

Simulations with MPS/MPO

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Model: Transverse Ising Chain

► Hamiltonian:

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

► Parameters Physics parameters:

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

Model:MPO

► **Hamiltonian:** In kron form:

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

► **MPO**

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

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

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

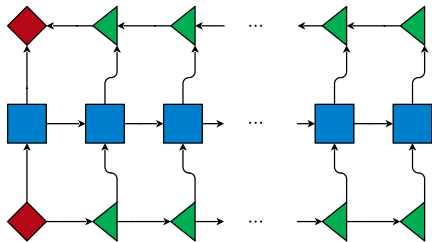
while AFM corresponds to state $C_{s_1 s_2 s_3 \dots s_N}$ with

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

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

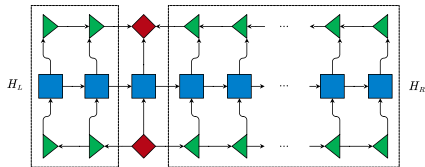
DMRG: 1-site update

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



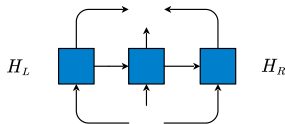
- Sweep at two direction (right - left - right - ...)

- Calculate the left/right environment H_L/H_R .

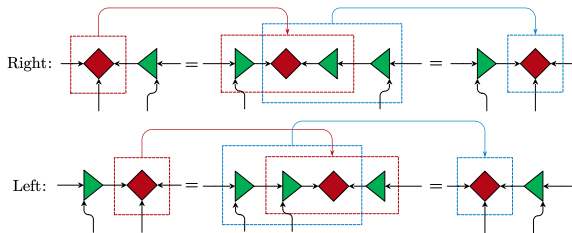


DMRG: 1-site update

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

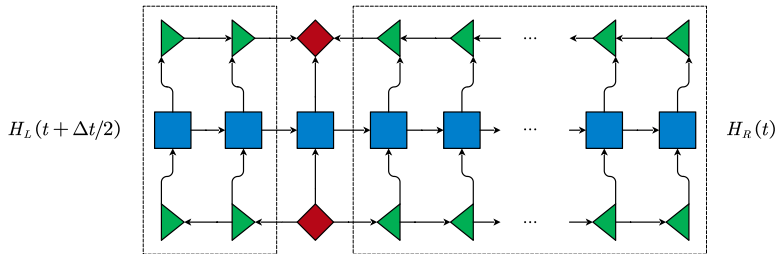


- ▶ OrientSVD and move the center to next site.



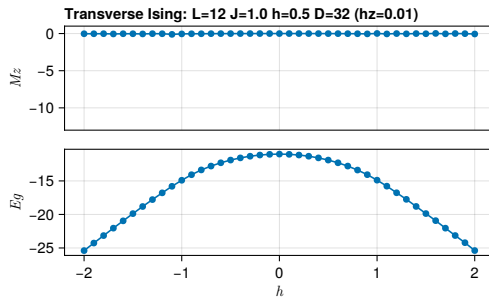
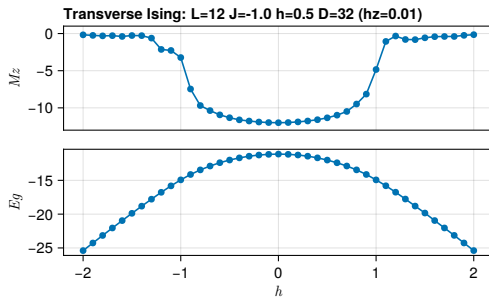
TDVP: 1-site integration

- ▶ 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

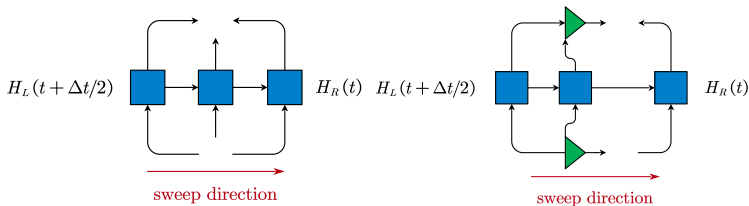
Simulation results:



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

TDVP: 1-site integration

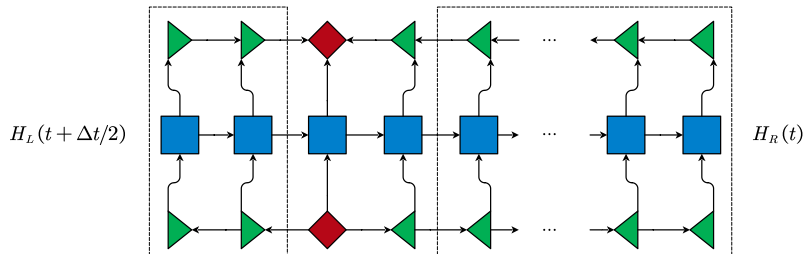
- ▶ Sweep at two direction (right - left - right - ...)
- ▶ Calculate the effective Hamiltonian $H_{eff}^{(1)}$
- ▶ Time evolution $A_i(t + \Delta t/2) = \exp\left(-i H_{eff}^{(1)} \Delta t/2\right) A_i(t)$
- ▶ OrientSVD and calculate the center with inverse evolution $C_i(t) = \exp\left(i H_{eff}^{(0)}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



TDVP: 2-site integration

Sweep schemes

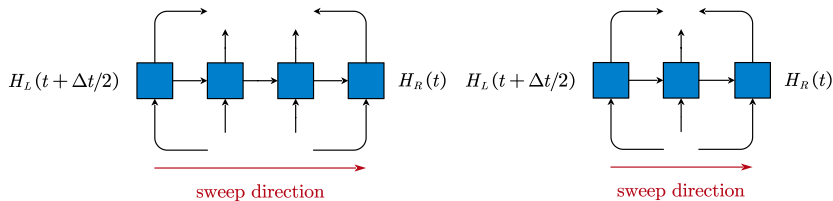
- Calculate the left/right environment $H_L(t + \Delta t/2)/H_R(t)$.



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.

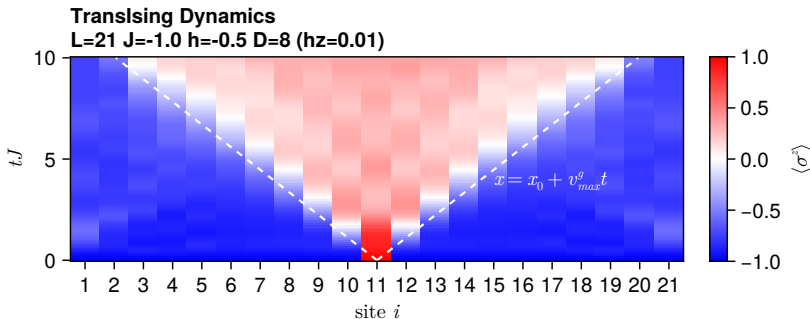


Results

- Choose initial state relevant is

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

- Simulation results: diffusion can be observed at site 11.



Model: Free Fermion on Square Lattice

► Hamiltonian:

$$H = t \sum_{\langle i,j \rangle} c_i^\dagger c_j + c_j^\dagger c_i \quad (11)$$

► Parameters Physics parameters:

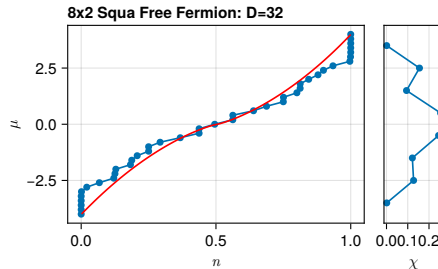
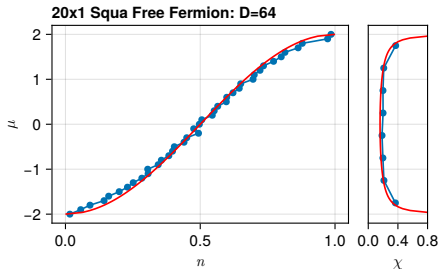
$$t = 1 \quad (12)$$

Results

- Charge susceptibility.

$$\chi = \frac{1}{N} \frac{\partial N}{\partial \mu} \quad (13)$$

- Simulation results: diffusion can be observed at site 11.



Observables

③ $t \sim D$

②

①

$\sim N$

$\| \Psi - H \Psi \|$

► Spectrum function



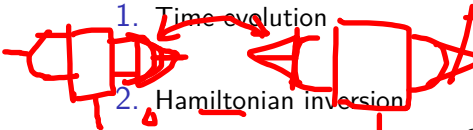
$$A(k, \omega) = -\frac{1}{\pi} \text{Im} G(k, \omega + 0^+) \quad (14)$$

there are two calculation schemes

X T K G.

1. Time evolution

2. Hamiltonian inversion



$$G(k, \omega) = \langle \Psi_0 | c_k(t) c_k^\dagger | \Psi_0 \rangle \quad (15)$$

$$G(k, \omega) = \langle \Psi_0 | c_k \frac{1}{\omega - H} c_k^\dagger | \Psi_0 \rangle \quad (16)$$

krylov

iso

D_{mpo} H

$p < 1 + \dots$