Matrix product states

d sites $\qquad \mathcal{F}_d = \{ |s_1, \cdots, s_d\rangle \mid s_i \in \{1,2\} \} \cong \mathbb{C}^{2^d}$.

$$|\Psi\rangle = \sum_{s} \psi(s_1, \cdots, s_d) \, |s_1 \cdots s_d\rangle .$$

SVD.

$$\psi(s_1, \underbrace{s_2, \cdots, s_d}_{\text{group}}) = \sum_{i=1}^{a_1} \left(A_1(s_1) \right)_i \; \hat{\psi}^{(1)}_i (s_2, \cdots, s_d))$$

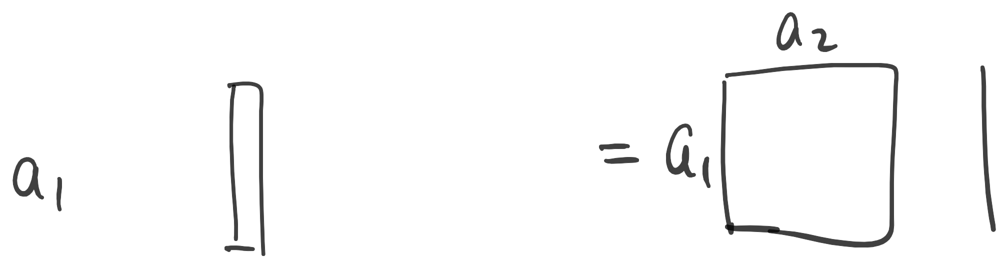
$$= A_1(s_1) \; \hat{\psi}^{(1)} (s_2, \cdots, s_d)$$

$$= A_1(s_1)_{a_0 = 1} \overset{a_1}{\text{——}} \quad \hat{\psi}^{(1)} \; a_1 \Big|$$

$a_1 \leq 2$.

$$\hat{\psi}^{(1)}_i(s_2, \cdots, s_d) = \sum_{j=1}^{a_2} \left(A_2(s_2)\right)_{ij} \hat{\psi}^{(2)}_j(s_3, \cdots, s_d)$$

$$\Rightarrow \hat{\psi}^{(1)}(s_2, \cdots, s_d) = A_2(s_2)\, \hat{\psi}^{(2)}(s_3, \cdots, s_d)$$



$a_2 \le 2^2$.

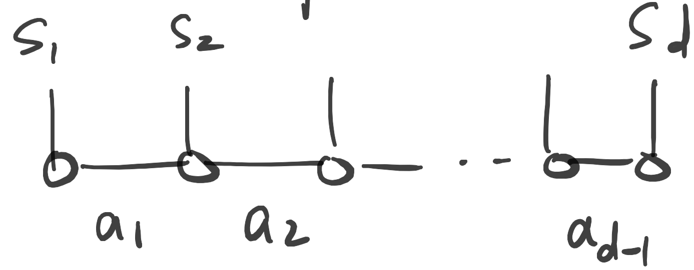
$$\Rightarrow \psi(s_1, \cdots, s_d) = A_1(s_1) A_2(s_2) \cdots A_d(s_d).$$

$A_i(s_i) \in \mathbb{C}^{a_{i-1} \times a_i}$, $a_0 = a_d = 1$.

$a_i \le 2^i$

MPS. $m = \max\{a_0, \cdots, a_d\}$ bond dimension.

graphical representation



edge : matrix-matrix multiplication.

Useful scenario.

$\psi(s_1, \cdots, s_d)$ well approximated by MPS

w. m weakly depending on d.

$$\mathcal{F}^{mps}_{m,d} = \{ A_1(s_1) \cdots A_d(s_d) \mid A_i \in \mathbb{C}^{a_{i-1} \times a_i}, a_0 = a_d = 1, a_i \le m \}.$$

Bounded MPS dimension?

Area law.

Essentially, 1D quantum systems

ground state

short range interaction

gapped.

$$E_0 \leq \inf_{\substack{\psi \in \mathcal{F}^{MPS}_{n,d} \\ \langle\psi|\psi\rangle = 1}} \langle\psi| H |\psi\rangle$$

H : lattice Hamiltonian.

e.g. 1D Heisenberg.

$$H = \sum_{i=1}^{d-1} \vec{S}_i \cdot \vec{S}_{i+1} = \sum_{i=1}^{d-1} \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y\right) + \sum_{i=1}^{d} S_i^z S_{i+1}^z$$

$$= \frac{1}{2} \sum_{i=1}^{d-1} \left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right) + \sum_{i=1}^{d} S_i^z S_{i+1}^z$$

$$S^+ = S_x + i S_y = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad S^- = S_x - i S_y = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$$

DMRG: an <u>algorithm</u> to solve optimization problem. (2-site version)

Ex. 2-site

$$|\psi\rangle = \sum_{K} A_1(s_1)\, C\, B_2(s_2)\, |s_1 s_2\rangle$$

$1 = a_0 \overset{a_1}{\text{———}}$ $\quad a_1 \big|$. $\quad a_1 = 2$

$a_2 = 1,$

o | o

L   R .

