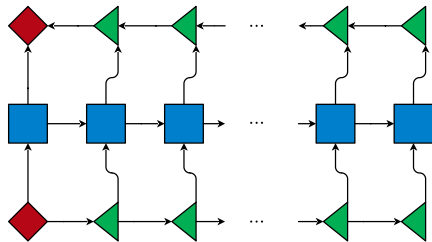# Simulations with MPS/MPO

Kunyang DU

Institue of Theoretical Physics
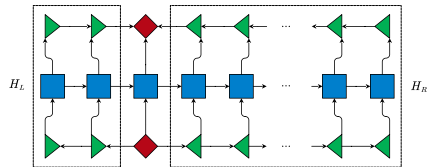
September 13, 2024

DMRG: 1-site update

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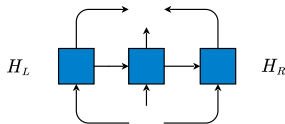

▶ Sweep at two direction (right - left - right - …)
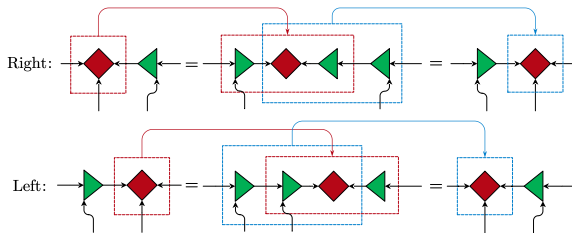
  ▶ Calculate the left/right environment H_L/H_R.

DMRG: 1-site update

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

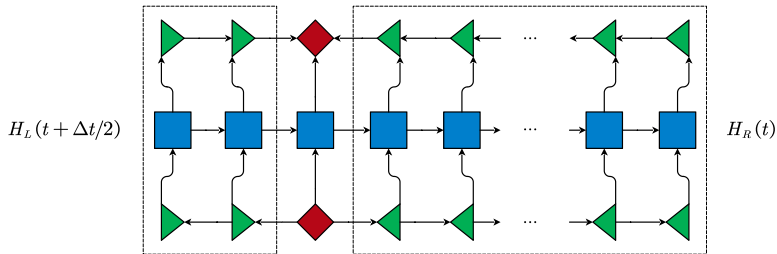▶ Calculate the effective Hamiltonian $H_{eff} = H_L H_i H_R$

▶ 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 $H_L(t + \Delta t/2)/H_R(t)$.

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.
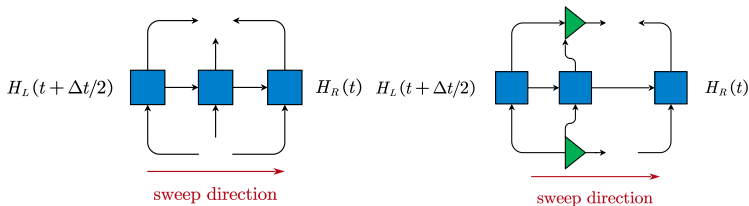
TDVP: 2-site integration

Sweep schemes

▶ Calculate the left/right environment $H_L(t + \Delta t/2)/H_R(t)$.
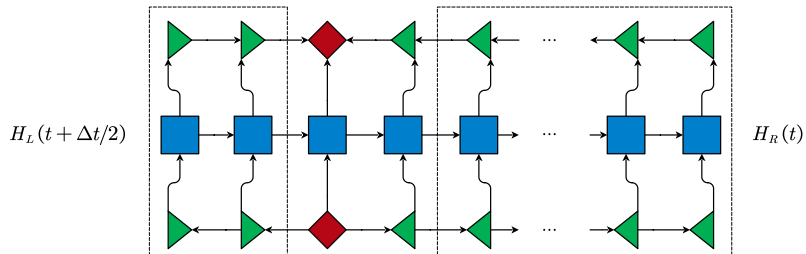
TDVP: 2-site integration

Sweep schemes

▶ Calculate the effective Hamiltonian $H_{eff}^{(2)}$

▶ Time evolution $A_i A_{i+1}(t + \Delta t/2) = \exp\left(-i H_{eff}^{(2)} \Delta t/2\right) A_i A_{i+1}(t)$

▶ 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.

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

sweep direction   sweep direction
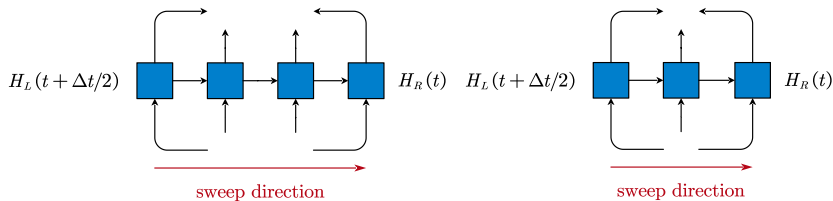
Model: Transverse Ising Chain

▶ **Hamiltonian:**

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

we always choose $J = \pm 1.0$.

▶ **Exact Solutions:** With **Jordan-Wigne** and **Bogoliubov** transformation, we can diagonalize H in fermion picture:

$$H = \sum_{k>0} \lambda(k) \gamma_k^\dagger \gamma_k, \quad \lambda(k) = \sqrt{\epsilon_k^2 + \Delta_k^2}, \quad \begin{pmatrix} \gamma_k^\dagger \\ \gamma_{-k} \end{pmatrix} = \mathbf{P}(k) \begin{pmatrix} c_k^\dagger \\ c_{-k} \end{pmatrix} \qquad (2)$$

$$\epsilon_k = -2J \cos ka - 2h, \quad \Delta_k = 2J \sin ka \qquad (3)$$

Model:MPO

▶ **Hamiltonian:** In kron form:

$$H = J\sigma_1^z \otimes \sigma_2^z \otimes \mathbb{1} \otimes \mathbb{1} \otimes \cdots + \mathbb{1} \otimes J\sigma_2^z \otimes \sigma_3^z \otimes \mathbb{1} \otimes \cdots$$
$$+ h\sigma_1^x \otimes \mathbb{1} \otimes \mathbb{1} \otimes \cdots + \mathbb{1} \otimes h\sigma_2^x \otimes \mathbb{1} \otimes \cdots \qquad (4)$$
$$+ h_z\sigma_1^z \otimes \mathbb{1} \otimes \mathbb{1} \otimes \cdots + \mathbb{1} \otimes h_z\sigma_2^z \otimes \mathbb{1} \otimes \cdots$$

▶ **MPO**

$$H_1 = \begin{pmatrix} h\sigma_1^x + h_z\sigma_1^z, & J\sigma_1^z, & \mathbb{1} \end{pmatrix},$$
$$H_i = \begin{pmatrix} \mathbb{1}, & \mathbb{0}, & \mathbb{0} \\ \sigma_i^z, & \mathbb{0}, & \mathbb{0} \\ h\sigma_i^x + h_z\sigma_i^z, & J\sigma_i^z, & \mathbb{1} \end{pmatrix}, \quad H_N = \begin{pmatrix} \mathbb{1} \\ \sigma_N^z \\ h\sigma_N^x + h_z\sigma_N^z \end{pmatrix} \qquad (5)$$

Model:MPO

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

$$M_z = \sigma_1^z \otimes \mathbb{1} \otimes \mathbb{1} \otimes \cdots + \mathbb{1} \otimes \sigma_2^z \otimes \mathbb{1} \otimes \cdots \qquad (6)$$

▶ **MPO**

$$H_1 = \begin{pmatrix} \sigma_1^z, & \mathbb{1} \end{pmatrix},$$
$$H_i = \begin{pmatrix} \mathbb{1}, & \mathbb{0} \\ \sigma_i^z, & \mathbb{1} \end{pmatrix}, \quad H_N = \begin{pmatrix} \mathbb{1} \\ \sigma_N^z \end{pmatrix} \qquad (7)$$

Model:MPS

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

▶ **Random Initialized State:** Random initial state

$$\psi_0 = \sum_{\{s_i\}} C_{s_1 s_2 s_3 \cdots s_N} |s_1 s_2 s_3 \cdots s_N\rangle \qquad (8)$$

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

$$C_{111\cdots1} = 1 \quad \text{or} \quad C_{-1-1-1\cdots-1} = 1 \qquad (9)$$
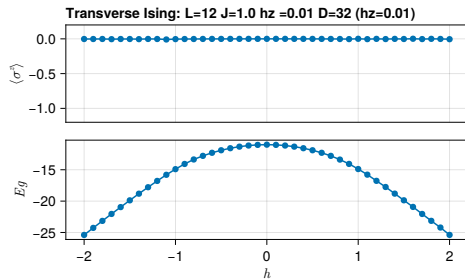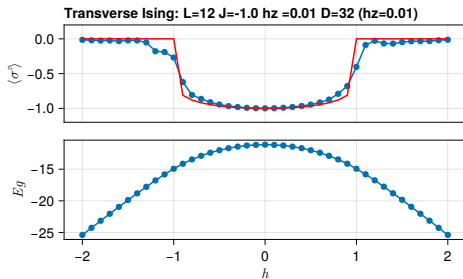
while AFM corresponds to state $C_{s_1 s_2 s_3 \cdots s_N}$ with

$$C_{1-11-1\cdots} = 1 \quad \text{or} \quad C_{-11-11\cdots} = 1 \qquad (10)$$

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

Results

Simulation results:

Transverse Ising: L=12 J=-1.0 hz =0.01 D=32 (hz=0.01)

Transverse Ising: L=12 J=1.0 hz =0.01 D=32 (hz=0.01)

Where exact solution can be obtained by calculating $\left\langle \sigma_i^z \sigma_j^z \right\rangle$ and let $|i - j| \to +\infty$, i.e.
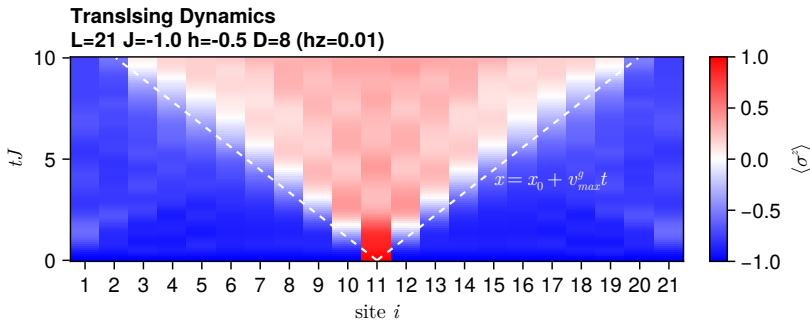
$$\langle \sigma^z \rangle = \left[1 - \left(\frac{h}{J} \right)^2 \right]^{1/8} \tag{11}$$

Results: Dynamics

▶ Choose initial state relevant is

$$\Psi_0 = |-1, -1, \cdots, -1, 1, -1, \cdots, -1, -1\rangle \qquad (12)$$

▶ Simulation results: $v_g^{max} = \max \partial \lambda(k)/\partial k$

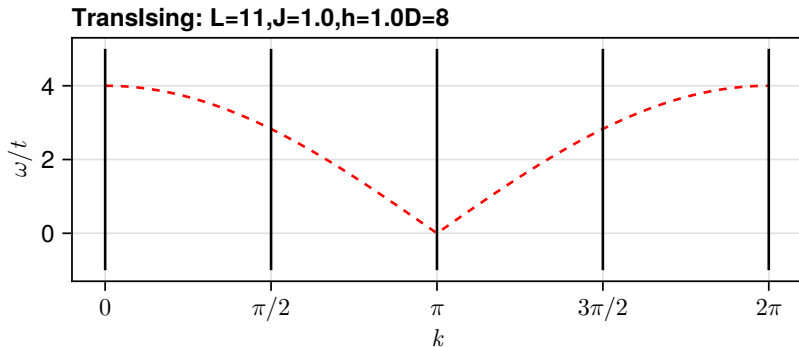**TransIsing Dynamics**
L=21 J=-1.0 h=-0.5 D=8 (hz=0.01)

Results: Spectrum Function

▶ Set

$$J = 1, \quad h = 1, \quad S(k, \omega) = -\frac{1}{\pi} \langle\langle \gamma_k; \gamma_k^\dagger \rangle\rangle_E^{ret} \tag{13}$$

