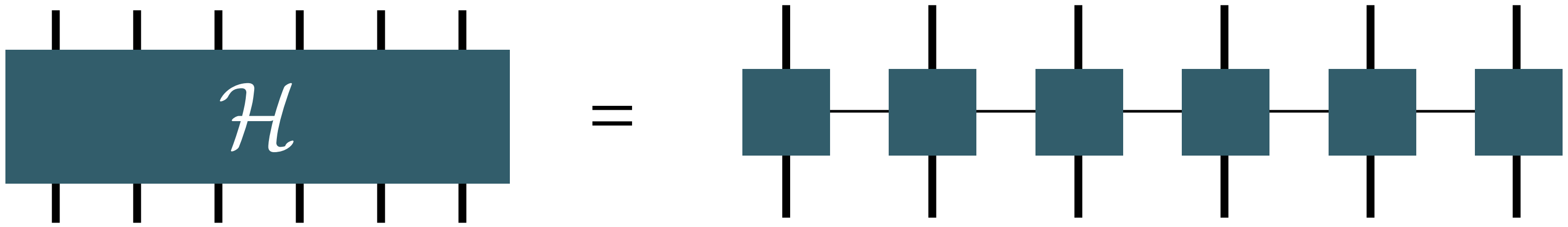
Compact representation of operators

- We are considering the situation where the whole Hamiltonian matrix can not be stored in the memory



$$a^N \times a^N$$

- Need of compact representation of Hamiltonian operator
  - typically, Hamiltonian is a sum of local Hamiltonians
  - or, we represent the matrix in a Matrix Product Operator (MPO) form



  - e.g.) Hamiltonian of the nearest-neighbor Heisenberg chain can be represented exactly by MPO with bond dimension $\chi = 5$

Review: U. Schollwöck, Annals. of Physics 326, 96 (2011)

Application to the time evolution of a quantum system:
Time evolution using tensor network representations

Time evolution of a quantum system

- Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = \mathcal{H}|\psi(t)\rangle$$

  - formal solution

$$|\psi(t)\rangle = \underline{e^{-it\mathcal{H}/\hbar}}|\psi(0)\rangle$$

time evolution operator (時間発展演算子)

- Time evolution calculation using MPS
  - multiply the time evolution operator to a MPS to generate a new state
  - find an approximate MPS representing the state

Time evolution using MPS

- Target: one-dimensional quantum system with short range interaction
  - typical examples: chains of quantum spins / qubits
  - transverse field Ising model

$$\mathcal{H} = -\sum_{i=1}^{N-1} S_i^z S_{i+1}^z - h\sum_{i=1}^{N} S_i^x$$

  - Heisenberg model

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

- Typical situation: quantum quench
  - initial state: ground state of a Hamiltonian which well approximated by a MPS
  - $t > 0$: Hamiltonian suddenly changes from the initial one
  - For a “short” time interval, evolving state is approximated by MPS efficiently

Suzuki-Trotter decomposition

- Systematic approximation of exponential operator $(\mathcal{A}\mathcal{B} \neq \mathcal{B}\mathcal{A})$

$$e^{\tau(\mathcal{A}+\mathcal{B})} = e^{\tau\mathcal{A}}e^{\tau\mathcal{B}} + O(\tau^2) \qquad \text{(1st order)}$$
$$= e^{\tau/2\mathcal{A}}e^{\tau\mathcal{B}}e^{\tau/2\mathcal{A}} + O(\tau^3) \qquad \text{(2nd order)}$$
$$= e^{\tau/2\mathcal{B}}e^{\tau\mathcal{A}}e^{\tau/2\mathcal{B}} + O(\tau^3) \qquad \text{(2nd order)}$$

- if our Hamiltonian is a sum of “local” operators

$$\mathcal{H} = \sum_i H_i$$

- time evolution operator can be approximated as

$$e^{-it\mathcal{H}/\hbar} = \left(e^{-i\delta\mathcal{H}}\right)^M = \left(\prod_j e^{-i\delta H_j}\right)^M + O(\delta)$$

$$\delta \equiv t/(M\hbar)$$

M. Suzuki, Commun. Math. Phys. 51, 183 (1976)

Graphical representation of ST decomposition

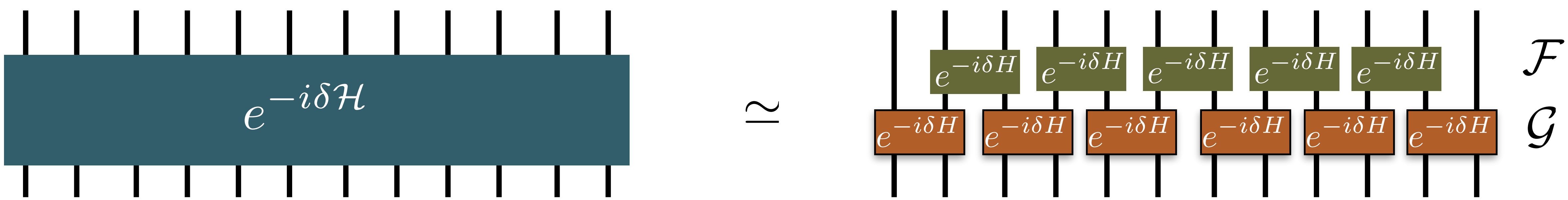
- Suppose the Hamiltonian is a sum of two-body local terms

