

# Selected Topics in Computational Quantum Physics

## 量子物理计算方法选讲

Shuo Yang (杨硕)

*Department of Physics, Tsinghua University*

Email: [shuoyang@tsinghua.edu.cn](mailto:shuoyang@tsinghua.edu.cn)

WeChat: condmat-ys

# Density Matrix Renormalization Group and Matrix Product States

- origin of Density Matrix Renormalization Group method (DMRG)
- many-body entanglement
- traditional DMRG method
- Matrix Product State (MPS) and Matrix Product Operator (MPO)
- MPS algorithms
- various applications

selected review articles:

U. Schollwock, arXiv: 1008.3477

N. Schuch, arXiv: 1306.5551.

F. Verstraete, J.I. Cirac, V. Murg, arXiv: 0907.2796.

# Infinite Time-Evolving Block Decimation method

- we consider the spin-1/2 anti-ferromagnetic Heisenberg chain

$$H = \sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z) = \sum_i \left[ \frac{1}{2} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + S_i^z S_{i+1}^z \right] = \sum_i h_{i,i+1}$$

- we are interested in evaluating the **time evolution** of a quantum state

$$|\psi(t)\rangle = U(t) |\psi(0)\rangle$$

the time evolution operator  $U$  can be either **real time evolution**  $U(t) = \exp(-iHt)$  or **imaginary time evolution**  $U(\tau) = \exp(-H\tau)$

which can be used to **find the ground state**  $|G\rangle = \lim_{\tau \rightarrow \infty} e^{-\tau H} |\psi_0\rangle$

- the Hamiltonian includes odd terms and even terms

$$H = H_{\text{odd}} + H_{\text{even}} = \sum_{i=\text{odd}} h_{i,i+1} + \sum_{i=\text{even}} h_{i,i+1},$$

$H_{\text{odd}}$  ( $H_{\text{even}}$ ) consists of a sum of commuting operators, but  $[H_{\text{odd}}, H_{\text{even}}] \neq 0$

- we may use the **Trotter-Suzuki decomposition**

to the first order  $e^{(V+W)\delta} = e^{V\delta} e^{W\delta} + \mathcal{O}(\delta^2)$

to the second order  $e^{(V+W)\delta} = e^{V\delta/2} e^{W\delta} e^{V\delta/2} + \mathcal{O}(\delta^3)$

# iTEBD method

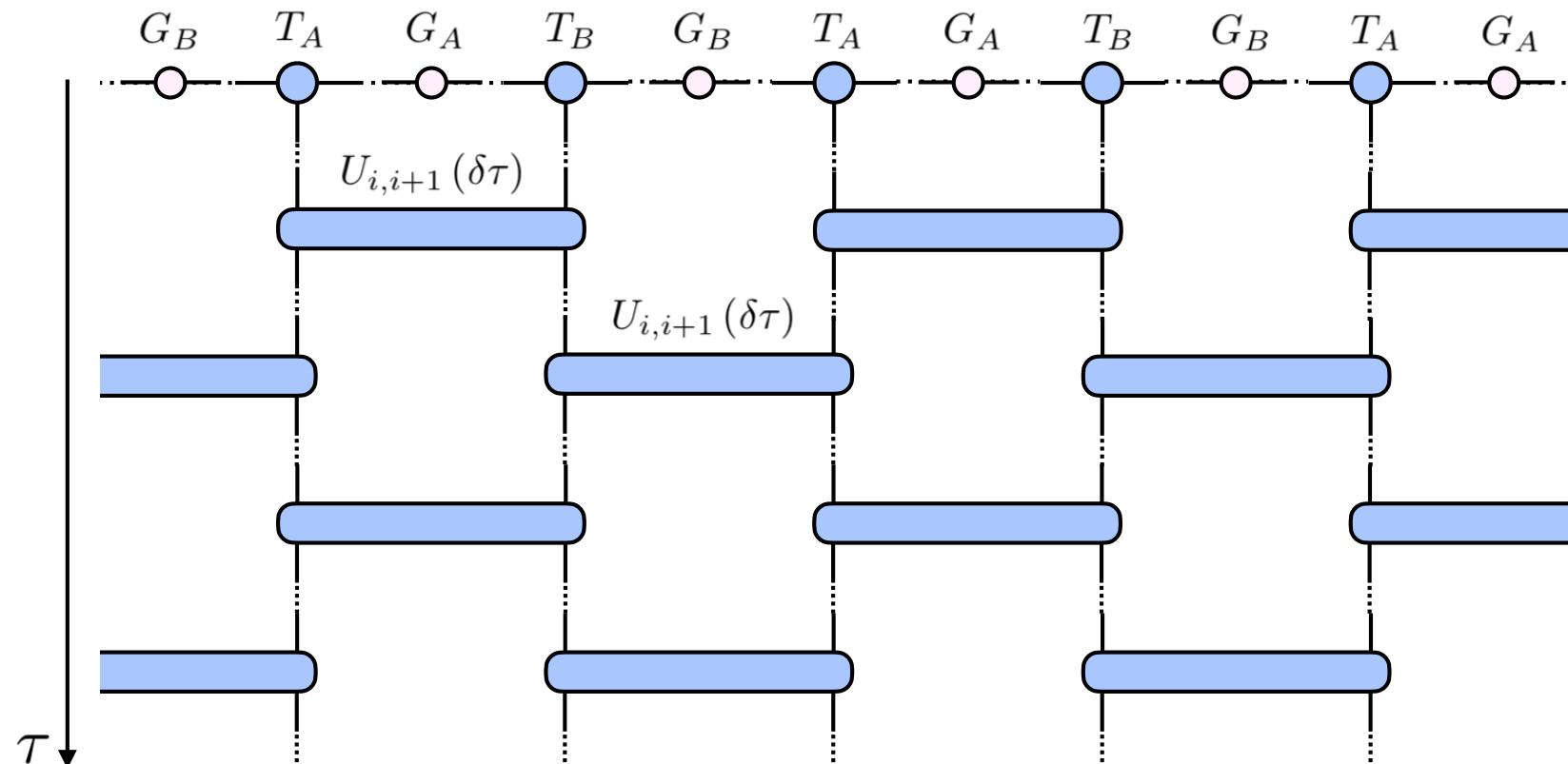
- to the first order, the evolution operator becomes

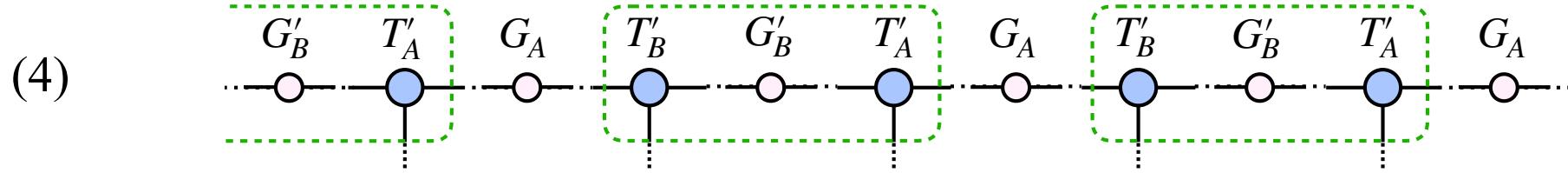
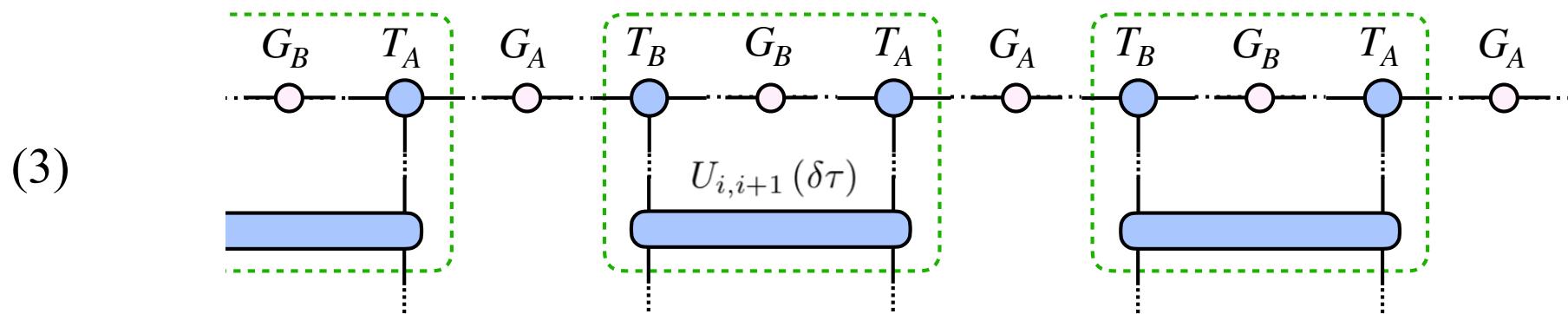
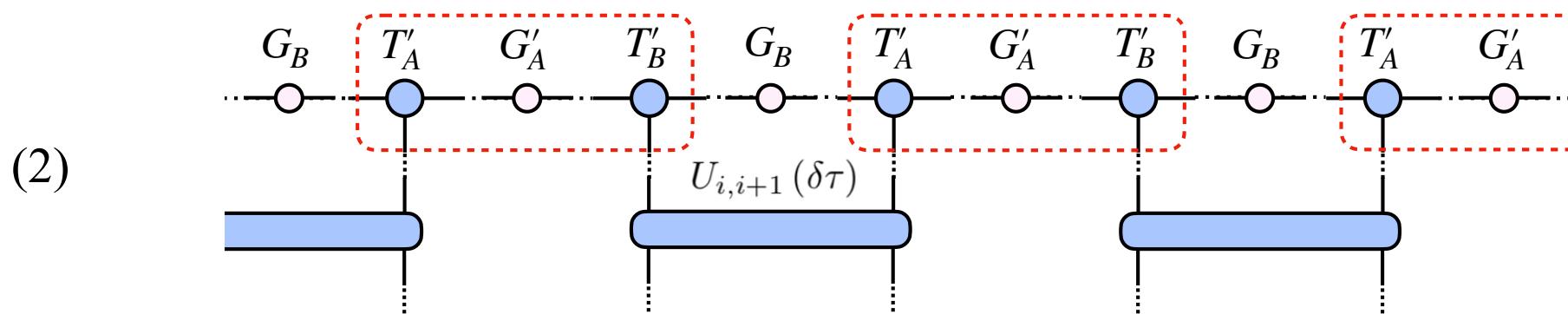
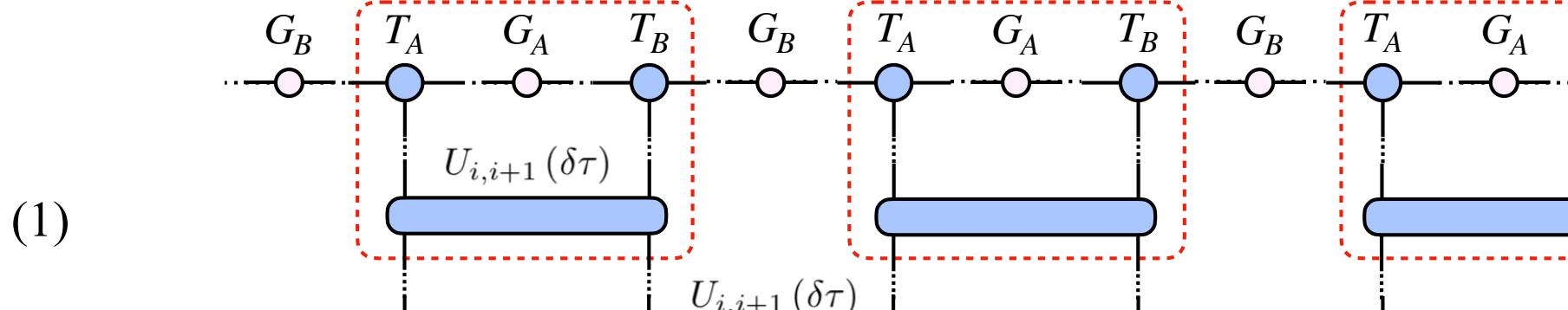
$$U = \prod_{M \rightarrow \infty} U(\delta\tau) = \prod_{M \rightarrow \infty} \left[ \prod_{i=\text{odd}} U_{i,i+1}(\delta\tau) \right] \left[ \prod_{i=\text{even}} U_{i,i+1}(\delta\tau) \right]$$

