Simulations with MPS/MPO

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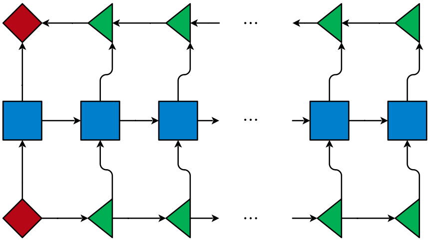
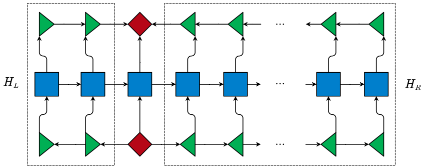
DMRG: 1-site update

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

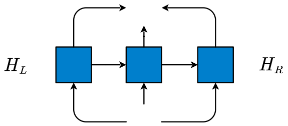


- Sweep at two direction (right - left - right - ...)
  - Calculate the left/right environment H_L/H_R.

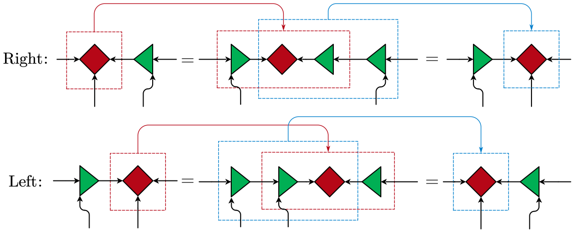


DMRG: 1-site update

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

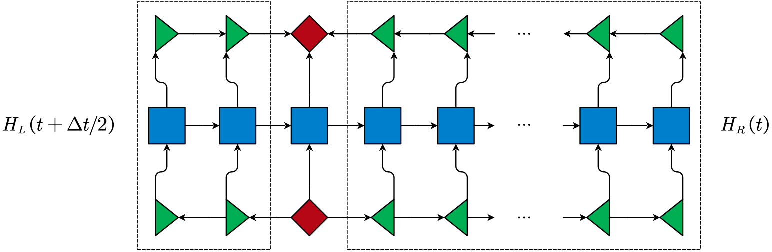


  - OrientSVD and move the center to next site.



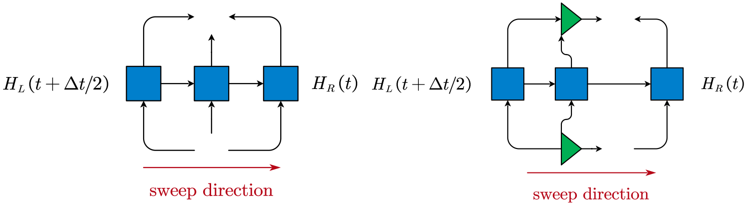
TDVP: 1-site integration

- 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

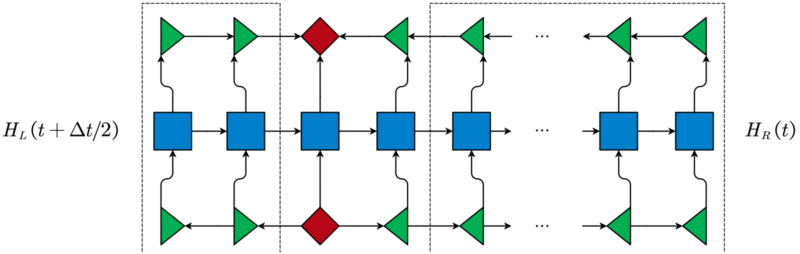
- Sweep at two direction (right - left - right - ...)
  - Calculate the effective Hamiltonian $H_{eff}^{(1)}$
  - Time evolution $A_i(t+\Delta t/2) = \exp\left(-iH_{eff}^{(1)}\Delta t/2\right)A_i(t)$
  - OrientSVD and calculate the center with inverse evolution $C_i(t) = \exp\left(iH_{eff}^{(0)}\Delta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



TDVP: 2-site integration

Sweep schemes

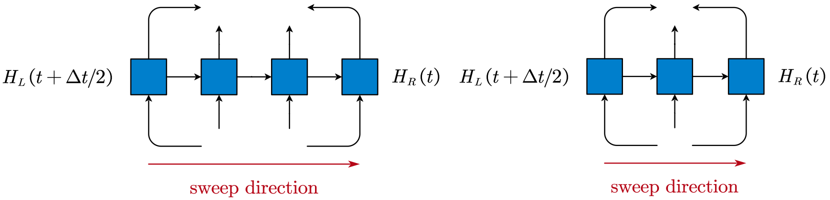
- Calculate the left/right environment $H_L(t + \Delta t/2)/H_R(t)$.



