

Simulations with MPS/MPO

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Model

► **Hamiltonian:** Transverse Ising Model

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

► **Parameters** Physics parameters:

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

Model:MPO

► **Hamiltonian:** In kron form:

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

► **MPO**

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

Model:MPO

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

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

► **MPO**

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

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

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

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 $C_{s_1 s_2 s_3 \dots s_N}$ with

$$C_{111\dots 1} = 1 \quad \text{or} \quad C_{-1-1-1\dots -1} = 1 \quad (8)$$

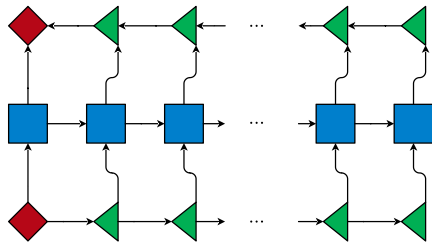
while AFM corresponds to state $C_{s_1 s_2 s_3 \dots s_N}$ with

$$C_{1-11-1\dots} = 1 \quad \text{or} \quad C_{-11-11\dots} = 1 \quad (9)$$

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

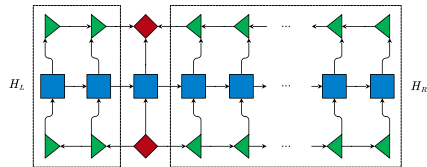
DMRG: 1-site update

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



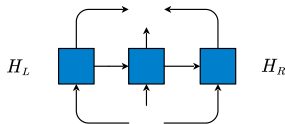
- Sweep at two direction (right - left - right - ...)

- Calculate the left/right environment H_L/H_R .

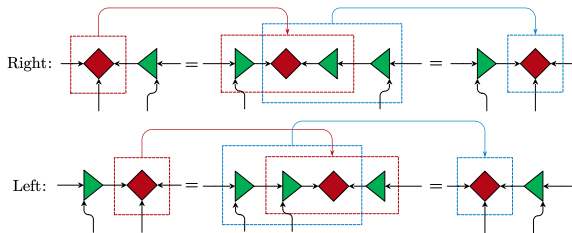


DMRG: 1-site update

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

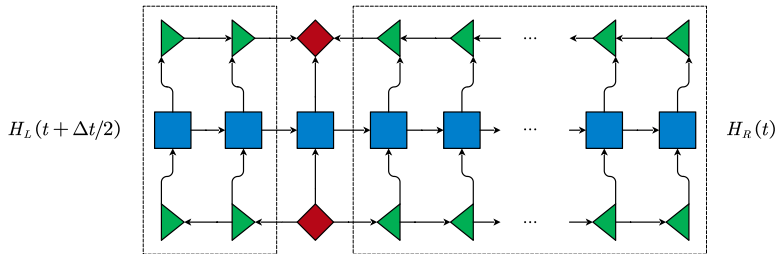


- ▶ OrientSVD and move the center to next site.



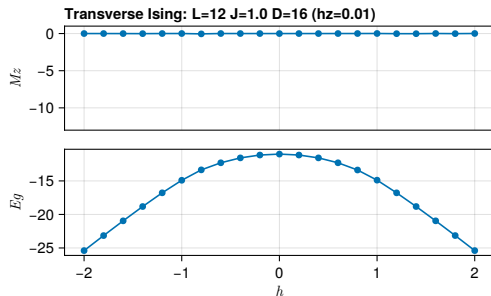
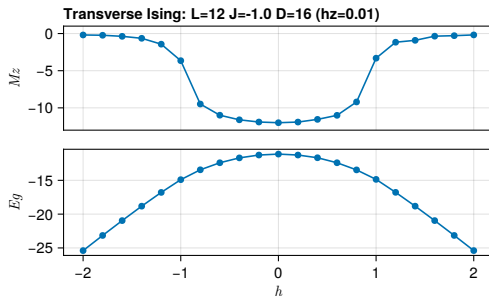
TDVP: 1-site integration

- ▶ 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

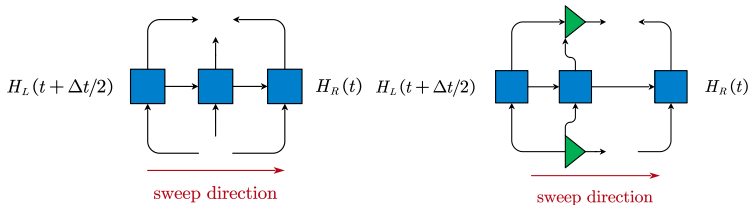
Simulation results:



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

TDVP: 1-site integration

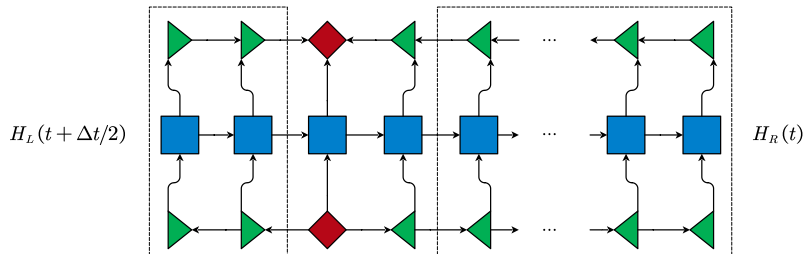
- ▶ Sweep at two direction (right - left - right - ...)
- ▶ Calculate the effective Hamiltonian $H_{eff}^{(1)}$
- ▶ Time evolution $A_i(t + \Delta t/2) = \exp\left(-i H_{eff}^{(1)} \Delta t/2\right) A_i(t)$
- ▶ OrientSVD and calculate the center with inverse evolution $C_i(t) = \exp\left(i H_{eff}^{(0)}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



TDVP: 2-site integration

Sweep schemes

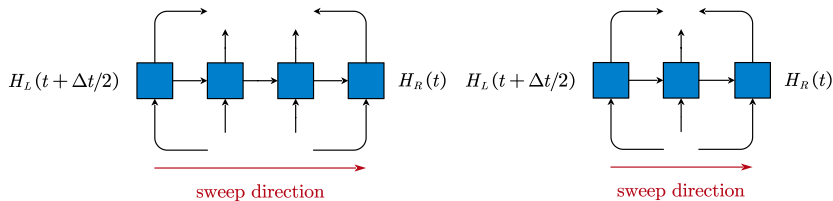
- Calculate the left/right environment $H_L(t + \Delta t/2)/H_R(t)$.



TDVP: 2-site integration

Sweep schemes

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



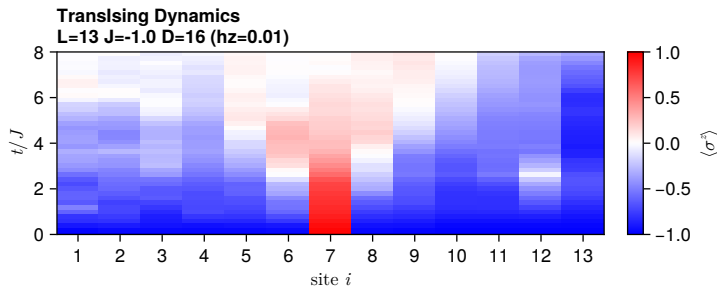
Results

- Choose initial state relevant parameters are

$$\Psi_0 = |-1, -1, -1, -1, -1, -1, 1, -1, -1, -1, -1, -1, -1\rangle \quad (10)$$

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

- Simulation results:



diffusion can be observed from site 7.