where

$$U_{i,i+1}(\delta\tau) = e^{-\delta\tau h_{i,i+1}}$$

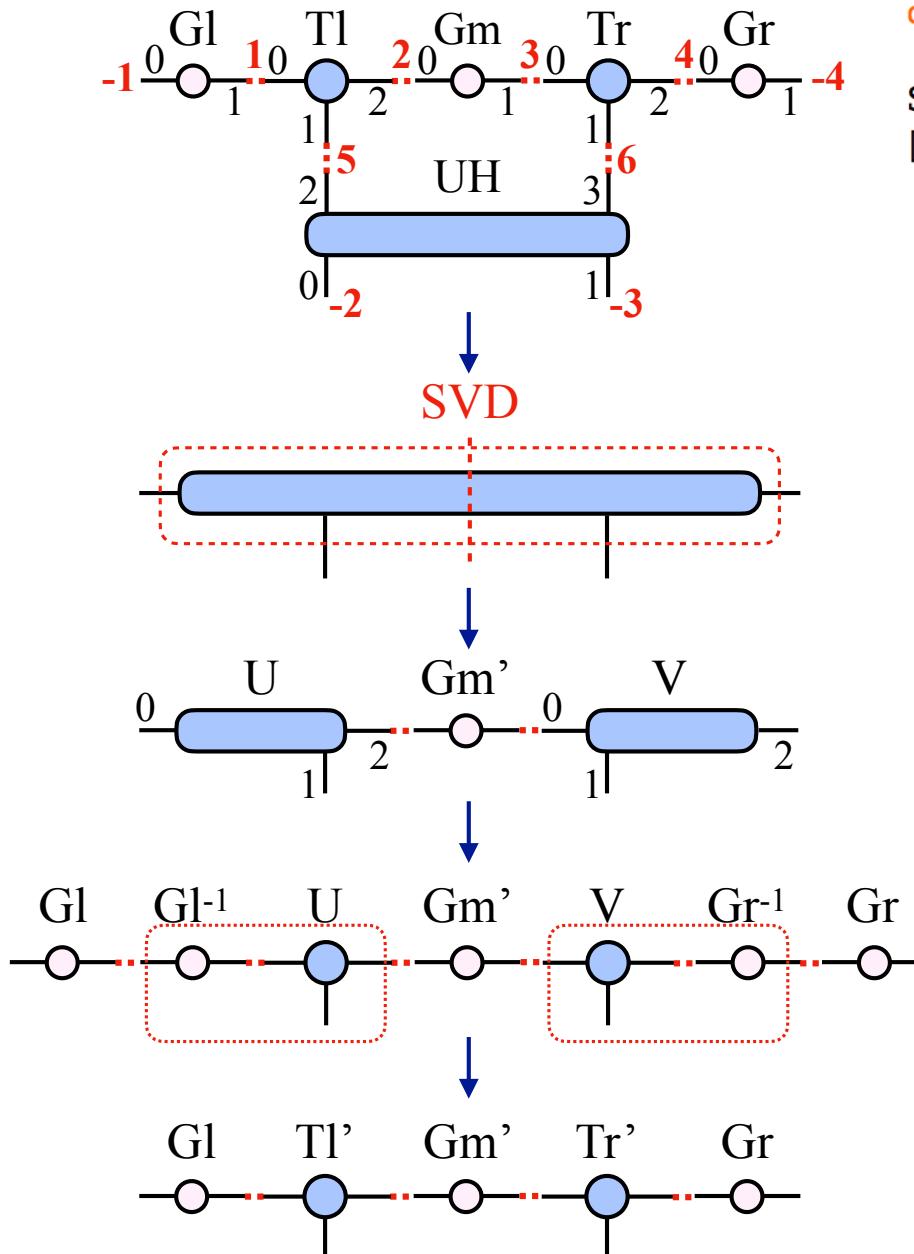
- this decomposition of the time evolution operator is





# iTEBD method

- local update of an MPS



```

def Evo_Bond(Tl,Tr,Gl,Gm,Gr,Ds,UH):
    A =
    Sub.NCon([np.diag(Gl),Tl,np.diag(Gm),Tr,np.diag(Gr),UH],
    [[-1,1],[1,5,2],[2,3],[3,6,4],[4,-4],[-2,-3,5,6]])
    DA = np.shape(A)
    A = Sub.Group(A,[[0,1],[2,3]])

    U,Gm,V,Dc = Sub.SplitSvd_Lapack(A,Ds,0,prec=1.0e-12)
    Gm /= np.sqrt(np.sum(Gm**2))

    U = np.reshape(U,[DA[0],DA[1],Dc])
    Tl = np.tensordot(np.diag(1.0/Gl),U,(1,0))
    V = np.reshape(V,[Dc,DA[2],DA[3]])
    Tr = np.tensordot(V,np.diag(1.0/Gr),(2,0))

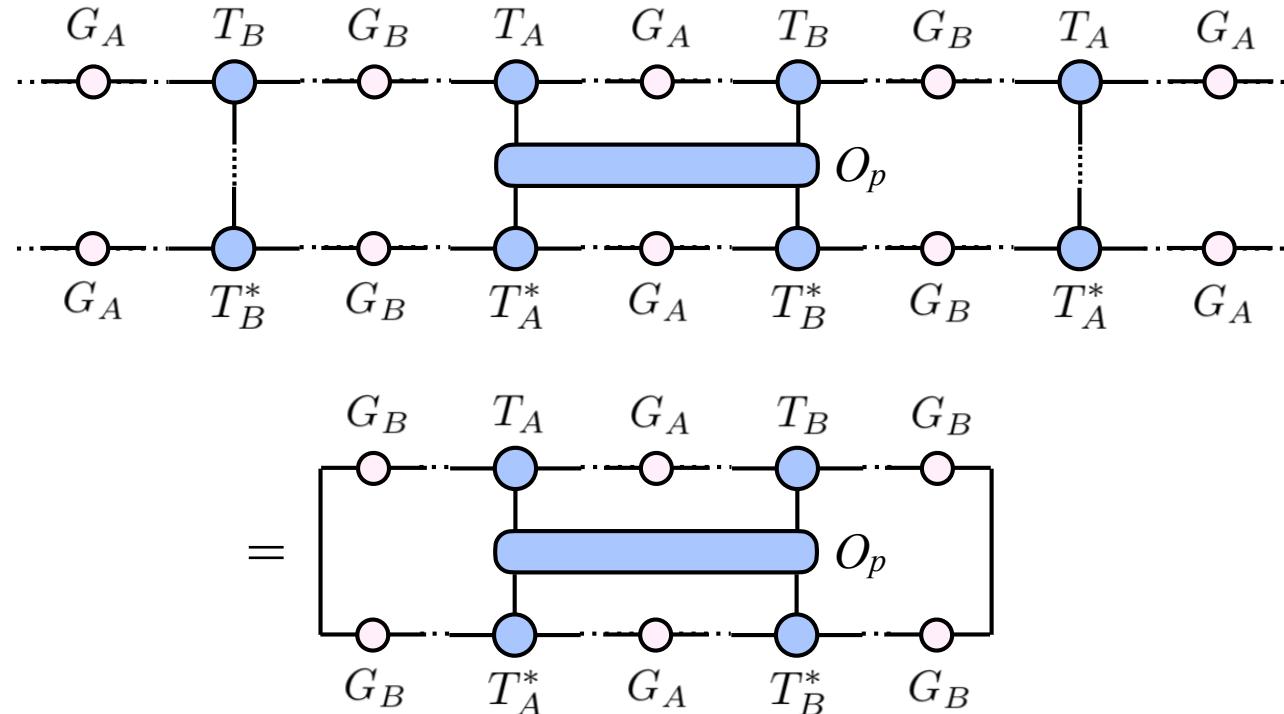
    return Tl,Tr,Gm

```

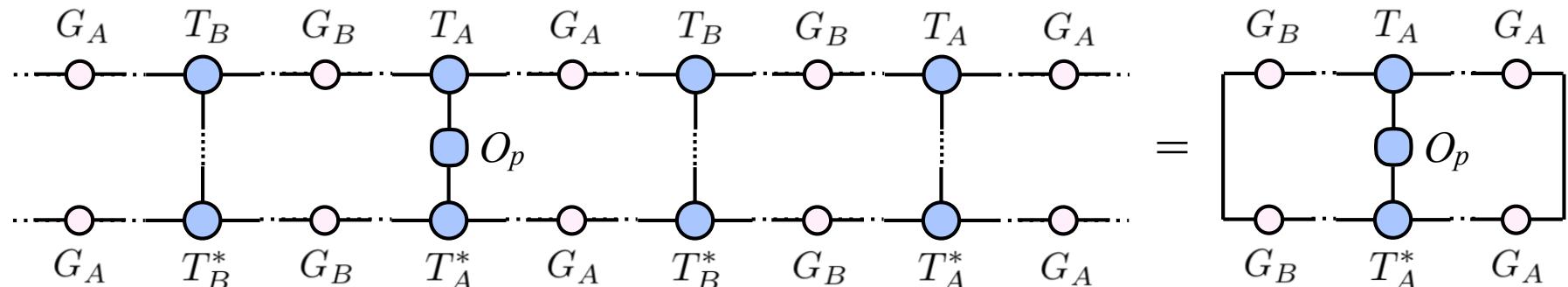
- $T_l$ ,  $G_m$ ,  $T_r$  are updated to new values  
 $G_l$  and  $G_r$  remain the same

# iTEBD method

- calculate physical quantities: two-body operator



- calculate physical quantities: single-body operator



# Homework rules

- this homework has only one task  
please submit through <http://learn.tsinghua.edu.cn>
- please submit the source code and a detailed note including:
  - (1) a brief summary of theory and algorithm
  - (2) the structure and technical details of the code
  - (3) problems encountered and solutions
  - (4) summary of results and your understanding
- deadline is Nov. 24, 23:00  
if you submit after the deadline, you will have less points
- if you are an expert in iTEBD method, this homework may be waived  
please contact me in person and submit something you have done before

# Homework

- read and understand the sample code  
2-site iTEBD method
- consider the 1D spin model with open boundary condition

$$H = \sum_j \left[ -(\sigma_j^x + \sigma_j^z \sigma_{j+1}^z) + g(\sigma_j^x \sigma_{j+1}^z \sigma_{j+2}^z + \sigma_j^z \sigma_{j+1}^z \sigma_{j+2}^x) \right]$$

where  $\sigma^x$ ,  $\sigma^y$  and  $\sigma^z$  are Pauli matrices

- write a code for the 3-site iTEBD method, choose  $D_s = 6$ ,  $g = 0.428$ 
  - (1) calculate the ground state energy  $E$  per site and the magnetization per site  $\langle \sigma_i^z \rangle$  and  $\langle \sigma_i^x \rangle$
  - (2) show the data of entanglement entropy  $S = - \sum_{\alpha} \lambda_{\alpha}^2 \ln \lambda_{\alpha}^2$  and entanglement spectrum  $-\ln \lambda_{\alpha}$ , where  $\lambda_{\alpha}$  are Schmidt weights

# Sample output

- please note the input parameters are **different** from homework

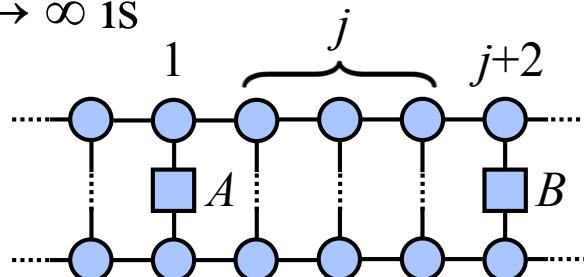
```
Ds=6 g= 1
(1) ground_state_energy_per_site: -1.2477387570215506
(1) sigmax_per_site: [0.76640054 0.76652721 0.76632992]
(1) sigmaz_per_site: [-5.10273065e-14 -1.07240567e-13 -5.39047973e-14]
(2) entanglement_entropy_per_site: [0.30850706 0.30892417 0.30892419]
(2) entanglement_spectrum_energy_per_site: [[0.03917548 1.37737216 2.389807    2.92539298 4.03577772 4.41704344]
[0.0392439 1.37663169 2.38850838 2.92375606 4.03450487 4.41651994]
[0.0392439 1.37663164 2.38850852 2.92375588 4.03450494 4.41651963]]
```

# Grading of this homework

- academic integrity [+50]  
completing assignments independently, creating and expressing your own ideas, DON'T copy answers from others or allow others to copy your answers
- the source code can be executed [+10] and can provide correct results [+10]  
the source code has high readability [+10]
- there is a detailed note file to explain the basic principle, source code and results [+10]  
the note file is well-written and easy to understand [+10]
- did not use the 3-site iTEBD method [-20]
- time-dependent score: after DDL: [-1 per day]
- self-motivation score: new ideas or extra results [+10]

# Transfer operator and correlation length

- we consider a uniform MPS  
the **correlation function** between operator  $A$  at site 1 and  $B$  at site  $j+2$  on a chain of length  $N \rightarrow \infty$  is

$$\langle A_1 B_{j+2} \rangle = \text{Tr} [\mathbb{E}_A \mathbb{E}^j \mathbb{E}_B \mathbb{E}^{N-j-2}] / \text{Tr} [\mathbb{E}^N]$$


where

$$\begin{aligned} \mathbb{E}_A &= \begin{array}{c} \text{---} \\ | \quad \quad \quad | \\ \text{---} \end{array} \\ \mathbb{E}_A &= \begin{array}{c} \text{---} \\ | \quad \quad \quad | \\ \text{---} \\ \text{---} \\ | \\ \text{---} \end{array} \end{aligned}$$

$$\begin{aligned} \mathbb{E}_B &= \begin{array}{c} \text{---} \\ | \quad \quad \quad | \\ \text{---} \\ \text{---} \\ | \\ \text{---} \end{array} \\ \mathbb{E}_B &= \begin{array}{c} \text{---} \\ | \quad \quad \quad | \\ \text{---} \\ | \\ \text{---} \end{array} \end{aligned}$$

$$\begin{aligned} \mathbb{E} &= \begin{array}{c} \text{---} \\ | \quad \quad \quad | \\ \text{---} \\ | \\ \text{---} \end{array} \\ \mathbb{E} &= \begin{array}{c} \text{---} \\ | \quad \quad \quad | \\ \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{array} \end{aligned}$$

- we assume  $\mathbb{E}$  has a unique maximal eigenvalues  $\lambda_1$ , which we normalize to  $\lambda_1 = 1$   
 $\mathbb{E} |r\rangle = |r\rangle$ ,  $\langle l| \mathbb{E} = \langle l|$ , for large  $N$ ,  $\mathbb{E}^N \rightarrow |r\rangle \langle l|$

we now expand  $\mathbb{E}^j = |r\rangle \langle l| + \sum_{k \geq 2} \lambda_k^j |r_k\rangle \langle l_k|$

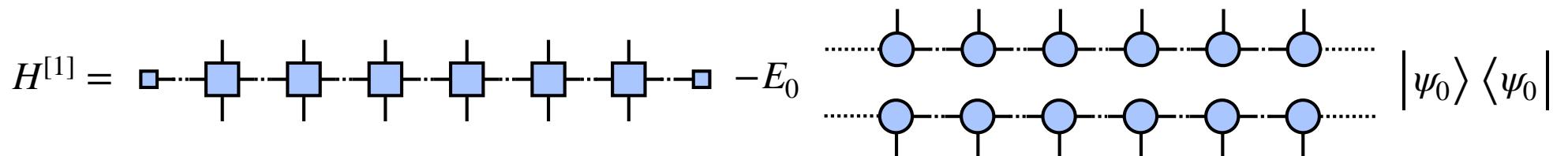
we find that  $\langle A_1 B_{j+2} \rangle = \langle l| \mathbb{E}_A |r\rangle \langle l| \mathbb{E}_B |r\rangle + \sum_{k \geq 2} \lambda_k^j \langle l| \mathbb{E}_A |r_k\rangle \langle l_k| \mathbb{E}_B |r\rangle$

and thus decays exponentially with  $j$ ,  $\langle A_1 B_{j+2} \rangle = e^{-j/\xi}$

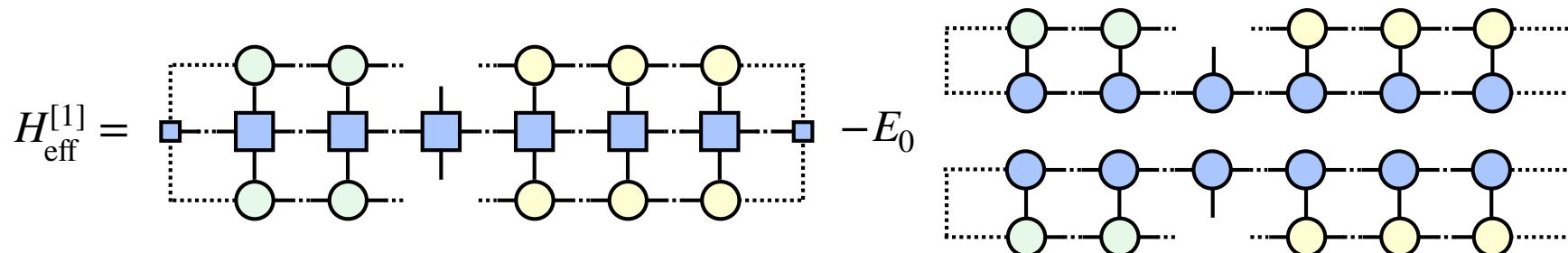
the **correlation length** is given by  $\xi = -1/\ln |\lambda_2|$

# Variational MPS for excited states

- suppose we have found out the ground state of  $H$ ,  $H |\psi_0\rangle = E_0 |\psi_0\rangle$
- we may construct  $H^{[1]} = H - E_0 |\psi_0\rangle \langle \psi_0|$   
the ground state of  $H^{[1]}$  is the first excited state of  $H$



- we construct **effective projector** at every site



- similarly, we construct  $H^{[2]} = H - E_0 |\psi_0\rangle \langle \psi_0| - E_1 |\psi_1\rangle \langle \psi_1|$   
the ground state of  $H^{[2]}$  is the second excited state of  $H$

# Quasiparticle ansatz for excitations

- consider a finite 1D spin chain of length  $N$  with open boundary conditions  
the optimal MPS approximation for the **ground state** can be found using  
the standard sweeping algorithm

$$|\Psi(A_1 \dots A_N)\rangle = \boxed{A_1^l} - \boxed{A_2^l} - \dots - \boxed{A_i^c} - \dots - \boxed{A_N^r}$$

- inspired by the success of the quasiparticle ansatz in the thermodynamic limit, we propose a similar ansatz for **excited states**

$$|\Phi(B_1, \dots, B_N)\rangle = \sum_i \boxed{A_1^l} - \dots - \boxed{B_i} - \dots - \boxed{A_N^r}$$

- to ensure the orthogonality of eigenstates,  $B_i$  lives in the null space of  $(A_i^l)^\dagger$   
the  $V_i$  tensor satisfies the conditions

$$-\boxed{B_i} = -\boxed{V_i} - \boxed{X_i}$$

$$\circlearrowleft \begin{array}{c} \boxed{V_i} \\ \downarrow \\ \boxed{\bar{A}_i^l} \end{array} = 0$$

$$\circlearrowleft \begin{array}{c} \boxed{V_i} \\ \downarrow \\ \boxed{\bar{V}_i} \end{array} = \circlearrowright$$

- see the following reference for details

M. Van Damme, R. Vanhove, J. Haegeman, F. Verstraete, and L. Vanderstraeten,  
Phys. Rev. B **104**, 115142 (2021)

# Excitation ansatz with OBC MPS

- we work in the MPO-representation of the Hamiltonian  
we will need the partially contracted environments of the state

$$\begin{aligned}
 \rho_{n+1}^l &= \rho_n^l \circledcirc O \circledast \bar{A}_n^l, & \rho_{n-1}^r &= A_n^r \circledast O \circledcirc \rho_n^r, \\
 \rho_{n+1}^{B,l} &= \rho_n^l \circledcirc B_n \circledast \bar{A}_n^l + \rho_n^{B,l} \circledcirc O \circledast \bar{A}_n^l, & \rho_{n-1}^{B,r} &= B_n \circledast O \circledcirc \rho_n^r + A_n^l \circledast O \circledcirc \rho_n^{B,r}.
 \end{aligned}$$

- all these quantities together make  $H_{\text{eff}}(\vec{X})$  take on a pleasant form  
for every site  $i$ , one calculate the following tensor  $T_i$  to get the derivative with respect to the tensor  $B'_i$

$$T_i = \rho_i^{B,l} \circledcirc A_i^r \circledast \rho_i^r + B_i \circledast O \circledcirc \rho_i^r + A_i^l \circledast O \circledcirc \rho_i^{B,r}.$$

# Excitation ansatz with OBC MPS

- $X'_i$  tensors can then be extracted by projecting down on  $V_i$

- the full action of  $H_{\text{eff}}$  is  $\vec{X}'_i = \sum_j (H_{\text{eff}})_{ij} \vec{X}_j$

the eigenvalue problem  $\sum_j (H_{\text{eff}})_{ij} \vec{X}_j = \omega \vec{X}_i$  can be solved iteratively

$$X'_i = \begin{array}{c} T \\ \square \\ \swarrow \curvearrowright \searrow \\ V_i \end{array} .$$

---

## Algorithm 1 Pseudocode for the action of $H_{\text{eff}}(\vec{X})$

---

```

1: Inputs  $(\vec{X}, \rho^l, \rho^r)$ 
2:  $\vec{X}' \leftarrow 0, \rho^{B,l} \leftarrow 0, \rho^{B,r} \leftarrow 0$                                 ▷ initialization
3: for  $i \in [1, \text{len}(\vec{X})]$  do                                              ▷ environments
4:     calculate  $\rho_{i+1}^{B,l}$  (A5)
5:     calculate  $\rho_{\text{end}-i}^{B,r}$  (A6)
6: for  $i \in [1, \text{len}(\vec{X})]$  do
7:     calculate  $T_i$  (A7)
8:     calculate  $X'_i$  (A8)
9: return  $\vec{X}'$ 

```

---

- this algorithm is simple, straightforward to implement, and requires similar contractions as in usual DMRG codes

# Multi-target MPS

- ground state

$$\psi_0 = \begin{array}{c} \sigma_1 \quad \sigma_i \quad \sigma_{i+1} \quad \sigma_L \\ | \quad | \quad | \quad | \\ \textcircled{C} \\ \hbox{\scriptsize A}_1 \quad \cdots \quad \hbox{\scriptsize A}_i \quad \hbox{\scriptsize B}_{i+1} \quad \cdots \quad \hbox{\scriptsize B}_L \end{array} .$$

- excited states

$$\psi_m = \begin{array}{c} \sigma_1 \quad \sigma_i \quad \sigma_{i+1} \quad \sigma_L \\ | \quad | \quad | \quad | \\ \textcircled{C} \\ \hbox{\scriptsize A}^1 \quad \cdots \quad \hbox{\scriptsize A}^i \quad \hbox{\scriptsize B}^{i+1} \quad \cdots \quad \hbox{\scriptsize B}^L \\ \hbox{\scriptsize m} \end{array} .$$

- canonical center at site  $i$

$$\begin{array}{c} \textcircled{C}^i \\ \hbox{\scriptsize m} \end{array} = \begin{array}{c} | \\ \text{---} \\ \boxed{A^i} \\ | \\ \textcircled{C} \\ \hbox{\scriptsize m} \end{array} .$$

$$\psi_m = \begin{array}{c} \sigma_1 \quad \sigma_{i-1} \quad \sigma_i \quad \sigma_{i+1} \quad \sigma_L \\ | \quad | \quad | \quad | \quad | \\ \textcircled{C}^i \\ \hbox{\scriptsize A}^1 \quad \cdots \quad \hbox{\scriptsize A}^{i-1} \quad \hbox{\scriptsize m} \quad \hbox{\scriptsize B}^{i+1} \quad \cdots \quad \hbox{\scriptsize B}^L \\ \hbox{\scriptsize m} \end{array} .$$

- applying the local projection operator  $\exp(-\tau H_{i,i+1})$  changes  $\psi_m$  to

$$\psi'_m = \begin{array}{c} \sigma_1 \quad \sigma_{i-1} \quad \sigma_i \quad \sigma_{i+1} \sigma_{i+2} \quad \sigma_L \\ | \quad | \quad | \quad | \quad | \\ \textcircled{T} \\ \hbox{\scriptsize A}^1 \quad \cdots \quad \hbox{\scriptsize A}^{i-1} \quad \hbox{\scriptsize m} \quad \hbox{\scriptsize B}^{i+2} \quad \cdots \quad \hbox{\scriptsize B}^L \end{array} ,$$

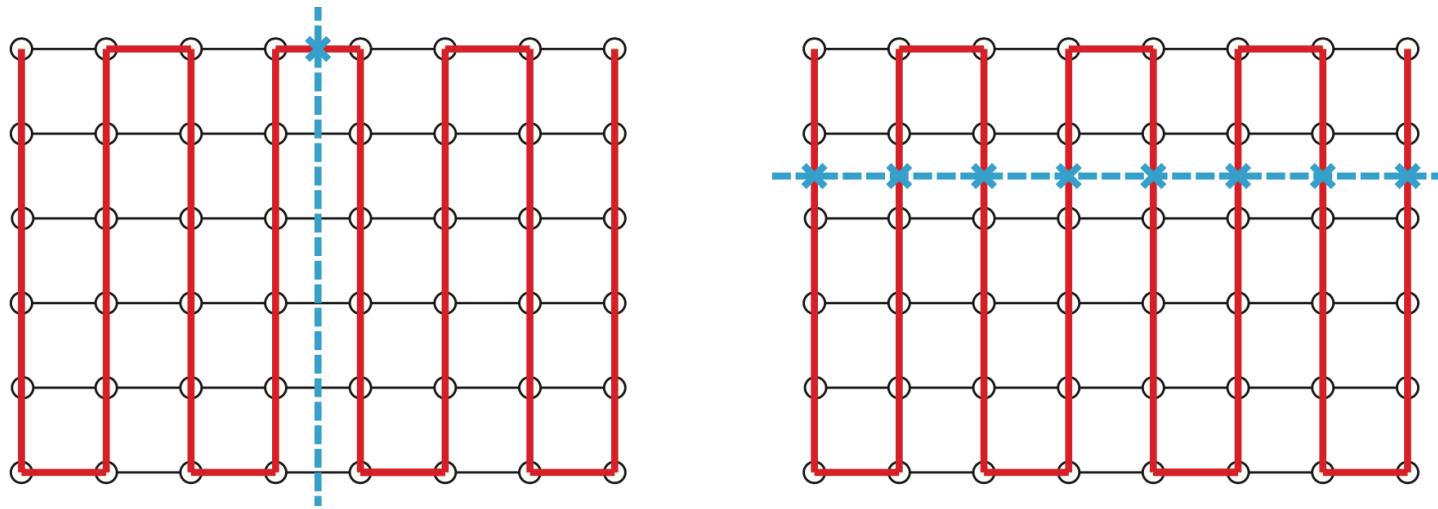
$$\begin{array}{c} | \\ \text{---} \\ \boxed{T} \\ \hbox{\scriptsize m} \end{array} = \begin{array}{c} | \\ \text{---} \\ \textcircled{C}^i \\ \hbox{\scriptsize m} \end{array} \quad \boxed{e^{-\tau H_{i,i+1}}} \quad \begin{array}{c} | \\ \text{---} \\ \textcircled{B}^{i+1} \end{array}$$

- take a QR decomposition to decouple  $T$

$$\begin{array}{c} | \\ \text{---} \\ \boxed{T} \\ \hbox{\scriptsize m} \end{array} = \begin{array}{c} | \quad | \\ \text{---} \quad \text{---} \\ \textcircled{\sigma_i} \quad \textcircled{\sigma_{i+1}} \\ \hbox{\scriptsize A}^i \quad \hbox{\scriptsize m} \end{array} \approx \begin{array}{c} | \quad | \\ \text{---} \quad \text{---} \\ \textcircled{\sigma_i} \quad \textcircled{\sigma_{i+1}} \\ \hbox{\scriptsize A}^i \quad \hbox{\scriptsize m} \end{array} \quad \begin{array}{c} | \\ \text{---} \\ \textcircled{\tilde{C}^{i+1}} \end{array} .$$

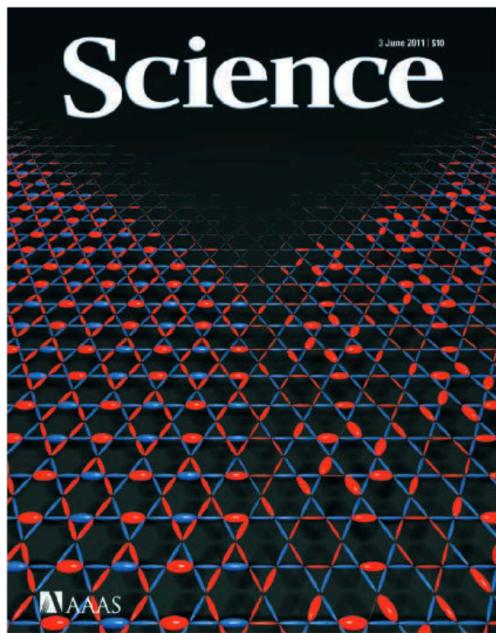
# DMRG in two dimensions

- 2D DMRG setup: the 2D lattice is explored by a 1D snake-shape MPS  
horizontal interactions become long-ranged



- **problem:** encoding the entanglement of vertically separated bi-partitions of the system becomes exponentially expensive
- **vertical cut** is crossed by the snake only once, we need MPS of huge dimension
- **horizontal cut** is crossed by the snake  $L$  times, each virtual bond has dimension  $D$   
we can encode entanglement  $S = L \ln D$

# Example of DMRG in two dimensions



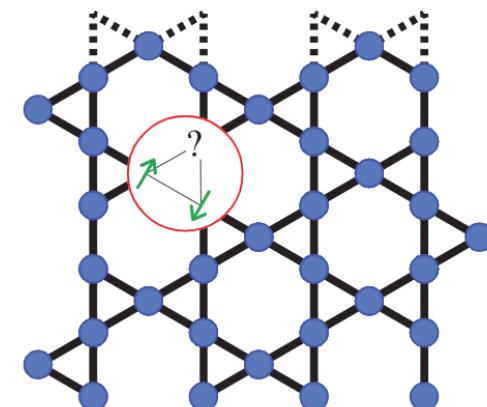
## Spin-Liquid Ground State of the $S = 1/2$ Kagome Heisenberg Antiferromagnet

Simeng Yan,<sup>1</sup> David A. Huse,<sup>2,3</sup> Steven R. White<sup>1\*</sup>

We use the density matrix renormalization group to perform accurate calculations of the ground state of the nearest-neighbor quantum spin  $S = 1/2$  Heisenberg antiferromagnet on the kagome lattice. We study this model on numerous long cylinders with circumferences up to 12 lattice spacings. Through a combination of very-low-energy and small finite-size effects, our results provide strong evidence that, for the infinite two-dimensional system, the ground state of this model is a fully gapped spin liquid.

### COVER

Three possible phases of the kagome Heisenberg antiferromagnet, a model of geometrically “frustrated” magnetism: the diamond-pattern valence bond crystal (lower left), honeycomb valence bond crystal (lower right), and quantum spin liquid (upper empty wedge). Deviations of bond strengths from their average values are shown by bond widths and colors (red, stronger; blue, weaker). The simulations of Yan *et al.* (p. 1173) show that the true ground-state phase is the quantum spin liquid.



S. Yan, D. A. Huse, S. R. White, Science 322, 1174 (2011).

# Example of DMRG in two dimensions

- solving the Hubbard model with DMRG

$$H = -\sum_{ij\sigma} t_{ij} (\hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} + h.c.) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

SUPERCONDUCTIVITY

## Superconductivity in the doped Hubbard model and its interplay with next-nearest hopping $t'$

Hong-Chen Jiang<sup>1\*</sup> and Thomas P. Devereaux<sup>1,2</sup>

The Hubbard model is widely believed to contain the essential ingredients of high-temperature superconductivity. However, proving definitively that the model supports superconductivity is challenging. Here, we report a large-scale density matrix renormalization group study of the lightly doped Hubbard model on four-leg cylinders at hole doping concentration  $\delta = 12.5\%$ . We reveal a delicate interplay between superconductivity and charge density wave and spin density wave orders tunable via next-nearest neighbor hopping  $t'$ . For finite  $t'$ , the ground state is consistent with a Luther-Emery liquid with power-law superconducting and charge density wave correlations associated with half-filled charge stripes. In contrast, for  $t' = 0$ , superconducting correlations fall off exponentially, whereas charge density and spin density modulations are dominant. Our results indicate that a route to robust long-range superconductivity involves destabilizing insulating charge stripes in the doped Hubbard model.

H.-C. Jiang and T. P. Devereaux, Science 365, 1424–1428 (2019).

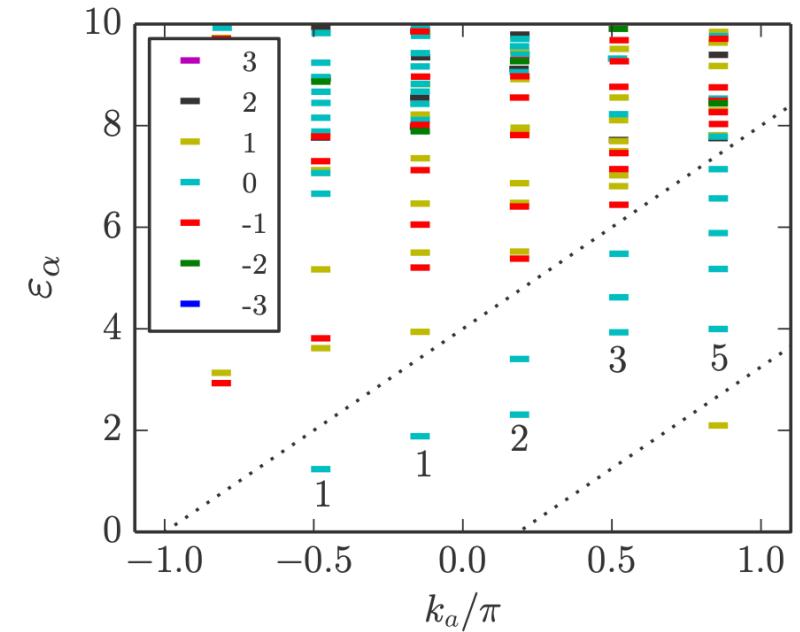
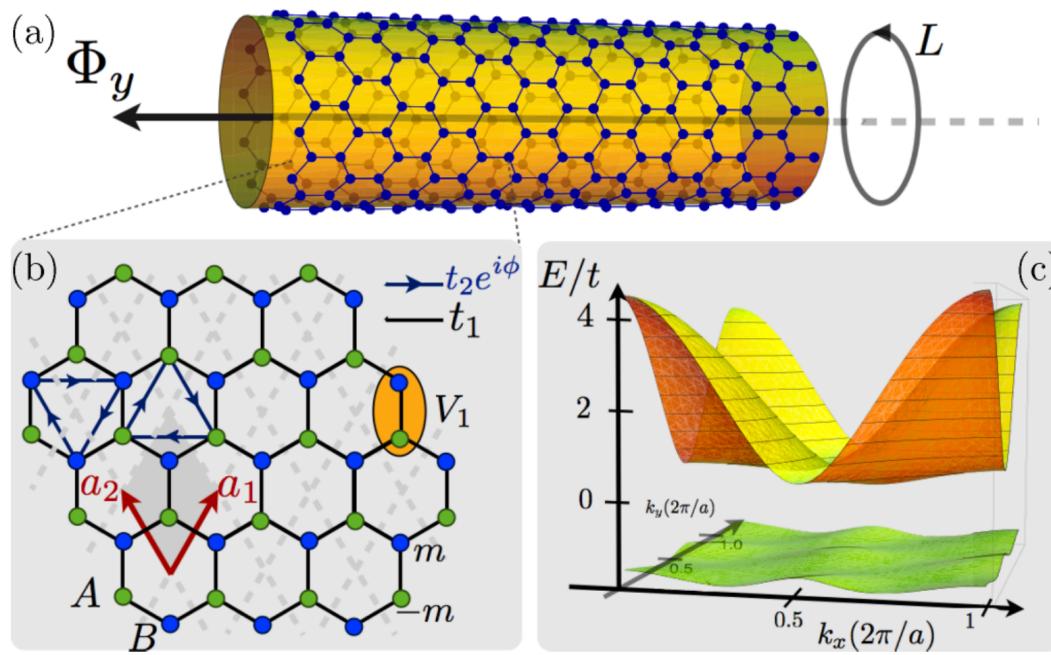
# Example of DMRG in two dimensions

- fractional Chern insulators  
the Haldane model for spinless fermions with nearest-neighbor interactions, 1/3 filling

$$H = H_0 + H_V,$$

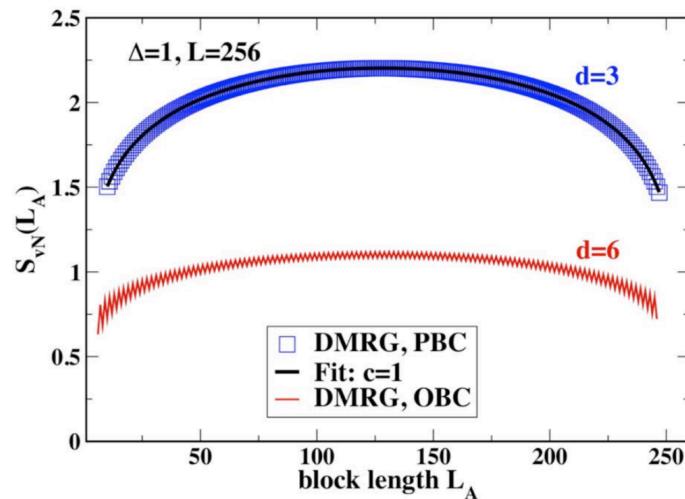
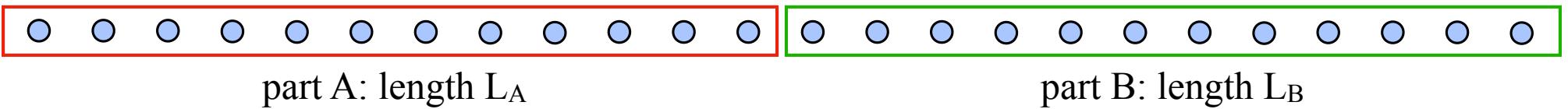
$$H_0 = - \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_i m(n_{A,i} - n_{B,i}),$$

$$H_V = V_1 \sum_{\langle ij \rangle} n_{A,i} n_{B,j}.$$



# Applications of MPS/DMRG

- critical systems in 1D: Heisenberg chain, Luttinger Liquid phase, ...  
measure entanglement entropy & central charge



$$S_{vN} = - \text{tr}(\rho_A \log_2 \rho_A)$$

$$S_{vN}(L_A) = \frac{c}{d} \ln \left[ \frac{N}{\pi} \sin \left( \frac{\pi L_A}{N} \right) \right] + c'$$

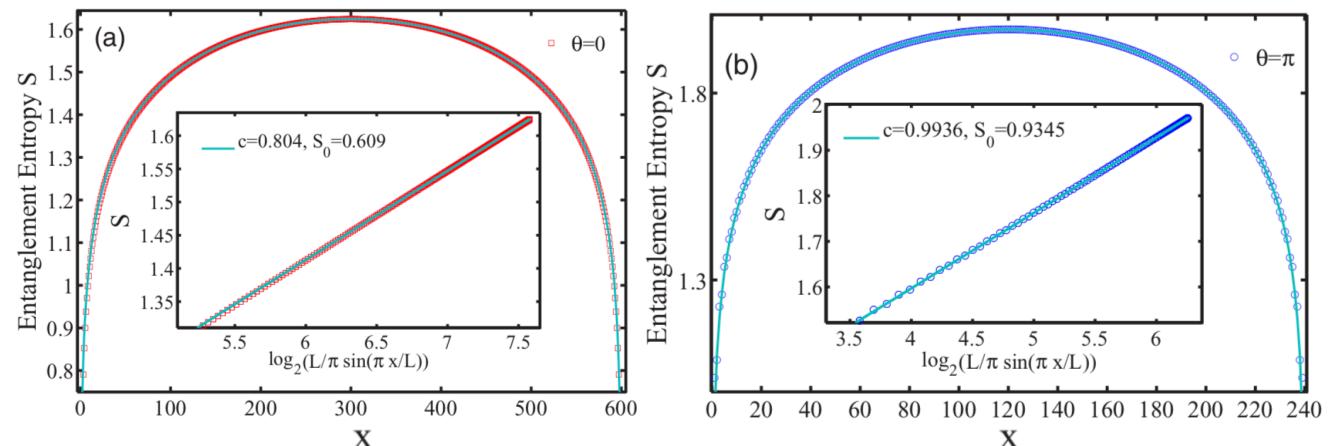
fit central charge  $c$

C. Holzhey et al., Nucl. Phys. B 424, 443 (1994).  
G. Vidal et al., PRL 90, 227902 (2003).  
P. Calabrese and J. Cardy, J. Phys. A 42, 504005 (2009).

- example

W. Li, S. Yang, H.-H. Tu, and M. Cheng, PRB 91, 115133 (2015).

FIG. 2. (Color online) Block entanglement entropy of the  $\mathbb{Z}_3$  FM( $\theta = 0$ ) and AF( $\theta = \pi$ ) Potts model. (a)  $\theta = 0$  with  $c = \frac{4}{5}$  and (b)  $\theta = \pi$  with  $c = 1$ . Open boundary conditions are adopted in both cases.

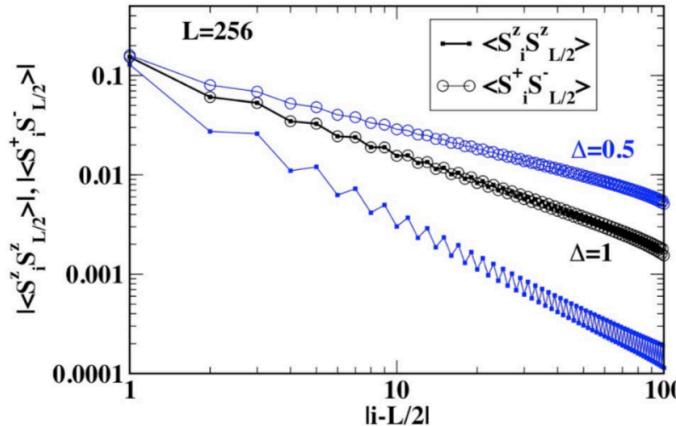


# Applications of MPS/DMRG

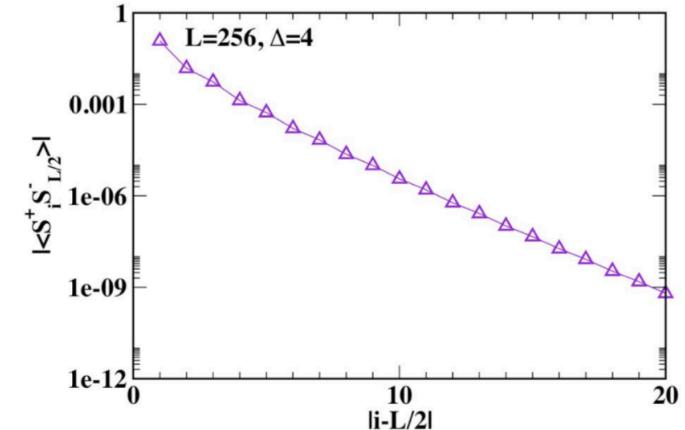
- correlation function

$$H = J \sum_{i=1}^L \left[ \frac{1}{2} (S_i^+ S_{i+1}^- + h.c.) + \Delta S_i^z S_{i+1}^z \right]$$