$$\mathcal{H} = \sum_i H_i = \sum_{i \in \mathrm{even}} H_i + \sum_{i \in \mathrm{odd}} H_i$$

$$= \mathcal{F} + \mathcal{G} \qquad [\mathcal{F}, \mathcal{G}] \neq 0$$

- Suzuki Trotter decomposition of time evolution opertor

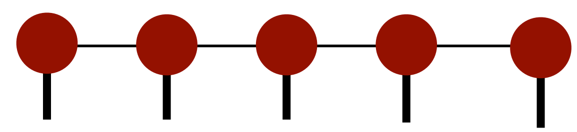
$$e^{-i\delta\mathcal{H}} = e^{-i\delta\mathcal{F}} e^{-i\delta\mathcal{G}} + O(\delta^2)$$



Multiplication of TE operator

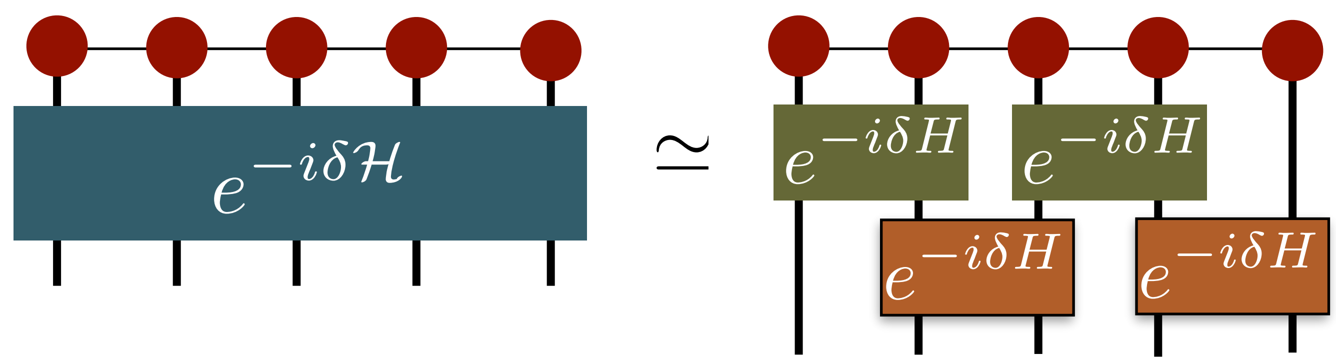
- For MPS representation of wave function

$$|\psi\rangle =$$

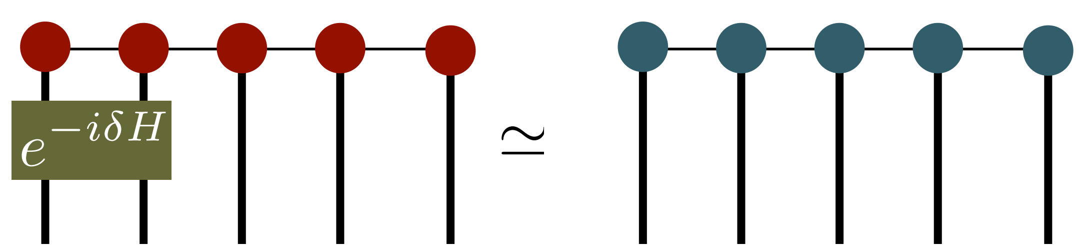


  - multiply time evolution operator using Suzuki Trotter decomposition

$$e^{-i\delta H}|\psi\rangle =$$



- If we can perform an approximate transformation as

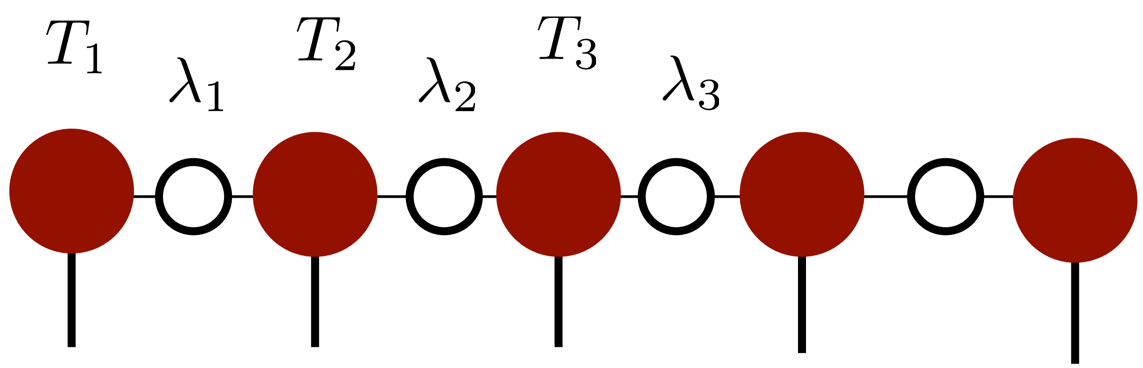


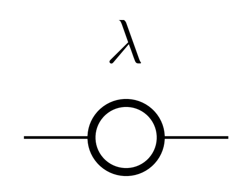
  - we can continue the time evolution repeatedly
  - (we want to keep the bond dimension χ after the time evolution)