▶ Simulation results: $S_{theo}(k, \omega) = \delta(\omega - \lambda(k))$

TransIsing: L=11,J=1.0,h=1.0D=8

Model:Free Fermion on Square Lattice

▶ **Hamiltonian:**

$$H = t \sum_{\langle i,j \rangle} c_i^\dagger c_j + c_j^\dagger c_i \tag{14}$$

▶ **Parameters:** Physics parameters:

$$t = 1 \tag{15}$$

▶ **J-W transformation:**

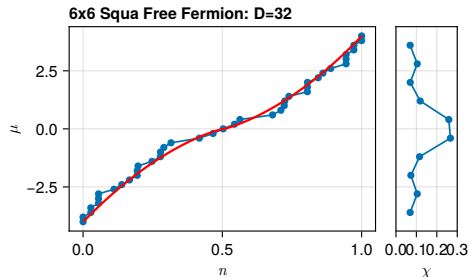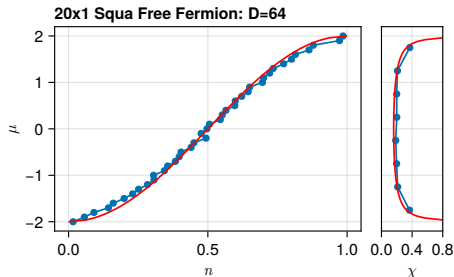$$c_i = \prod_{j=1}^{i-1} F_j b_i, \quad c_i^\dagger = \prod_{j=1}^{i-1} F_j b_i^\dagger \tag{16}$$

$$F_j = -\sigma_j^z, \quad b_i = \sigma_i^-, \quad b_i = \sigma_i^+ \tag{17}$$

Results

▶ Charge susceptibility.

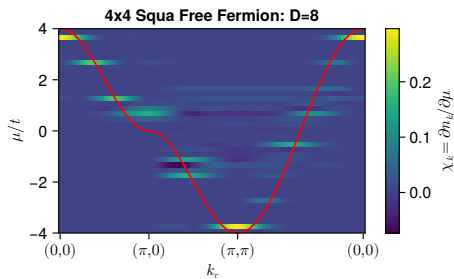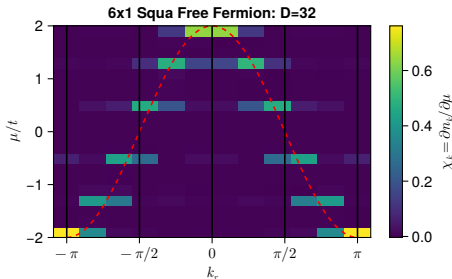$$\chi = \frac{1}{N}\frac{\partial N}{\partial \mu} \tag{18}$$

▶ Simulation results:

Results

▶ k dependent Charge susceptibility.

$$\chi_k = \frac{1}{N}\frac{\partial N_k}{\partial \mu} \tag{19}$$

▶ Simulation results:

Obserables

▶ Spectrum function

$$S(\mathbf{k}, E) = -\frac{1}{\pi}\mathrm{Im}G^{ret}(\mathbf{k}, E), \quad G^{ret}(\mathbf{k}, E) = \int_{-\infty}^{+\infty} G^{ret}(\mathbf{k}, t)\mathrm{e}^{iEt}\mathrm{d}t \quad (20)$$

$$\begin{aligned}
G^{ret}(\mathbf{k}, t) = & -i\Theta(t)\langle\Psi_0|\left[c_k(t)c_k^\dagger(0)\right]|\Psi_0\rangle \\
= & -i[\mathrm{e}^{iE_0 t}\left(\langle\Psi_0|c_k\right)\mathrm{e}^{-iHt}\left(c_k^\dagger|\Psi_0\rangle\right) \\
& + \mathrm{e}^{-iE_0 t}\left(\langle\Psi_0|c_k^\dagger\right)\mathrm{e}^{iHt}\left(c_k|\Psi_0\rangle\right)]
\end{aligned} \quad (21)$$

with

$$c_k = \sum_j \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{R}_j}c_j \quad (22)$$

Results

▶ Simulation Results: