# Simulations with MPS/MPO

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# Model:Transverse Ising Chain

- **Hamiltonian:**

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

- **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 $\sigma_i^z$ 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

$$C_{111\dots1} = 1 \quad \text{or} \quad C_{-1-1-1\dots-1} = 1 \tag{8}$$

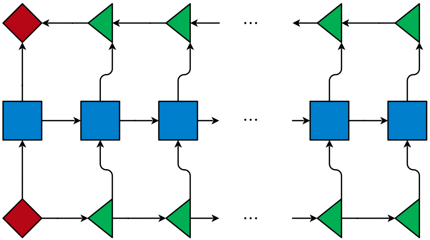
while AFM corresponds to state $C_{s_1 s_2 s_3 \cdots s_N}$ with

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

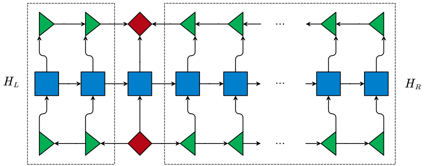
Then orientSVD in the same way as that in Random Initialized State.

# DMRG: 1-site update

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

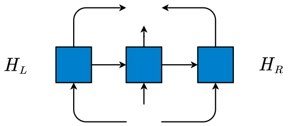


- Sweep at two direction (right - left - right - ...)
  - Calculate the left/right environment $H_L/H_R$.

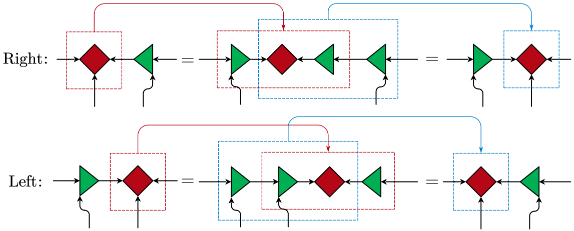


# DMRG: 1-site update

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

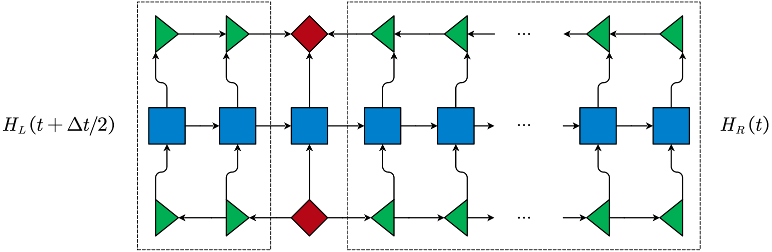



  - OrientSVD and move the center to next site.



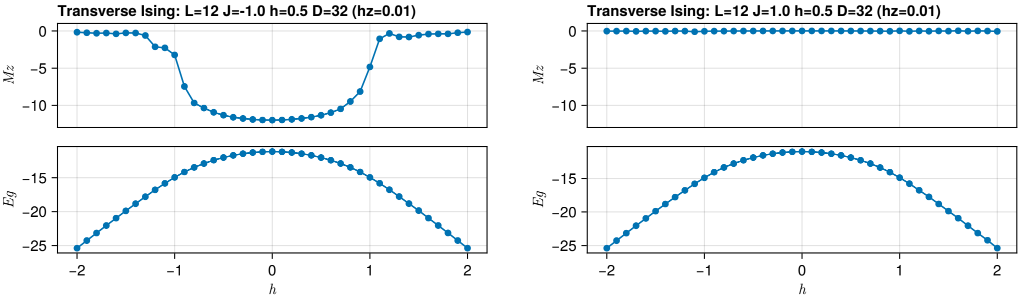
# TDVP: 1-site integration

- 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

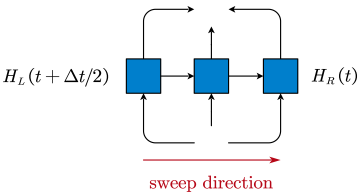
Simulation results:

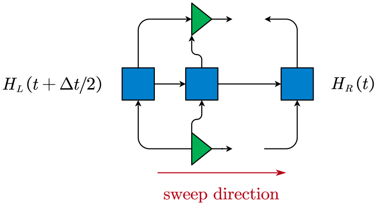



a quantum phase transition can be observed near $h \sim 1.0$

# TDVP: 1-site integration

- Sweep at two direction (right - left - right - ...)
  - Calculate the effective Hamiltonian $H_{eff}^{(1)}$
  - 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.

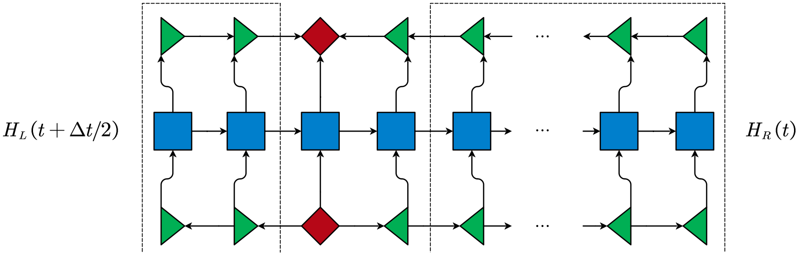


# TDVP: 2-site integration

Sweep schemes

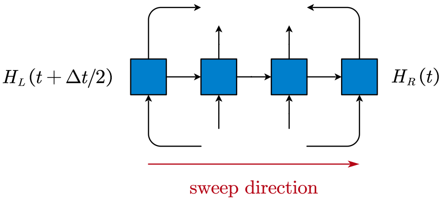
- Calculate the left/right environment $H_L(t+\Delta t/2)/H_R(t)$.

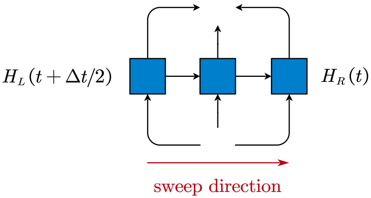


# TDVP: 2-site integration

Sweep schemes

- 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.



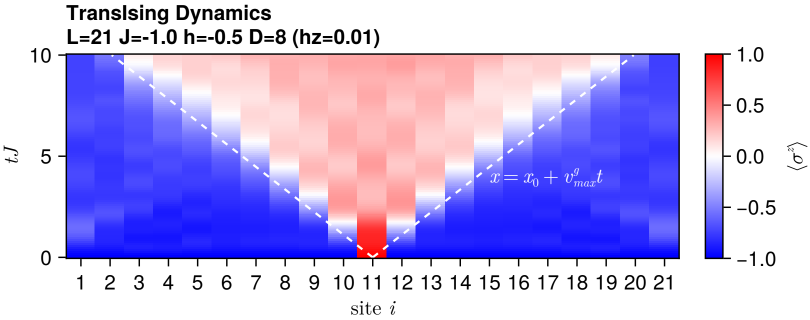



# Results

- Choose initial state relevant is

$$\Psi_0 = |-1, -1, \cdots, -1, 1, -1, \cdots, -1, -1\rangle \tag{10}$$

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



## Model:Free Fermion on Square Lattice

- **Hamiltonian:**

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

- **Parameters:** Physics parameters:

$$t = 1 \tag{12}$$

- **J-W transformation:**

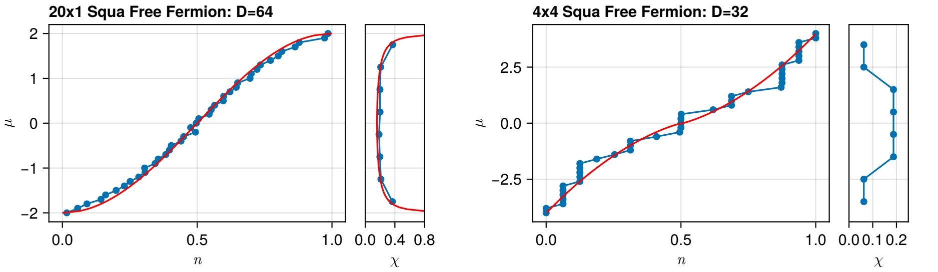
$$c_i = \prod_{k=1}^{i-1} b_i, \quad c_i^\dagger = \prod_{k=1}^{i-1} b_i^\dagger \tag{13}$$

# Results

- Charge susceptibility.

$$\chi = \frac{1}{N}\frac{\partial N}{\partial \mu} \tag{14}$$

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



# Obserables: Spectrum function

- Spectrum function

$$S(\boldsymbol{k}, E) = -\frac{1}{\pi}\mathrm{Im}G^{ret}(\boldsymbol{k}, E) \tag{15}$$

where the retarded Green function is

$$\begin{aligned} G^{ret}(\boldsymbol{k}, E) &= \int_{-\infty}^{+\infty} G^{ret}(\boldsymbol{k}, t)\mathrm{e}^{iEt}\mathrm{d}t \\ G^{ret}(\boldsymbol{k}, t) &= -\,i\Theta(t)\left\langle\Psi_0\right|\left[c_k(t)c_k^\dagger(0)\right]\left|\Psi_0\right\rangle \\ &= \begin{cases} -i\mathrm{e}^{iE_0t}\left(\left\langle\Psi_0\right| c_k\right)\mathrm{e}^{-iHt}\left(c_k^\dagger\left|\Psi_0\right\rangle\right) & \text{if } t > 0 \\ -i\mathrm{e}^{-iE_0t}\left(\left\langle\Psi_0\right| c_k^\dagger\right)\mathrm{e}^{iHt}\left(c_k\left|\Psi_0\right\rangle\right) & \text{if } t < 0 \end{cases} \end{aligned} \tag{16}$$

with

$$c_k = \sum_j \mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{R}_j} c_j \tag{17}$$

# Obserables: Spectrum function

The final observables:

$$\left(\langle\Psi_0\right| c_i) \, \mathrm{e}^{-iHt} \left(c_j^\dagger \left|\Psi_0\rangle\right.\right) \tag{18}$$

$$\left(\langle\Psi_0\right| c_i^\dagger\Big) \, \mathrm{e}^{iHt} \left(c_j \left|\Psi_0\rangle\right.\right) \tag{19}$$

i.e. calculate the $2L$ MPO*MPS, then TDVP by all-to-all inner product.