Application to the time evolution of a quantum system:
TEBD algorithm

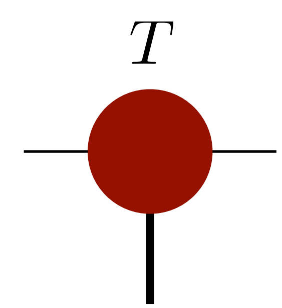
Vidal canonical form

- Another canonical form of MPS (Vidal canonical form)



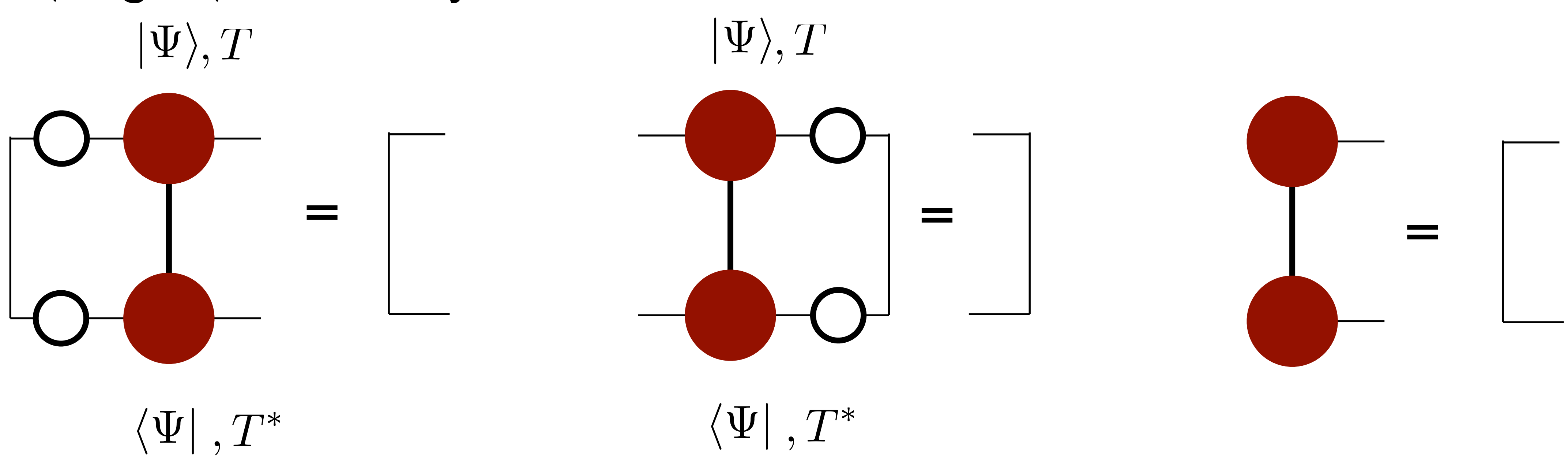


diagonal matrix
corresponding to
Schmidt coefficient



Virtual indices
corresponding to
Schmidt basis

- Left / right / boundary canonical conditions

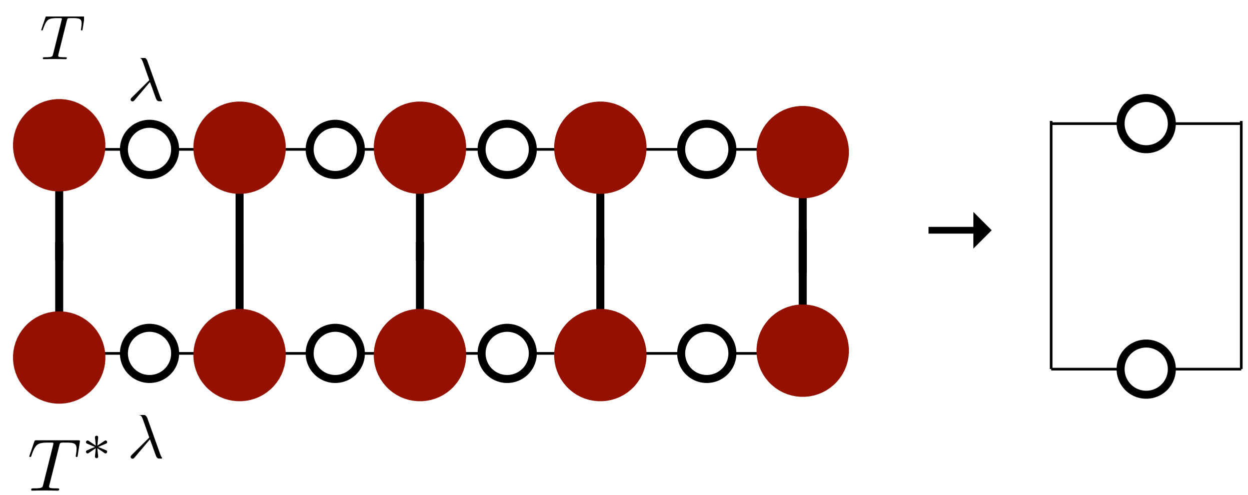


G. Vidal, Phys. Rev. Lett. 91, 147902 (2003)

Expectation values of MPS with canonical form

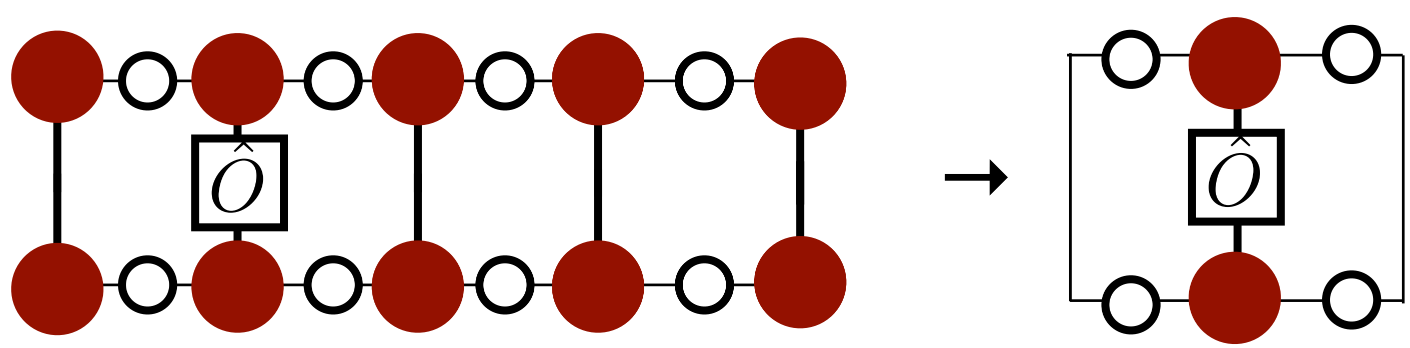
- Evaluation of expectation values becomes extremely simple under canonical condition

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



$$= \sum_i \lambda_i^2 = 1$$

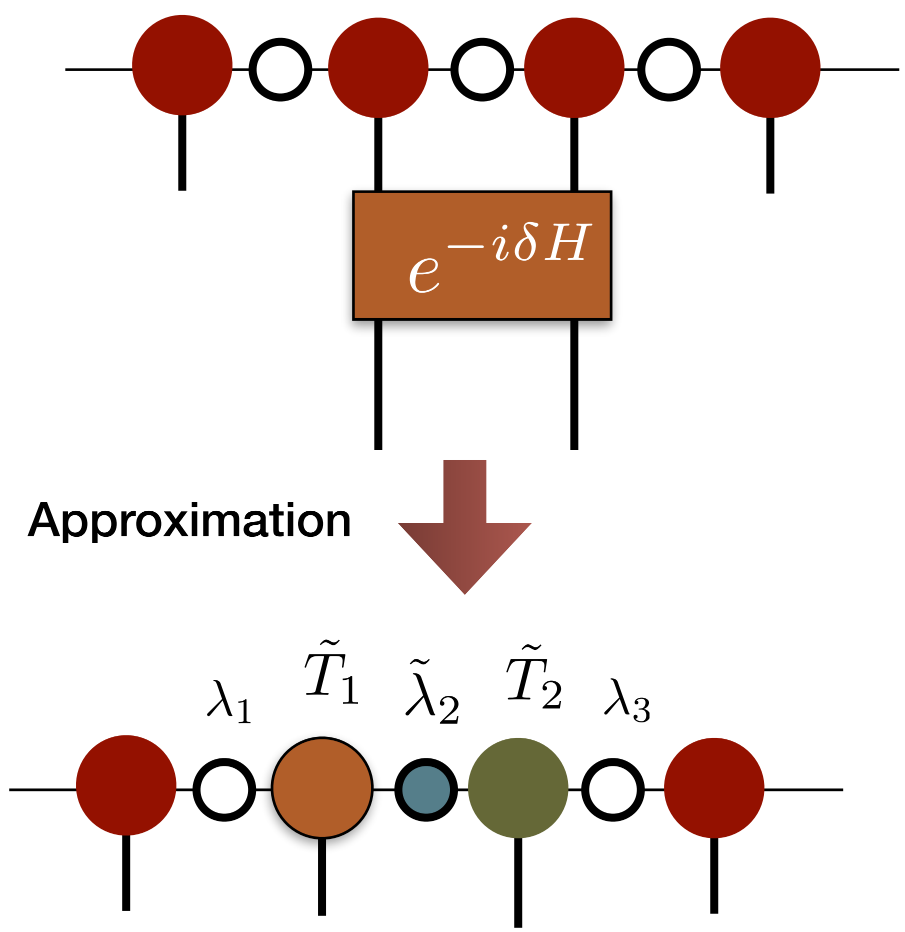
$$\langle \Psi | \hat{O} | \Psi \rangle =$$



- similar simple diagram can also be obtained with mixed canonical form

TEBD algorithm

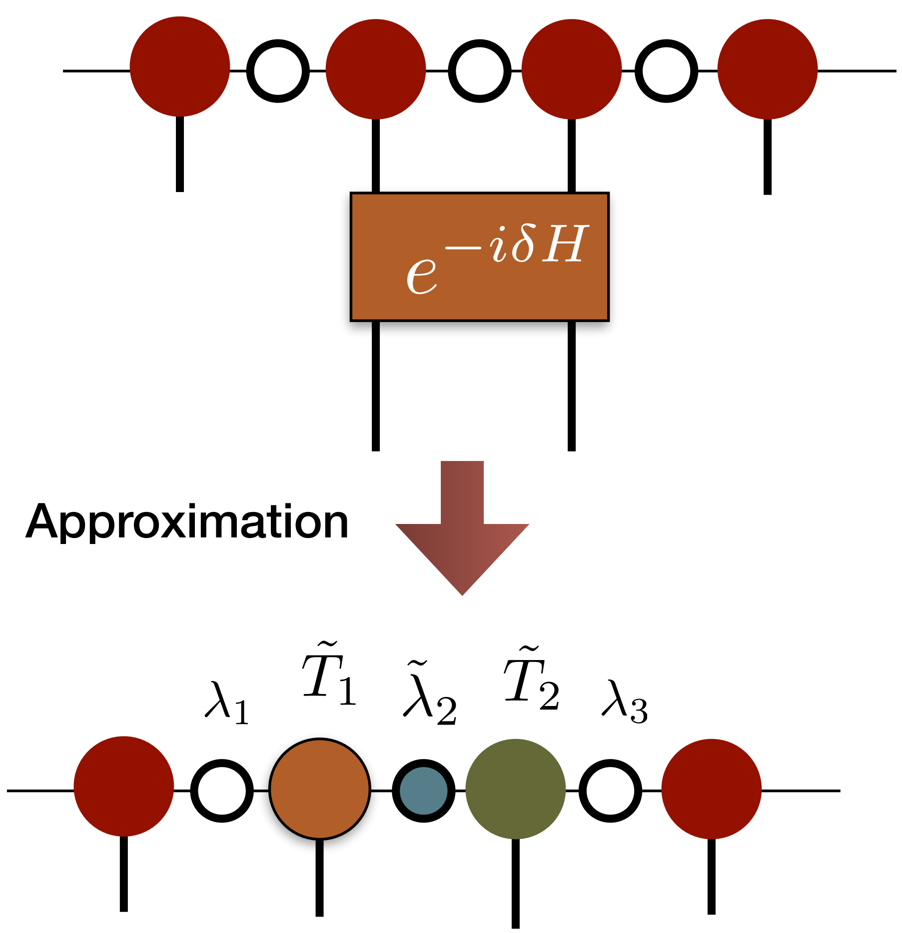
- Time Evolving Block Decimation (TEBD)
  - perform accurate transformation locally by using canonical MPS

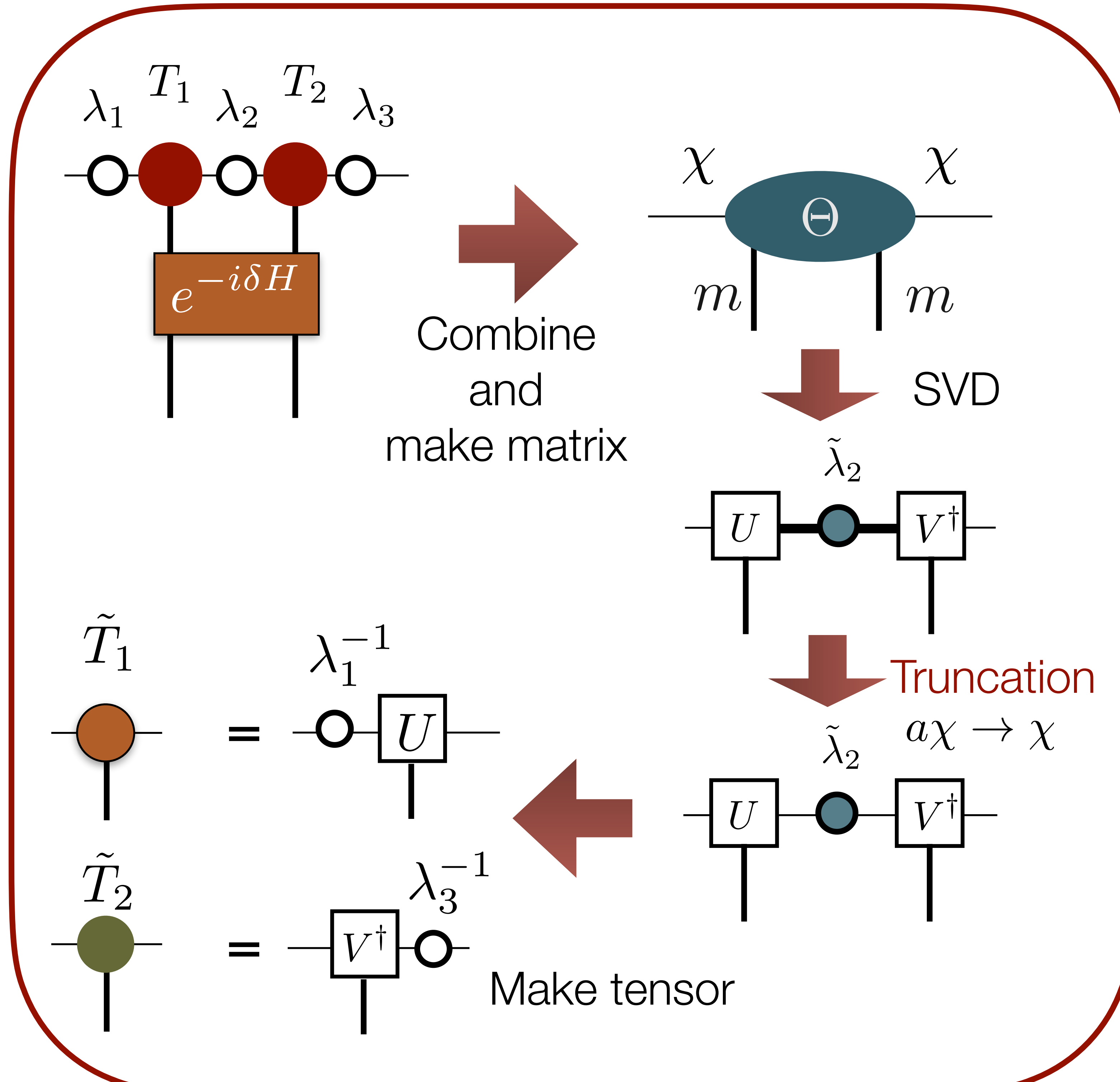


  - only two matrices that are directly applied TE operator change

G. Vidal, Phys. Rev. Lett. 91, 147902 (2003)

TEBD algorithm

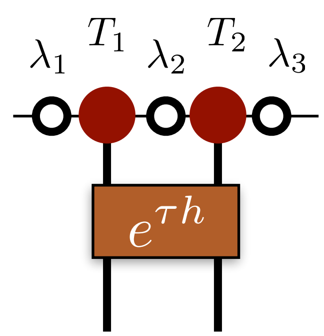




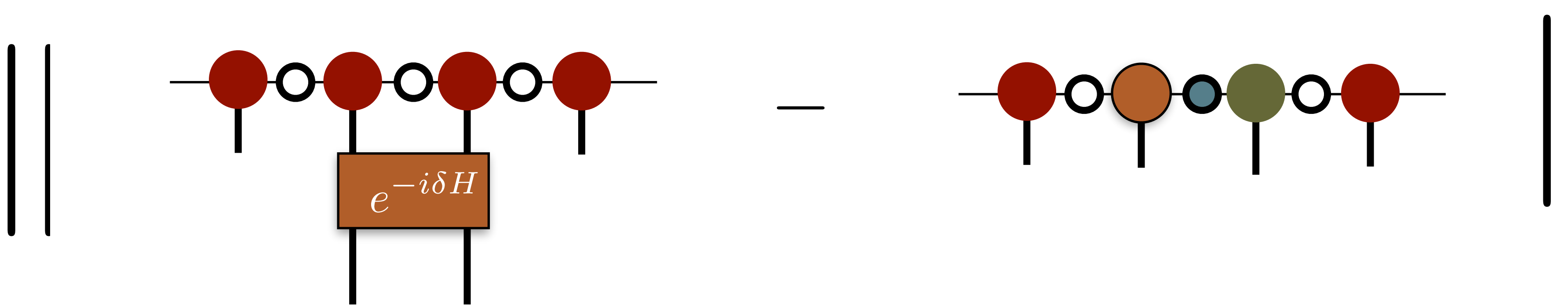
G. Vidal, Phys. Rev. Lett. 91, 147902 (2003)

Why TEBD is accurate?