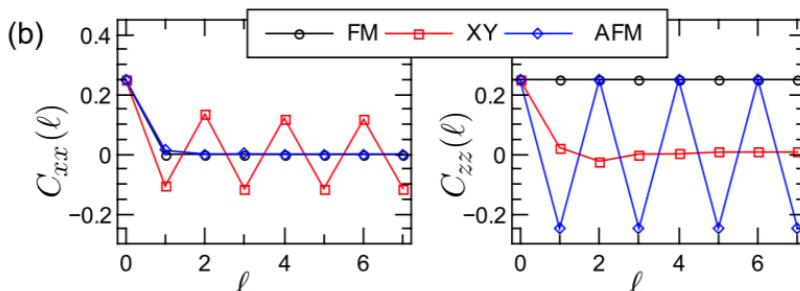
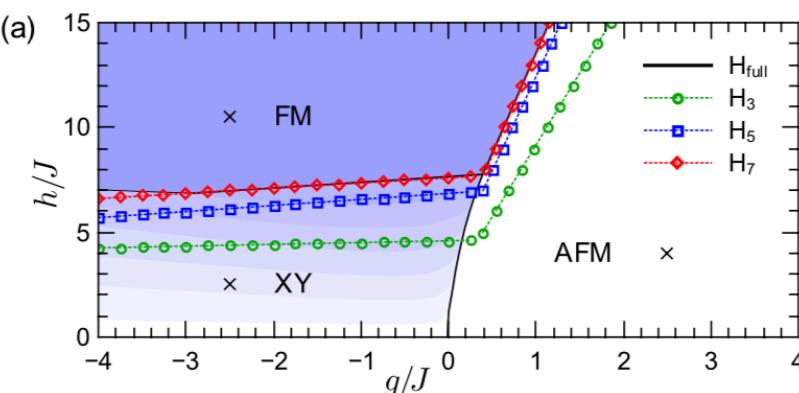
critical phase: power-law decay



AFM/Ising phase: exponential decay



- example



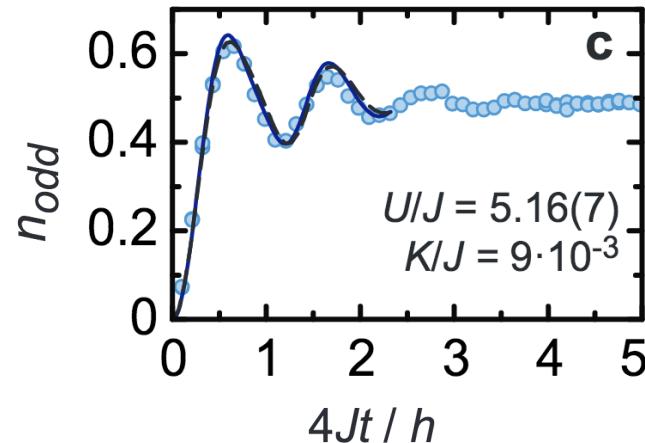
$$\mathcal{H}_g \approx \sum_{\ell \geq 1} \left[ \gamma_\ell \sum_i S_i^z S_{i+\ell}^z + \frac{\eta_\ell - \gamma_\ell}{3} \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+\ell} \right]$$

FIG. 3 (color online). Edge Hamiltonian for the perturbed AKLT model, Eq. (1). (a) Phase diagram as a function of anisotropy  $g/J$  and field  $h/J$ , for  $J > 0$ . Three phases are observed: a fully polarized ferromagnetic (FM) phase (with magnetization  $m_z = \frac{1}{2}$ ), an antiferromagnetic (AFM) phase ( $m_z = 0$ ), and an XY Luttinger liquid phase. The shading shows  $m_z$  for the ground state of the full edge Hamiltonian  $\mathcal{H}$  for  $N_v = 14$ ; the solid lines give phase boundaries determined analytically using fully polarized and mean-field AFM Ansätze, both for  $\mathcal{H}$  and Hamiltonians  $\mathcal{H}_k$  where the sum in (2) and (3) is restricted to  $\ell < k$ . (b) Correlation functions  $C_{xx}(\ell) = \langle S_i^x S_{i+\ell}^x \rangle$  and  $C_{zz}(\ell) = \langle S_i^z S_{i+\ell}^z \rangle$  for the three phases, computed at the points marked  $\times$  in (a). DMRG calculations for  $\mathcal{H}_k$  show that in the XY phase,  $C_{xx}$  decays algebraically.

S. Yang et al.,  
PRL 112,  
036402 (2014).

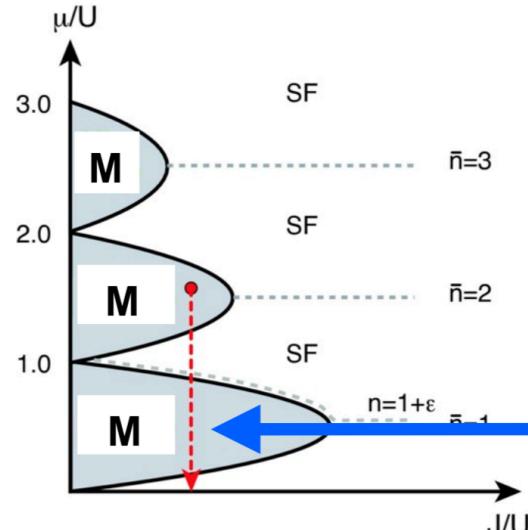
# Applications of tDMRG

- non-equilibrium in quantum gases



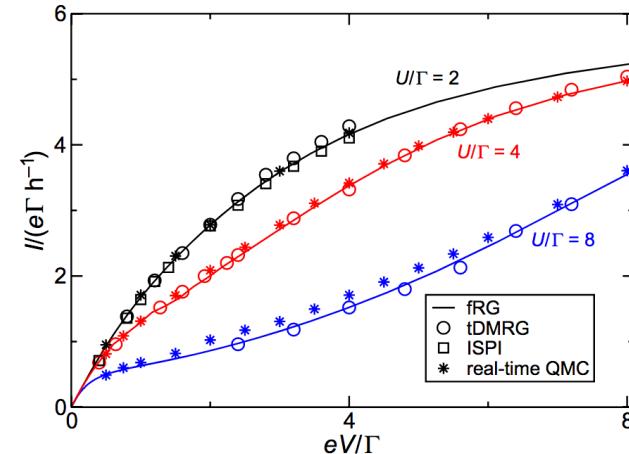
Trotzky et al., Nature Phys. 8, 330 (2012).

- thermalization & relaxation dynamics



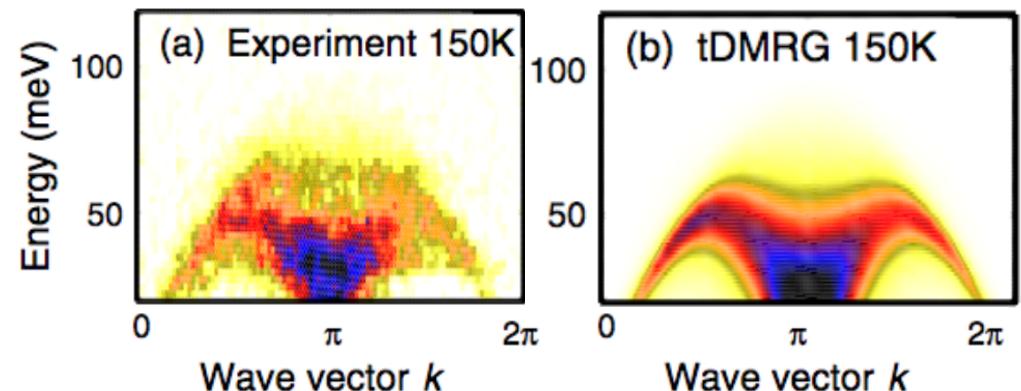
Kollath, et al., PRL 98, 180601 (2007).

- steady-state transport



Eckel et al., New. J Phys. 12, 043042 (2010).

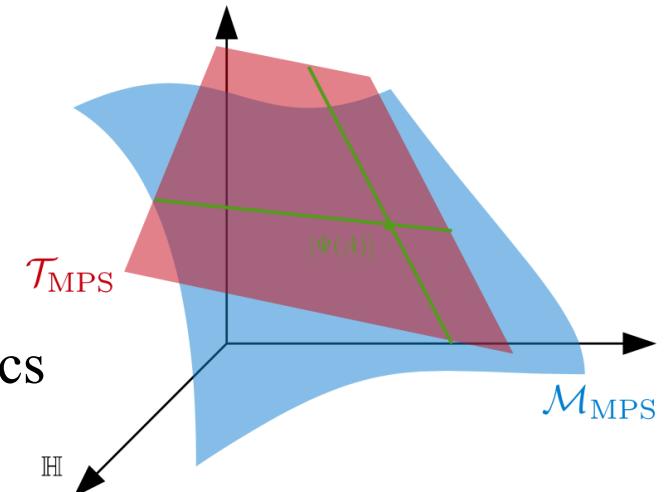
- time-dependent correlation functions



Lake et al., PRL 111, 137205 (2013).

# Tangent-space methods for uniform MPS

- state-of-the-art DMRG/MPS algorithms
- take an MPS in the **thermodynamic limit**  
construct the tangent space on the MPS manifold  
this is the space that contains the low-energy dynamics  
real time evolution, elementary excitations



- we represent a **uniform MPS** as

$$|\Psi(A)\rangle = \dots - \boxed{A} - \boxed{A} - \boxed{A} - \boxed{A} - \boxed{A} - \dots$$