TDVP: 2-site integration

Sweep schemes

- Calculate the effective Hamiltonian $H_{eff}^{(2)}$
- Time evolution $A_i A_{i+1}(t+\Delta t/2) = \exp\left(-iH_{eff}^{(2)}\Delta t/2\right) A_i A_{i+1}(t)$
- 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.



Model:Transverse Ising Chain

- **Hamiltonian:**

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

  we always choose $J = \pm 1.0$.

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

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

$$\epsilon_k = -2J \cos ka - 2h, \quad \Delta_k = 2J \sin ka \tag{3}$$

Model:MPO

- **Hamiltonian:** In kron form:

$$
\begin{aligned}
H =& J\sigma_1^z \otimes \sigma_2^z \otimes \mathbb{1} \otimes \mathbb{1} \otimes \cdots + \mathbb{1} \otimes J\sigma_2^z \otimes \sigma_3^z \otimes \mathbb{1} \otimes \cdots \\
&+ h\sigma_1^x \otimes \mathbb{1} \otimes \mathbb{1} \otimes \cdots + \mathbb{1} \otimes h\sigma_2^x \otimes \mathbb{1} \otimes \cdots \\
&+ h_z\sigma_1^z \otimes \mathbb{1} \otimes \mathbb{1} \otimes \cdots + \mathbb{1} \otimes h_z\sigma_2^z \otimes \mathbb{1} \otimes \cdots
\end{aligned} \tag{4}
$$

- **MPO**

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

Model:MPO

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

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

- **MPO**

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

Model:MPS

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

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

$$\psi_0 = \sum_{\{s_i\}} C_{s_1 s_2 s_3 \cdots s_N} \left|s_1 s_2 s_3 \cdots s_N\right\rangle \tag{8}$$

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

$$C_{111\cdots 1} = 1 \quad \text{or} \quad C_{-1-1-1\cdots -1} = 1 \tag{9}$$

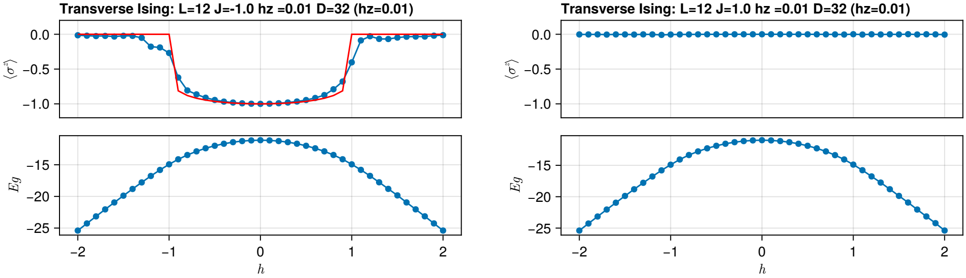
while AFM corresponds to state $C_{s_1 s_2 s_3 \cdots s_N}$ with

$$C_{1-11-1\cdots} = 1 \quad \text{or} \quad C_{-11-11\cdots} = 1 \tag{10}$$

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

Results

Simulation results:



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.

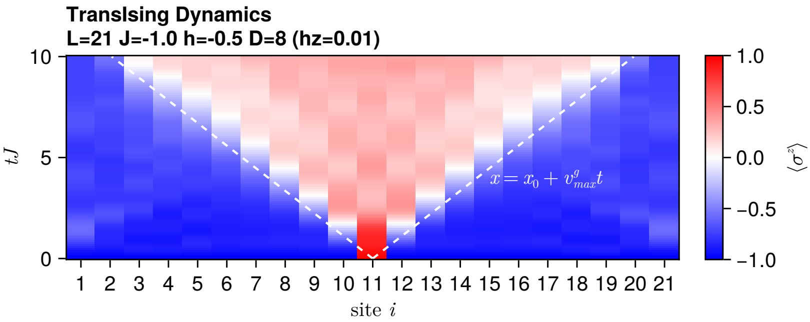
$$\langle \sigma^z \rangle = \left[1 - \left(\frac{h}{J} \right)^2 \right]^{1/8} \tag{11}$$

Results: Dynamics

- Choose initial state relevant is

$$\Psi_0 = |-1, -1, \cdots, -1, 1, -1, \cdots, -1, -1\rangle \tag{12}$$

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



Model: Heisenberg Chain

- **Hamiltonian:**

$$H = -J \sum_{i=1}^{N-1} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+1} \tag{13}$$

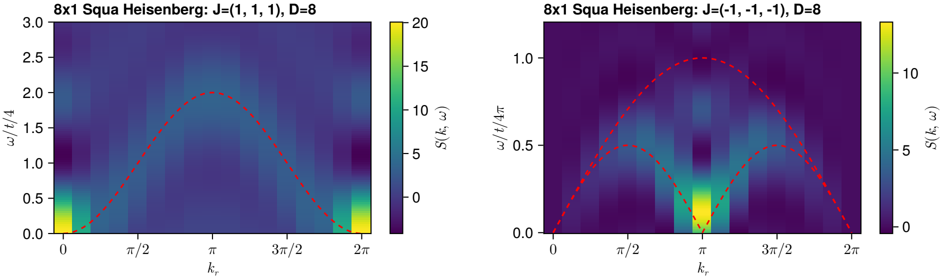
we always choose $J = \pm 1.0$.

Results: Dynamical Spin Structure Factor

- Set

$$J = \pm 1.0, \quad S(\mathbf{q}, \omega) = \int_{-\infty}^{+\infty} \left\langle \boldsymbol{\sigma}_{\mathbf{q}}(t) \cdot \boldsymbol{\sigma}_{-\mathbf{q}}(0) \right\rangle e^{i\omega t} dt \tag{14}$$

- Simulation results:



Model:Free Fermion on Square Lattice

- **Hamiltonian:**

$$H = t \sum_{\langle i,j \rangle} c_i^\dagger c_j + c_j^\dagger c_i \tag{15}$$

- **Parameters:** Physics parameters:

$$t = 1 \tag{16}$$

- **J-W transformation:**

$$c_i = \prod_{j=1}^{i-1} F_j b_i, \quad c_i^\dagger = \prod_{j=1}^{i-1} F_j b_i^\dagger \tag{17}$$

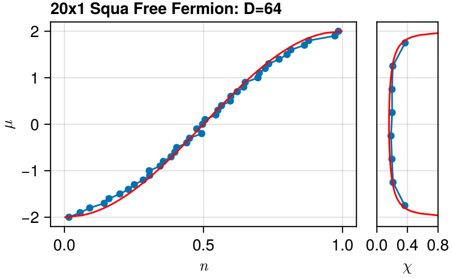
$$F_j = -\sigma_j^z, \quad b_i = \sigma_i^-, \quad b_i = \sigma_i^+ \tag{18}$$

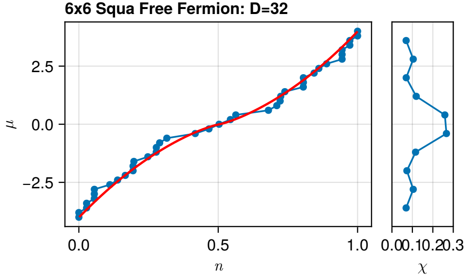
Results

- Charge susceptibility.

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

- Simulation results:



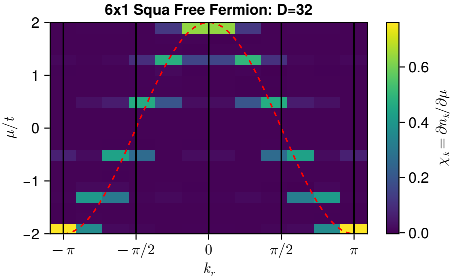


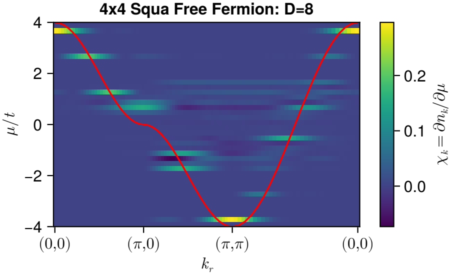
Results

- k dependent Charge susceptibility.

$$\chi_k = \frac{1}{N}\frac{\partial N_k}{\partial \mu} \tag{20}$$

- Simulation results:





Obserables

- Spectrum function

$$S(\boldsymbol{k},E)=-\frac{1}{\pi}\mathrm{Im}G^{ret}(\boldsymbol{k},E),\quad G^{ret}(\boldsymbol{k},E)=\int_{-\infty}^{+\infty}G^{ret}(\boldsymbol{k},t)\mathrm{e}^{iEt}\mathrm{d}t \tag{21}$$

$$\begin{aligned}G^{ret}(\boldsymbol{k},t)=&-i\Theta(t)\left\langle\Psi_0\middle|\left[c_k(t)c_k^\dagger(0)\right]\middle|\Psi_0\right\rangle\\=&-i[\mathrm{e}^{iE_0t}\left(\left\langle\Psi_0\right|c_k\right)\mathrm{e}^{-iHt}\left(c_k^\dagger\left|\Psi_0\right\rangle\right)\\&+\mathrm{e}^{-iE_0t}\left(\left\langle\Psi_0\right|c_k^\dagger\right)\mathrm{e}^{iHt}\left(c_k\left|\Psi_0\right\rangle\right)]\end{aligned} \tag{22}$$

with

$$c_k=\sum_j\mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{R}_j}c_j \tag{23}$$

Results

- Simulation Results: