# Simulations with MPS/MPO

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### Model

► Hamiltonian: Transverse Ising Model

$$H = -J \sum_{i=1}^{N-1} \sigma_i^z \sigma_{i+1}^z - h \sum_{i=1}^{N} \sigma_{i=1}^x + h_z \sum_{i=1}^{N} \sigma_i^z$$
 (1)

Parameters Physics parameters:

$$J = \pm 1.0, \quad h = 0.5, \quad N = 12$$
 (2)

### Model:MPO

**Hamiltonian:** In kron form:

$$H = J\sigma_1^z \otimes \sigma_2^z \otimes \mathbb{1} \otimes \mathbb{1} \otimes \cdots + \mathbb{1} \otimes J\sigma_2^z \otimes \sigma_3^z \otimes \mathbb{1} \otimes \cdots + h\sigma_1^x \otimes \mathbb{1} \otimes \mathbb{1} \otimes \cdots + \mathbb{1} \otimes h\sigma_2^x \otimes \mathbb{1} \otimes \cdots + h_z\sigma_1^z \otimes \mathbb{1} \otimes \mathbb{1} \otimes \cdots + \mathbb{1} \otimes h_z\sigma_2^z \otimes \mathbb{1} \otimes \cdots$$

$$(3)$$

▶ MPO

$$H_{1} = \begin{pmatrix} h\sigma_{1}^{x} + h_{z}\sigma_{1}^{z}, & J\sigma_{1}^{z}, & 1 \end{pmatrix},$$

$$H_{i} = \begin{pmatrix} 1, & 0, & 0 \\ \sigma_{i}^{z}, & 0, & 0 \\ h\sigma_{i}^{x} + h_{z}\sigma_{i}^{z}, & J\sigma_{i}^{z}, & 1 \end{pmatrix}, \quad H_{N} = \begin{pmatrix} 1 \\ \sigma_{N}^{z} \\ h\sigma_{N}^{x} + h_{z}\sigma_{N}^{z} \end{pmatrix}$$

$$(4)$$

### Model:MPO

**Total Magnetic Moment:** In kron form:

$$M_z = \sigma_1^z \otimes \mathbb{1} \otimes \mathbb{1} \otimes \cdots + \mathbb{1} \otimes \sigma_2^z \otimes \mathbb{1} \otimes \cdots$$
 (5)

▶ MPO

$$H_{1} = \begin{pmatrix} \sigma_{1}^{z}, & \mathbb{1} \end{pmatrix},$$

$$H_{i} = \begin{pmatrix} \mathbb{1}, & \mathbb{0} \\ \sigma_{i}^{z}, & \mathbb{1} \end{pmatrix}, \quad H_{N} = \begin{pmatrix} \mathbb{1} \\ \sigma_{N}^{z} \end{pmatrix}$$
(6)

### Model:MPS

 $|s_i\rangle$  denote that site i is in eigenstate of  $\sigma_i^z$  with eigenvalue  $s_i=\pm 1$ .  $|s_1s_2s_3\cdots s_N\rangle$  is corresponding many body basis of system.

Random Initialized State: Random initial state

$$\psi_0 = \sum_{\{s_i\}} C_{s_1 s_2 s_3 \cdots s_N} | s_1 s_2 s_3 \cdots s_N \rangle$$
 (7)

equals the random tensor  $C_{s_1s_2s_3...s_N}$ . Then orientSVD:



### Model:MPS

**Assigned Initialized State** FM corresponds to state  $C_{s_1s_2s_3\cdots s_N}$  with

$$C_{111...1} = 1$$
 or  $C_{-1-1-1...-1} = 1$  (8)

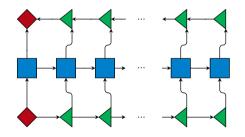
while AFM corresponds to state  $C_{s_1s_2s_3\cdots s_N}$  with

$$C_{1-11-1...} = 1$$
 or  $C_{-11-11...} = 1$  (9)

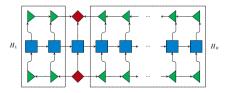
Then orientSVD in the same way as that in Random Initialized State.

## DMRG: 1-site update

Initialize MPS with diagonalization center at i = 1.

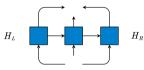


- Sweep at two direction (right left right ...)
  - Calculate the left/right environment  $H_L/H_R$ .

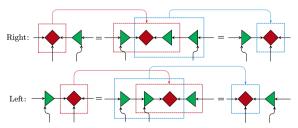


## DMRG: 1-site update

- Sweep at two direction (right left right ...)
  - Calculate the effective Hamiltonian  $H_{eff} = H_L H_i H_R$

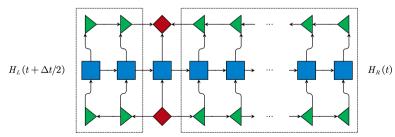


OrientSVD and move the center to next site.



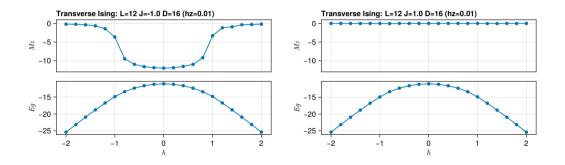
## TDVP: 1-site integration

- Initialize MPS with diagonalization center at i = 1.
- Sweep at two direction (right left right ...)
  - Calculate the left/right environment  $H_L(t + \Delta t/2)/H_R(t)$ .



#### Results

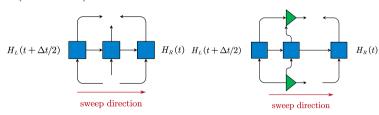
#### Simulation results:



a quantum phase transition can be observed near  $h \sim 1.0$ 

## TDVP: 1-site integration

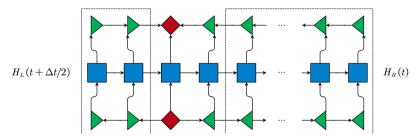
- Sweep at two direction (right left right ...)
  - Calculate the effective Hamiltonian  $H_{eff}^{(1)}$
  - Time evolution  $A_i(t + \Delta t/2) = \exp\left(-iH_{eff}^{(1)}\Delta t/2\right)A_i(t)$
  - OrientSVD and calculate the center with inverse evolution  $C_i(t) = \exp\left(iH_{eff}^{(0)}\Delta t/2\right)C_i(t+\Delta t/2)$ , then absorb it into nextsite.



### TDVP: 2-site integration

#### Sweep schemes

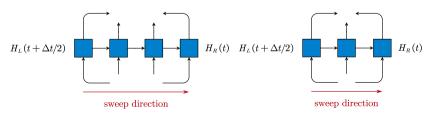
Calculate the left/right environment  $H_L(t + \Delta t/2)/H_R(t)$ .



## TDVP: 2-site integration

#### Sweep schemes

- lacksquare Calculate the effective Hamiltonian  $H_{eff}^{(2)}$
- Time evolution  $A_i A_{i+1}(t + \Delta t/2) = \exp\left(-iH_{eff}^{(2)} \Delta t/2\right) A_i A_{i+1}(t)$
- OrientSVD and calculate the center with inverse evolution  $A_{i+1}(t) = \exp\left(iH_{eff}^{(1)}\Delta t/2\right)A_{i+1}(t+\Delta t/2)$ , then regard it as nextsite.



#### Results

Choose initial state relevant parameters are

$$t = 5/|J|, \quad L = 13, \quad D = 16$$
 (11)

Simulation results:

