

Simulations with MPS/MPO

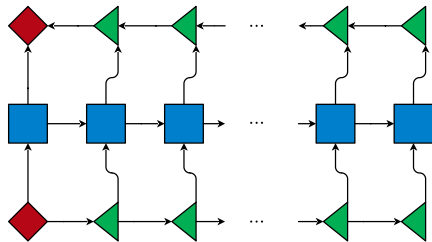
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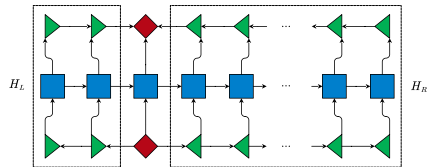
September 20, 2024

DMRG: 1-site update

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

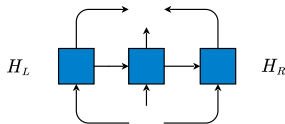


- Sweep at two direction (right - left - right - ...)
- Calculate the left/right environment H_L/H_R .

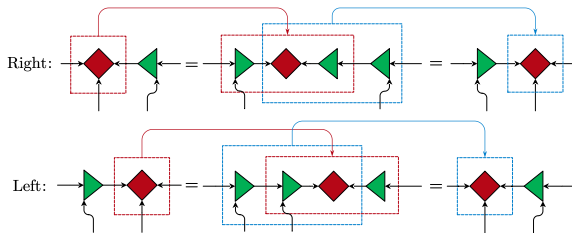


DMRG: 1-site update

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

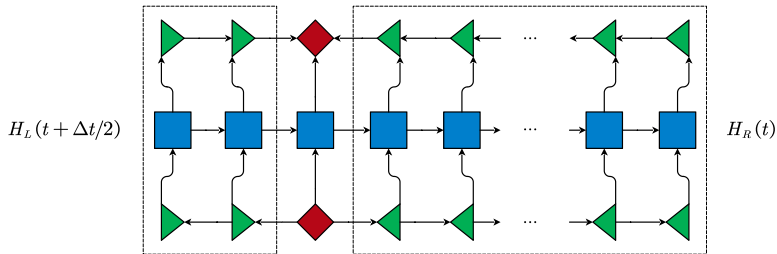


- ▶ OrientSVD and move the center to next site.



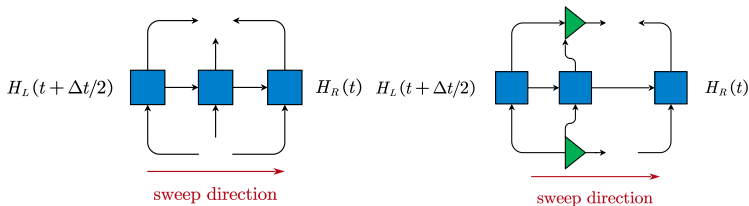
TDVP: 1-site integration

- ▶ 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

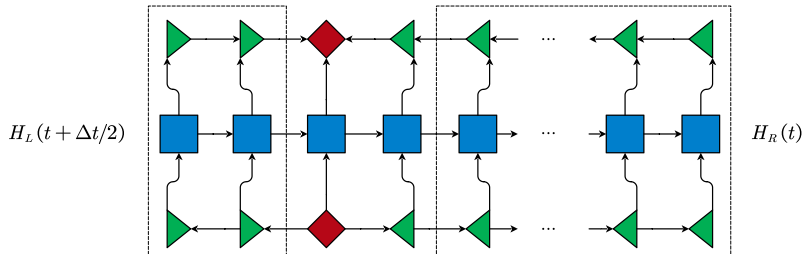
- ▶ Sweep at two direction (right - left - right - ...)
- ▶ Calculate the effective Hamiltonian $H_{eff}^{(1)}$
- ▶ Time evolution $A_i(t + \Delta t/2) = \exp\left(-i H_{eff}^{(1)} \Delta t/2\right) A_i(t)$
- ▶ OrientSVD and calculate the center with inverse evolution $C_i(t) = \exp\left(i H_{eff}^{(0)}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



TDVP: 2-site integration

Sweep schemes

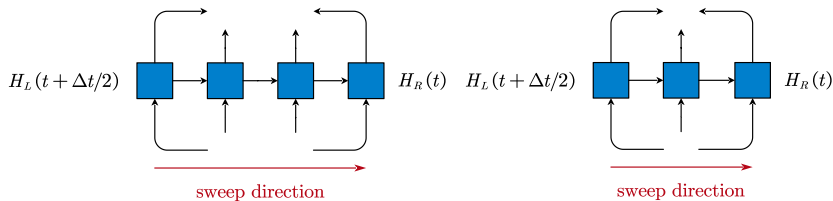
- ▶ Calculate the left/right environment $H_L(t + \Delta t/2)/H_R(t)$.



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.



SETTN

Write ρ in series expansion:

$$\rho = e^{-\beta H} = \sum_{k=0}^{+\infty} \frac{(-\beta H)^k}{k!} \quad (1)$$

calculate the $\{H^k\}$, $k = 0, 1, 2, \dots$

Suppose $X_\rho \in T_\rho M$

$$\frac{d\rho}{d\beta} = \arg \min |X_\rho + H\rho| \quad (2)$$

i.e., project the $H\rho$ onto the tangent space of M at ρ

Model: Transverse Ising Chain

► Hamiltonian:

$$H = -J \sum_{i=1}^{N-1} \sigma_i^z \sigma_{i+1}^z - h \sum_i^N \sigma_{i=1}^x + h_z \sum_{i=1}^N \sigma_i^z \quad (3)$$

we always choose $J = \pm 1.0$.

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

$$H = \sum_{k>0} \lambda(k) \gamma_k^\dagger \gamma_k, \quad \lambda(k) = \sqrt{\epsilon_k^2 + \Delta_k^2}, \quad \begin{pmatrix} \gamma_k^\dagger \\ \gamma_{-k} \end{pmatrix} = \mathbf{P}(k) \begin{pmatrix} c_k^\dagger \\ c_{-k} \end{pmatrix} \quad (4)$$

$$\epsilon_k = -2J \cos ka - 2h, \quad \Delta_k = 2J \sin ka \quad (5)$$

Model:MPO

► **Hamiltonian:** In kron form:

$$\begin{aligned} H = & J\sigma_1^z \otimes \sigma_2^z \otimes 1 \otimes 1 \otimes \dots + 1 \otimes J\sigma_2^z \otimes \sigma_3^z \otimes 1 \otimes \dots \\ & + h\sigma_1^x \otimes 1 \otimes 1 \otimes \dots + 1 \otimes h\sigma_2^x \otimes 1 \otimes \dots \\ & + h_z\sigma_1^z \otimes 1 \otimes 1 \otimes \dots + 1 \otimes h_z\sigma_2^z \otimes 1 \otimes \dots \end{aligned} \quad (6)$$

► **MPO**

$$\begin{aligned} H_1 = & (h\sigma_1^x + h_z\sigma_1^z, \quad J\sigma_1^z, \quad 1), \\ H_i = & \begin{pmatrix} 1, & 0, & 0 \\ \sigma_i^z, & 0, & 0 \\ h\sigma_i^x + h_z\sigma_i^z, & J\sigma_i^z, & 1 \end{pmatrix}, \quad H_N = \begin{pmatrix} 1 \\ \sigma_N^z \\ h\sigma_N^x + h_z\sigma_N^z \end{pmatrix} \end{aligned} \quad (7)$$

Model:MPO

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

$$M_z = \sigma_1^z \otimes \mathbb{1} \otimes \mathbb{1} \otimes \dots + \mathbb{1} \otimes \sigma_2^z \otimes \mathbb{1} \otimes \dots \quad (8)$$

► **MPO**

$$H_1 = (\sigma_1^z, \mathbb{1}),$$
$$H_i = \begin{pmatrix} \mathbb{1} & 0 \\ \sigma_i^z & \mathbb{1} \end{pmatrix}, \quad H_N = \begin{pmatrix} \mathbb{1} \\ \sigma_N^z \end{pmatrix} \quad (9)$$

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

$$\psi_0 = \sum_{\{s_i\}} C_{s_1 s_2 s_3 \cdots s_N} |s_1 s_2 s_3 \cdots s_N\rangle \quad (10)$$

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

$$C_{111\dots 1} = 1 \quad \text{or} \quad C_{-1-1-1\dots -1} = 1 \quad (11)$$

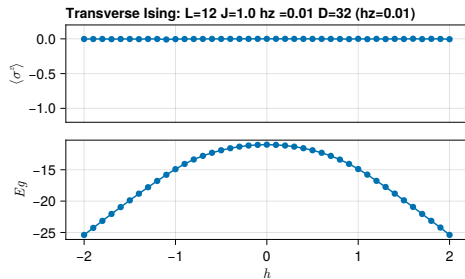
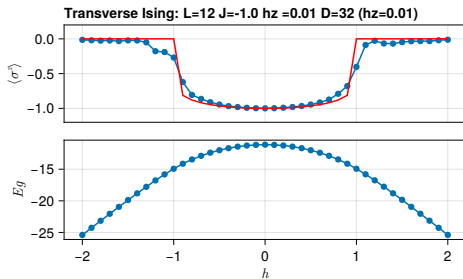
while AFM corresponds to state $C_{s_1 s_2 s_3 \dots s_N}$ with

$$C_{1-11-1\dots} = 1 \quad \text{or} \quad C_{-11-11\dots} = 1 \quad (12)$$

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

Results

Simulation results:



Where exact solution can be obtained by calculating $\langle \sigma_i^z \sigma_j^z \rangle$ and let $|i - j| \rightarrow +\infty$, i.e.

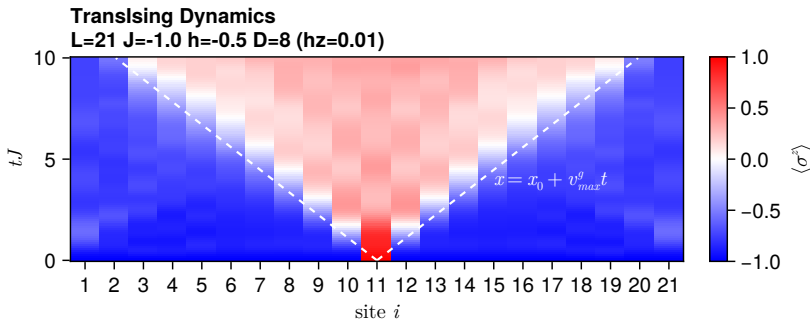
$$\langle \sigma^z \rangle = \left[1 - \left(\frac{h}{J} \right)^2 \right]^{1/8} \quad (13)$$

Results: Dynamics

- Choose initial state relevant is

$$\Psi_0 = |-1, -1, \dots, -1, 1, -1, \dots, -1, -1\rangle \quad (14)$$

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



Model: Heisenberg Chain

► Hamiltonian:

$$H = -J \sum_{i=1}^{N-1} \sigma_i \cdot \sigma_{i+1} \quad (15)$$

we always choose $J = \pm 1.0$.

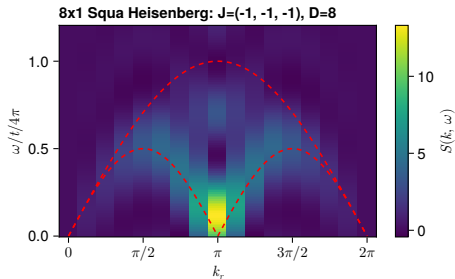
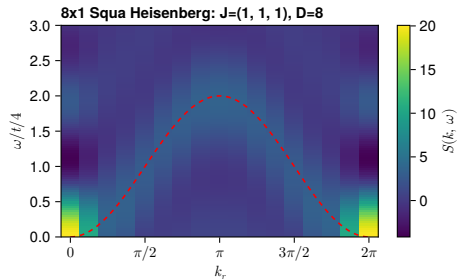
Results: Dynamical Spin Structure Factor

► Set

$$J = \pm 1.0, \quad S(\mathbf{q}, \omega) = \int_{-\infty}^{+\infty} \langle \boldsymbol{\sigma}_{\mathbf{q}}(t) \cdot \boldsymbol{\sigma}_{-\mathbf{q}}(0) \rangle e^{i\omega t} dt \quad (16)$$

► Simulation results:

L=16, D?



Model: Free Fermion on Square Lattice

► Hamiltonian:

$$H = t \sum_{\langle i,j \rangle} c_i^\dagger c_j + c_j^\dagger c_i \quad (17)$$

► Parameters: Physics parameters:

$$t = 1 \quad (18)$$

► J-W transformation:

$$c_i = \prod_{j=1}^{i-1} F_j b_i, \quad c_i^\dagger = \prod_{j=1}^{i-1} F_j b_i^\dagger \quad (19)$$

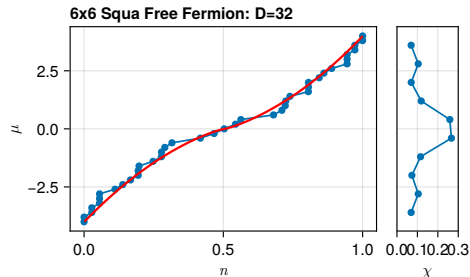
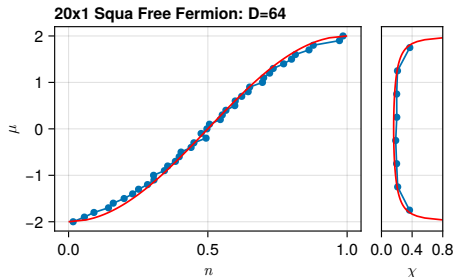
$$F_j = -\sigma_j^z, \quad b_i = \sigma_i^-, \quad b_i = \sigma_i^+ \quad (20)$$

Results

- Charge compressibility.

$$\chi = \frac{1}{N} \frac{\partial N}{\partial \mu} \quad (21)$$

- Simulation results:

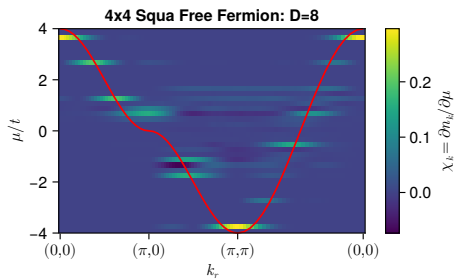
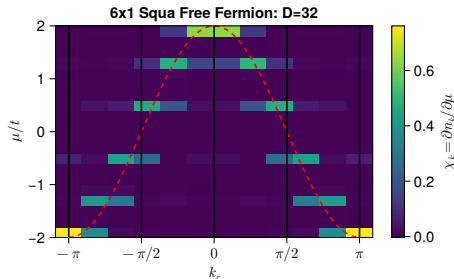


Results

- ▶ k dependent Charge compressibility.

$$\chi_k = \frac{1}{N} \frac{\partial N_k}{\partial \mu} \quad (22)$$

- ▶ Simulation results:



Observables

► Spectrum function

$$S(\mathbf{k}, E) = -\frac{1}{\pi} \text{Im} G^{ret}(\mathbf{k}, E), \quad G^{ret}(\mathbf{k}, E) = \int_{-\infty}^{+\infty} G^{ret}(\mathbf{k}, t) e^{iEt} dt \quad (23)$$

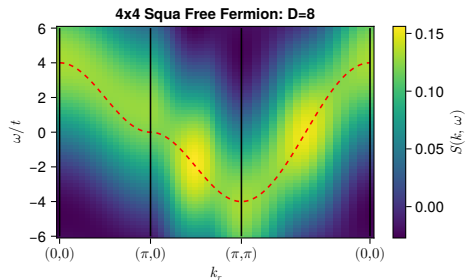
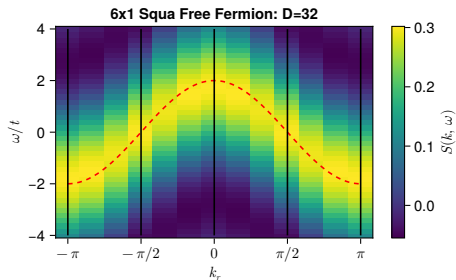
$$\begin{aligned} G^{ret}(\mathbf{k}, t) &= -i\Theta(t) \langle \Psi_0 | [c_{\mathbf{k}}(t) c_{\mathbf{k}}^{\dagger}(0)] | \Psi_0 \rangle \\ &= -i[e^{iE_0 t} (\langle \Psi_0 | c_{\mathbf{k}}) e^{-iHt} (c_{\mathbf{k}}^{\dagger} | \Psi_0 \rangle) \\ &\quad + e^{-iE_0 t} (\langle \Psi_0 | c_{\mathbf{k}}^{\dagger}) e^{iHt} (c_{\mathbf{k}} | \Psi_0 \rangle)] \end{aligned} \quad (24)$$

with

$$c_{\mathbf{k}} = \sum_j e^{-i\mathbf{k} \cdot \mathbf{R}_j} c_j \quad (25)$$

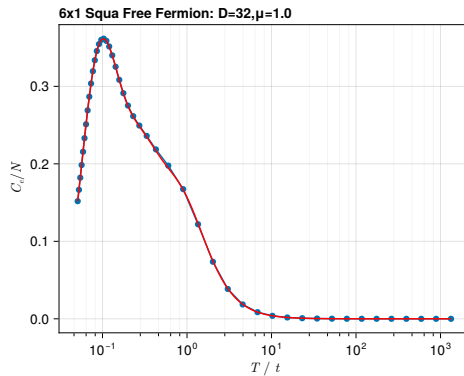
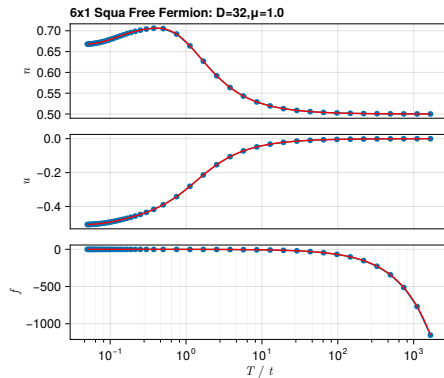
Results

► Simulation Results:



Results

► Finite Temperature Results:



Model: Hubbard Model on Square Lattice

► **Hamiltonian:**

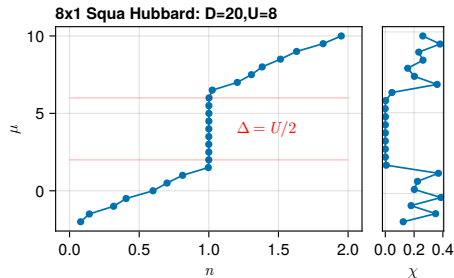
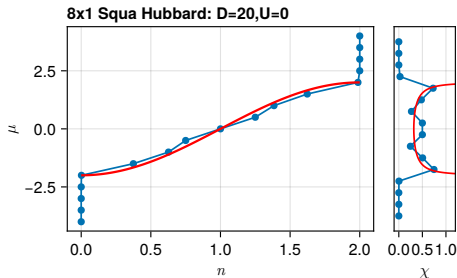
$$H = t \sum_{\langle i,j \rangle} \left(c_i^\dagger c_j + c_j^\dagger c_i \right) + \frac{U}{2} \sum_{\langle i \rangle} n_{i,\sigma} n_{i,\hat{\sigma}} \quad (26)$$

Results

- Charge compressibility.

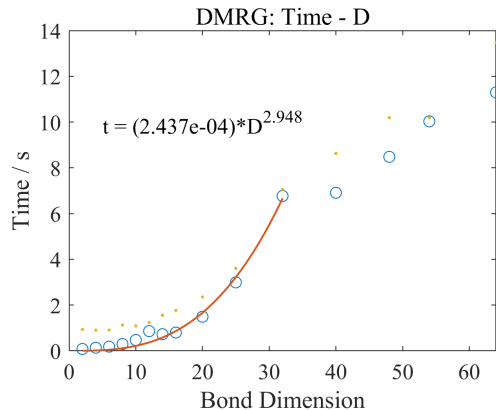
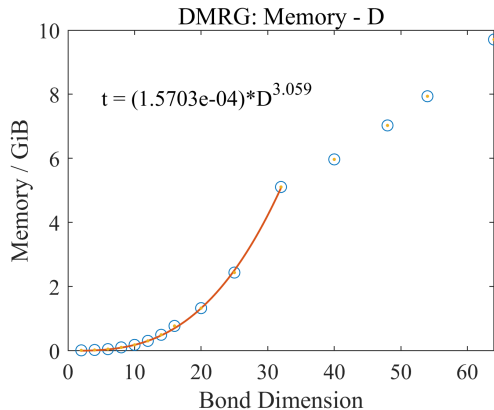
$$\chi = \frac{1}{N} \frac{\partial N}{\partial \mu} \quad (27)$$

- Simulation results:



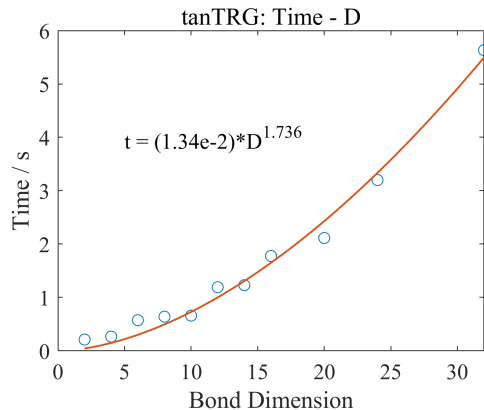
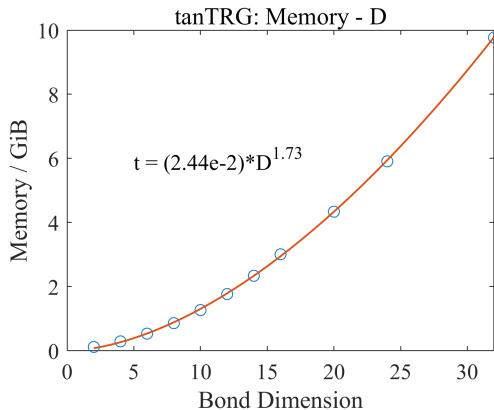
Benchmark

► DMRG complexity:



Benchmark

► tanTRG + SETTN complexity:



Source code

Can be found at <https://github.com/KunyangDU/iMPS.git>, where dev branch is the latest version, but is still under developemnt.