Simulations with MPS/MPO

Kunyang DU

Institue of Theoretical Physics

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Model

- **Hamiltonian:** Transverse Ising Model

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

- **Parameters** Physics parameters:

$$J = \pm 1.0, \quad h = 0.5, \quad N = 12 \tag{2}$$

Model:MPO

- **Hamiltonian:** In kron form:

$$
\begin{aligned}
H =& J\sigma_1^z \otimes \sigma_2^z \otimes \mathbb{1} \otimes \mathbb{1} \otimes \cdots + \mathbb{1} \otimes J\sigma_2^z \otimes \sigma_3^z \otimes \mathbb{1} \otimes \cdots \\
&+ h\sigma_1^x \otimes \mathbb{1} \otimes \mathbb{1} \otimes \cdots + \mathbb{1} \otimes h\sigma_2^x \otimes \mathbb{1} \otimes \cdots \\
&+ h_z\sigma_1^z \otimes \mathbb{1} \otimes \mathbb{1} \otimes \cdots + \mathbb{1} \otimes h_z\sigma_2^z \otimes \mathbb{1} \otimes \cdots
\end{aligned} \tag{3}
$$

- **MPO**

$$
\begin{gathered}
H_1 = \left(h\sigma_1^x + h_z\sigma_1^z, \quad J\sigma_1^z, \quad \mathbb{1} \right), \\
H_i = \begin{pmatrix} \mathbb{1}, & \mathbb{0}, & \mathbb{0} \\ \sigma_i^z, & \mathbb{0}, & \mathbb{0} \\ h\sigma_i^x + h_z\sigma_i^z, & J\sigma_i^z, & \mathbb{1} \end{pmatrix}, \quad H_N = \begin{pmatrix} \mathbb{1} \\ \sigma_N^z \\ h\sigma_N^x + h_z\sigma_N^z \end{pmatrix}
\end{gathered} \tag{4}
$$

Model:MPO

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

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

- **MPO**

$$\begin{gathered} H_1 = \begin{pmatrix} \sigma_1^z, & \mathbb{1} \end{pmatrix}, \\ H_i = \begin{pmatrix} \mathbb{1}, & \mathbb{0} \\ \sigma_i^z, & \mathbb{1} \end{pmatrix}, \quad H_N = \begin{pmatrix} \mathbb{1} \\ \sigma_N^z \end{pmatrix} \end{gathered} \tag{6}$$

Model:MPS

$|s_i\rangle$ denote that site i is in eigenstate of σ_i^z with eigenvalues$s_i = \pm 1$.
$|s_1 s_2 s_3 \cdots s_N\rangle$is corresponding many body basis of system.

- **Random Initialized State:** Random initial state

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

equals the random tensor $C_{s_1 s_2 s_3 \cdots s_N}$. Then orientSVD:

Model:MPS

- **Assigned Initialized State** FM corresponds to state $C_{s_1 s_2 s_3 \cdots s_N}$ with

$$C_{111\ldots1} = 1 \quad \text{or} \quad C_{-1-1-1\ldots-1} = 1 \tag{8}$$

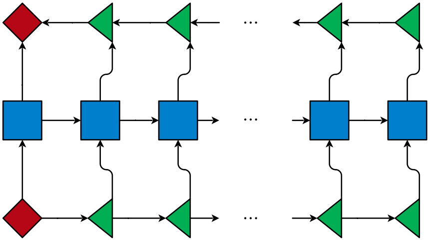
while AFM corresponds to state $C_{s_1 s_2 s_3 \cdots s_N}$ with

$$C_{1-11-1\ldots} = 1 \quad \text{or} \quad C_{-11-11\ldots} = 1 \tag{9}$$

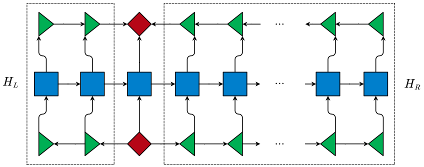
Then orientSVD in the same way as that in Random Initialized State.

DMRG: 1-site update

- Initialize MPS with diagonalization center at $i = 1$.

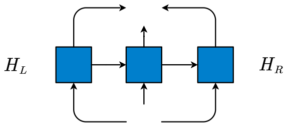


- Sweep at two direction (right - left - right - ...)
  - Calculate the left/right environment H_L/H_R.

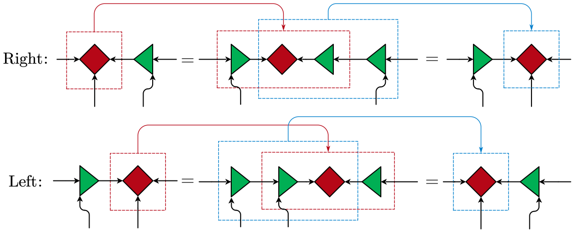


DMRG: 1-site update

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

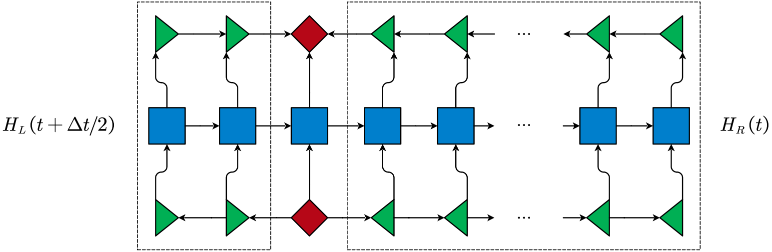


  - OrientSVD and move the center to next site.



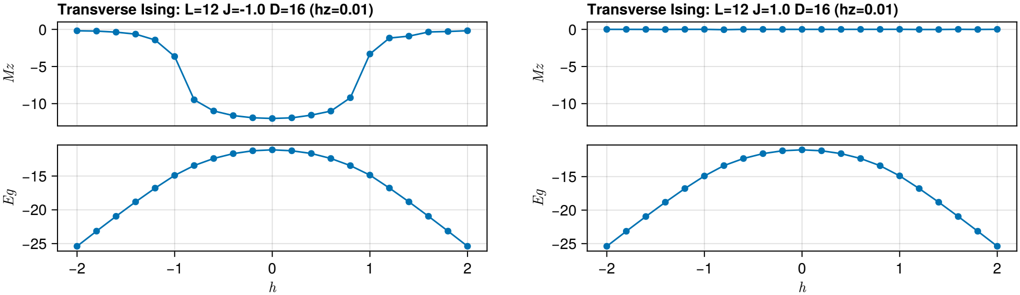
TDVP: 1-site integration

- 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

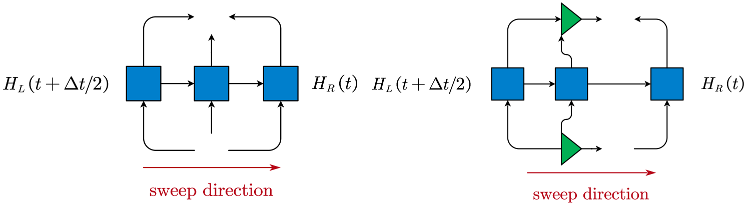
Simulation results:



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

TDVP: 1-site integration

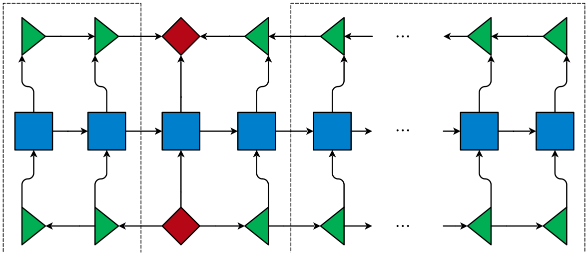
- Sweep at two direction (right - left - right - ...)
  - Calculate the effective Hamiltonian $H^{(1)}_{eff}$
  - Time evolution $A_i(t+\Delta t/2) = \exp\left(-iH^{(1)}_{eff}\Delta t/2\right)A_i(t)$
  - OrientSVD and calculate the center with inverse evolution $C_i(t) = \exp\left(iH^{(0)}_{eff}\Delta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



TDVP: 2-site integration

Sweep schemes

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

$H_L(t+\Delta t/2)$  $H_R(t)$

TDVP: 2-site integration

Sweep schemes

- 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.