- For accurate calculation, the canonical form is important
  - If λ is equal to the Schmidt coefficient, it contains all information of the remaining part of the system

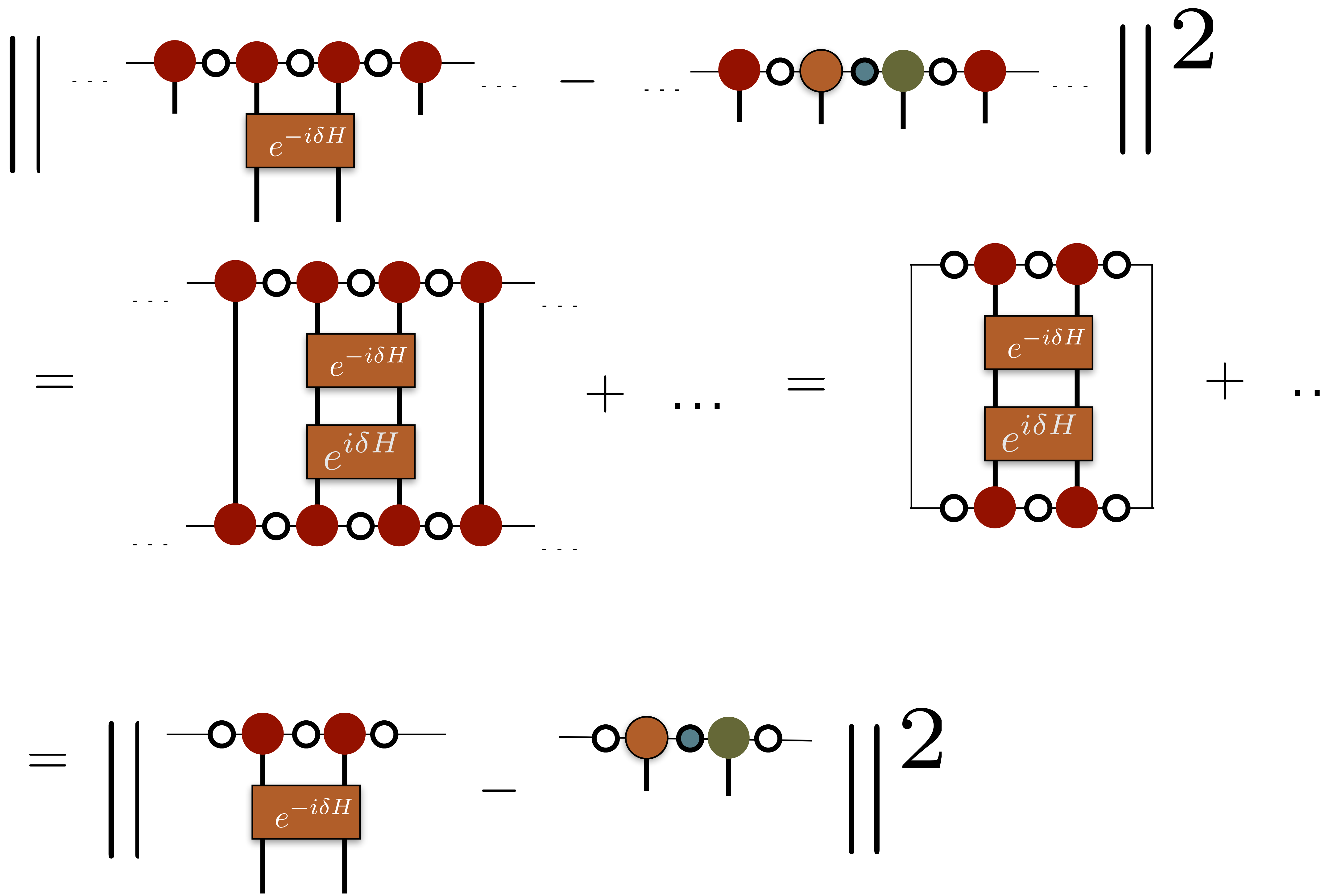


  - due to the canonical form, we can prove that TEBD algorithm minimize the distance of two quantum states:



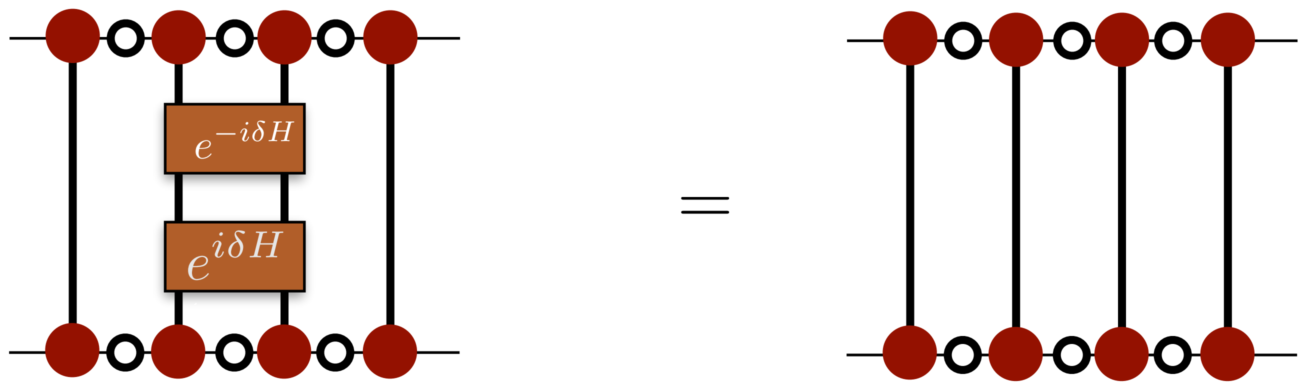
  - truncation based on local SVD can be globally optimal, even if we look at a part of the MPS

Distance between MPS's



Why TEBD is accurate?

- If the operator is unitary, MPS keeps canonical form even after approximation



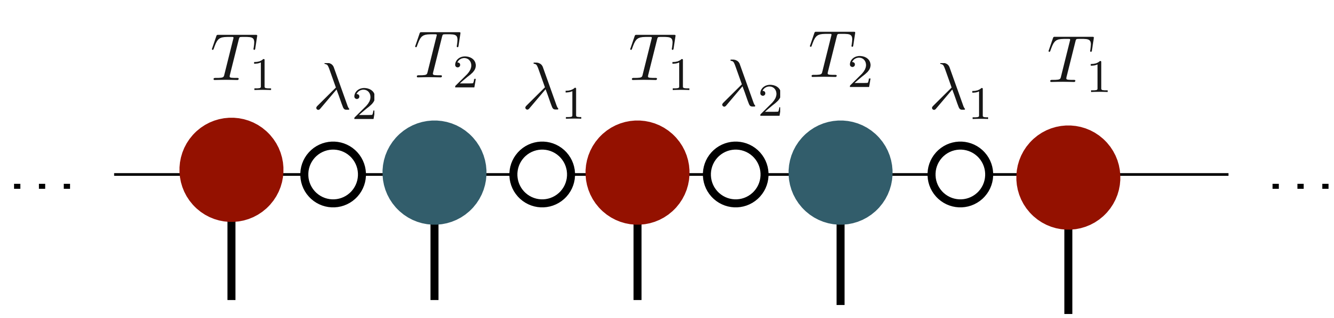
  - Unitary operator does not affect to the other Schmidt coefficients
  - If we choose the initial MPS as the canonical form, TEBD algorithm almost keeps it
  - (So, TEBD is almost “globally optimal”)

Application to the time evolution of a quantum system: iTEBD and (i)TEBD for eigenvalue problems

Extension of TEBD to infinite system

- Finite system: TEBD
  - Sequentially apply TE operators → O(N) SVD for each step
- Infinite system: iTEBD
  - Due to the translational invariance of the system, all SVD's are equivalent → O(1) SVD for each step

- Note
  - Because SVD in TEBD algorithm update two adjacent matrices at the same time, we need at least two independent matrices even in translationally invariant system



(i)TEBD for eigenvalue problem

- Method to optimize MPS for GS of a specific Hamiltonian
  - variational optimization
    - change matrix elements to minimize the energy $$\min_{T,\lambda} \frac{\langle\Psi|\mathcal{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$
  - imaginary time evolution
    - simulate imaginary time evolution (虚時間発展) by (i)TEBD

$$|\Psi_{\mathrm{GS}}\rangle \propto \lim_{\beta\to\infty} e^{-\beta\mathcal{H}}|\Psi_0\rangle$$ for an initial state $\langle\Psi_{\mathrm{GS}}|\Psi_0\rangle \neq 0$

    - by replacing the time evolution operator with the imaginary time evolution operator

$$e^{-i\mathcal{H}t} \to e^{-\tau\mathcal{H}} \quad (t \to -i\tau)$$

    - we can use TEBD (or iTEBD) algorithm for eigenvalue problem

(i)TEBD for eigenvalue problem

- Difference between time evolution and imaginary time evolution
  - time evolution $e^{-i\mathcal{H}t}$: unitary
  - imaginary time evolution $e^{-\mathcal{H}\tau}$: non-unitary
- In general, by multiplying imaginary time evolution operator to MPS, the canonical form is destroyed and TEBD becomes less accurate
  - we have to keep τ small enough so that the canonical property of MPS is kept effectively
  - for small enough τ, TEBD is almost "globally optimal" even in the case of the imaginary time evolution

- Instead, we can transform the MPS into the canonical form after multiplying ITE operator at each step

Notice

- No classes on Nov. 3, Nov. 17, and Nov. 22
- Classes will also be held on Jan. 5 and Jan. 19

Next (Dec. 1)

1. Computational science, quantum computing, and data compression
2. Review of linear algebra
3. Singular value decomposition
4. Application of SVD and generalization to tensors
5. Entanglement of information and matrix product states
6. Application of MPS to eigenvalue problems
7. Tensor network representation
8. Data compression in tensor network
9. Tensor network renormalization
10. Quantum mechanics and quantum computation
11. Simulation of quantum computers
12. Quantum-classical hybrid algorithms and tensor network
13. Quantum error correction and tensor network