- **mixed gauge**

$$|\Psi(A)\rangle = \dots - \boxed{A_L} - \boxed{A_L} - \circled{C} - \boxed{A_R} - \boxed{A_R} - \dots$$

$$= \dots - \boxed{A_L} - \boxed{A_L} - \boxed{A_C} - \boxed{A_R} - \boxed{A_R} - \dots$$

where

$$-\boxed{A_L} - \circled{C} - = -\circled{C} - \boxed{A_R} - = -\boxed{A_C} -$$

# Tangent vector and tangent space

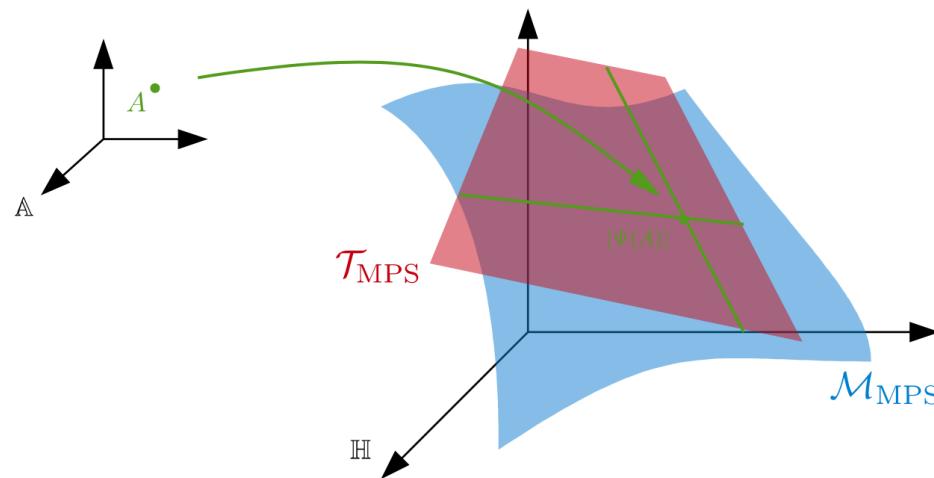
- if MPS is parameterized by tensor  $A$ , a general tangent vector has the form

$$|\Phi(B; A)\rangle = B^i \frac{\partial}{\partial A_i} |\Psi(A)\rangle = \sum_n \dots - \boxed{A} - \boxed{A} - \boxed{B} - \boxed{A} - \boxed{A} - \dots$$

$\dots$        $s_{n-1}$        $s_n$        $s_{n+1}$        $\dots$

in the mixed gauge       $|\Phi(B; A_L, A_R)\rangle = \sum_n \dots - \boxed{A_L} - \boxed{A_L} - \boxed{B} - \boxed{A_R} - \boxed{A_R} - \dots$

$\dots$        $s_{n-1}$        $s_n$        $s_{n+1}$        $\dots$



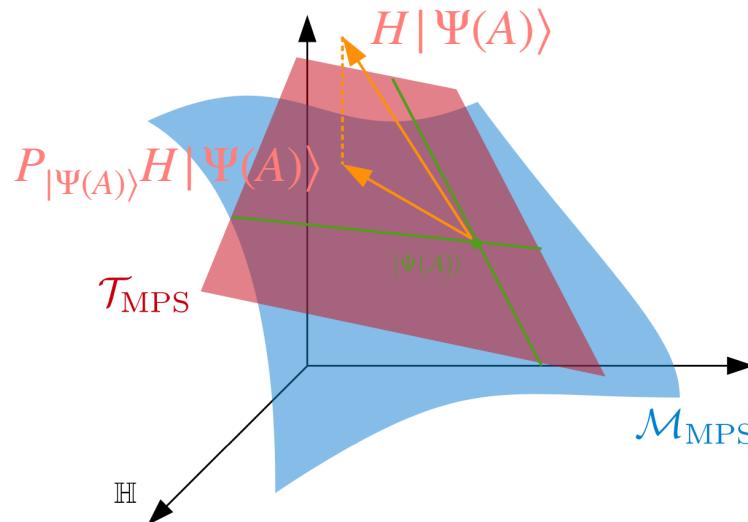
- at every point we can define a tangent space
- we interpret it as a **local perturbation** on a strongly correlated background state  
this perturbation is non-extensive, carries the notion of a **quasi-particle**  
tangent space parameterizes the **low-energy subspace** on a given reference state

# Time-dependent variational principle (TDVP)

- start from Schroedinger equation  $i\frac{\partial}{\partial t}|\Psi(A)\rangle = H|\Psi(A)\rangle$
- the left-hand side is a tangent vector

$$i\frac{\partial}{\partial t}|\Psi(A(t))\rangle = i\dot{A}\frac{\partial}{\partial A}|\Psi(A(t))\rangle = i|\Phi(\dot{A}; A)\rangle$$

but the right-hand side points out of the manifold



- TDVP: project time evolution onto the tangent space

$$\frac{\partial}{\partial t}|\Psi(A(t))\rangle = -iP_{|\Psi(A(t))\rangle}H|\Psi(A(t))\rangle$$

$$|\Phi(\dot{A}(t); A(t))\rangle = -iP_{|\Psi(A(t))\rangle}H|\Psi(A(t))\rangle$$

# Time-dependent variational principle (TDVP)

- in terms of the mixed gauge, the tangent space projector is given by

$$P_{\{A_L, A_R\}} = \sum_n \dots - \sum_n \dots - \sum_n \dots - \dots$$

- to see why  $P$  is the tangent space projector, we introduce  $V_L$

- we may construct the tangent vector as

$$|\Phi(B; A_L, A_R)\rangle = \sum_n \dots - \langle A_L | \dots | s_{n-1} | s_n | B | s_{n+1} | \dots | A_R \rangle$$

- $X$  contains the variational parameters for elementary excitations

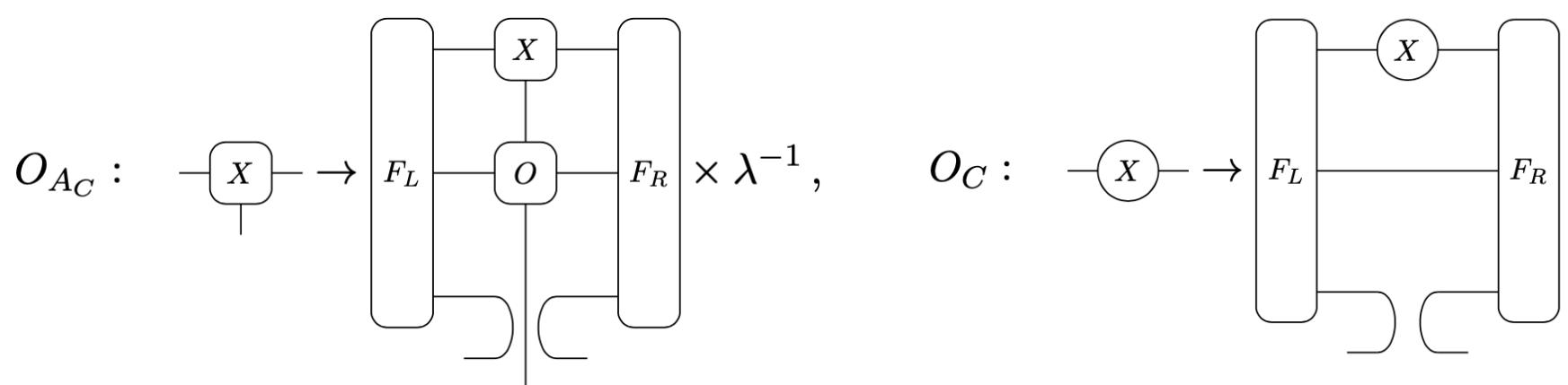
# Finding ground states using VUMPS

- we can derive the expression for the tangent-space gradient from the tangent-space projector

$$|\Psi(G; A)\rangle = \mathcal{P}_A \left( H - \langle \Psi(\bar{A}) | H | \Psi(A) \rangle \right) |\Psi(A)\rangle$$

$$|\Phi(G; A_L, A_R)\rangle = \sum_n \left( \dots \begin{array}{c} \text{---} \\ \boxed{A_L} \text{---} \boxed{A_L} \text{---} \boxed{A_C} \text{---} \boxed{A_R} \text{---} \boxed{A_R} \\ \text{---} \\ \boxed{O} \text{---} \boxed{O} \text{---} \boxed{O} \text{---} \boxed{O} \text{---} \boxed{O} \\ \text{---} \\ \boxed{\bar{A}_L} \text{---} \boxed{\bar{A}_L} \text{---} \text{---} \text{---} \text{---} \text{---} \\ \text{---} \\ \boxed{A_L} \text{---} \boxed{A_L} \end{array} \dots \right) - \left( \dots \begin{array}{c} \text{---} \\ \boxed{A_L} \text{---} \boxed{A_L} \text{---} \text{---} \text{---} \text{---} \text{---} \\ \text{---} \\ \boxed{O} \text{---} \boxed{O} \text{---} \text{---} \text{---} \text{---} \text{---} \\ \text{---} \\ \boxed{\bar{A}_L} \text{---} \boxed{\bar{A}_L} \text{---} \text{---} \text{---} \text{---} \text{---} \\ \text{---} \\ \boxed{A_L} \text{---} \boxed{A_L} \end{array} \dots \right)$$

- we only need to solve eigenvalue equations for  $A_C$  and  $C$



# New progress

## Site Basis Excitation Ansatz for Matrix Product States

Steven R. White<sup>1</sup>

<sup>1</sup>*Department of Physics and Astronomy, University of California, Irvine, California 92697, USA*

We introduce a simple and efficient variation of the tangent-space excitation ansatz used to compute elementary excitation spectra of one-dimensional quantum lattice systems using matrix product states (MPS). A small basis for the excitation tensors is formed based on a single diagonalization analogous to a single site DMRG step but for multiple states. Once overlap and Hamiltonian matrix elements are found, obtaining the excitation for any momentum only requires diagonalization of a tiny matrix, akin to a non-orthogonal band-theory diagonalization. The approach is based on an infinite MPS description of the ground state, and we introduce an extremely simple alternative to variational uniform matrix product states (VUMPS) based on finite system DMRG. For the  $S = 1$  Heisenberg chain, our method—site basis excitation ansatz (SBEA)—efficiently produces the one-magnon dispersion with high accuracy. We also examine the role of MPS gauge choices, finding that not imposing a gauge condition—leaving the basis nonorthogonal—is crucial for the approach, whereas imposing a left-orthonormal gauge (as in prior work) severely hampers convergence. We also show how one can construct Wannier excitations, analogous to the Wannier functions of band theory, where one Wannier excitation, translated to all sites, can reconstruct the single magnon modes exactly for all momenta.

arXiv:2509.06241v1