$$|\tilde{\phi}^{L(1)}_{\alpha}\rangle = |s_1\rangle \quad , \quad \alpha = s_1$$

$$|\tilde{\phi}^{R(2)}_{\beta}\rangle = |s_2\rangle \quad , \quad \beta = s_2$$

$$|\Psi\rangle = \sum_{\alpha\beta} \tilde{C}_{\alpha\beta} \, |\tilde{\phi}^{L(1)}_{\alpha} \tilde{\phi}^{R(2)}_{\beta}\rangle$$

$$\langle \tilde{\phi}^{L(1)}_{\alpha} \tilde{\phi}^{R(2)}_{\beta} | \tilde{\phi}^{L(1)}_{\alpha'} \tilde{\phi}^{R(2)}_{\beta'} \rangle = \delta_{\alpha\alpha'} \delta_{\beta\beta'}$$

Solve $\sum_{\alpha'\beta'} \langle \tilde{\phi}^{L(1)}_{\alpha} \tilde{\phi}^{R(2)}_{\beta} | H | \tilde{\phi}^{L(1)}_{\alpha'} \tilde{\phi}^{R(2)}_{\beta'} \rangle \tilde{C}_{\alpha'\beta'} = E \tilde{C}_{\alpha\beta}$

$$\tilde{C}_{\alpha\beta} = \sum_{K} U_{\alpha,K} \, \sigma_K \, \bar{V}_{\beta,K}$$

$$(A(s_1))_{1,K} = U_{s_1,K} \qquad (B(s_2))_{K,1} = \bar{V}_{s_2,K}$$

$$C_{KK'} = \sigma_K \delta_{KK'}$$

$$\sum_{s_1} A_1(s_1)^* A_1(s_1) = \delta_{\alpha\alpha'}$$

$$\sum_{s_2} B_2(s_2) B_2^*(s_2) = \delta_{\beta\beta'}.$$

change of basis

$$|\phi_\alpha^{L(1)}\rangle = \sum_{s_1} \left(A_1(s_1)\right)_{1,\alpha} |s_1\rangle$$

$$|\phi_\beta^{R(2)}\rangle = \sum_{s_2} \left(B_2(s_2)\right)_{\beta,1} |s_2\rangle$$

Ex. 4-site.

$$\begin{array}{cc|cc} 1 & 2 & 3 & 4 \\ \circ & \circ & \circ & \circ \end{array}$$

$$|\tilde{\phi}^{L(2)}_{\tilde{\alpha}}\rangle = |\phi^{L(1)}_{\alpha}\rangle \otimes |S_2\rangle . \qquad \tilde{\alpha} = (\alpha, S_2)$$

extended basis

$$|\tilde{\phi}^{R(3)}_{\tilde{\beta}}\rangle = |S_3\rangle \otimes |\phi^{R(4)}_{\beta}\rangle . \qquad \tilde{\beta} = (S_3, \beta)$$

$$\langle \tilde{\phi}^{L(2)}_{\tilde{\alpha}} \tilde{\phi}^{R(3)}_{\tilde{\beta}} | \tilde{\phi}^{L(2)}_{\tilde{\alpha}'} \tilde{\phi}^{R(3)}_{\tilde{\beta}'} \rangle = \delta_{\tilde{\alpha}\tilde{\alpha}'} \delta_{\tilde{\beta}\tilde{\beta}'}$$

$$|\Psi\rangle = \sum_{\tilde{\alpha}\tilde{\beta}} \tilde{C}_{\tilde{\alpha}\tilde{\beta}} \, |\phi^{L(2)}_{\tilde{\alpha}} \phi^{R(3)}_{\tilde{\beta}}\rangle$$

$$\sum_{\tilde{\alpha}'\tilde{\beta}'} \langle \phi^{L(2)}_{\tilde{\alpha}} \phi^{R(3)}_{\tilde{\beta}} | H | \phi^{L(2)}_{\tilde{\alpha}'} \phi^{R(3)}_{\tilde{\beta}'} \rangle \tilde{C}_{\tilde{\alpha}'\tilde{\beta}'} = \epsilon \, \tilde{C}_{\tilde{\alpha}'\tilde{\beta}'}$$

superblock Hamiltonian

SVD

$$\tilde{C}_{\tilde{\alpha}\tilde{\beta}} = \sum_{k=1}^{m} U_{\tilde{\alpha}k} \, \sigma_k \, V^*_{\tilde{\beta}k} . \qquad (m \le 2^2)$$

Link w. MPS.

$$\left(A_2(S_2)\right)_{\alpha',k} = U_{(\alpha', S_2), k} .$$

$$\left(B_3\,(S_3)\right)_{k,\beta'} = \bar{V}_{(S_3, \beta'), k} .$$

k : bond dimension

$k = 1, \cdots, m$

$$|\phi^{L(2)}_{\alpha}\rangle = \sum_{\alpha'=1}^{a_1}\sum_{s_2} \left(A_2(s_2)\right)_{\alpha',\alpha} |\phi^{L(1)}_{\alpha'}\rangle \otimes |s_2\rangle .$$

$\alpha = 1, \cdots, a_2 = m$

$$|\phi^{R(3)}_{\beta}\rangle = \sum_{\beta'=1}^{a_3}\sum_{s_3} \left(B_3(s_3)\right)_{\beta,\beta'} |s_3\rangle \otimes |\phi^{R(4)}_{\beta'}\rangle$$

$\beta = 1, \cdots, b_3 = m .$

$$\langle \phi^{L(2)}_{\alpha} | \phi^{L(2)}_{\alpha'} \rangle = \sum_{s_2} \left(A_2^{*}(s_2)\, A_2(s_2) \right)_{\alpha,\alpha'} = \delta_{\alpha\alpha'} ,$$

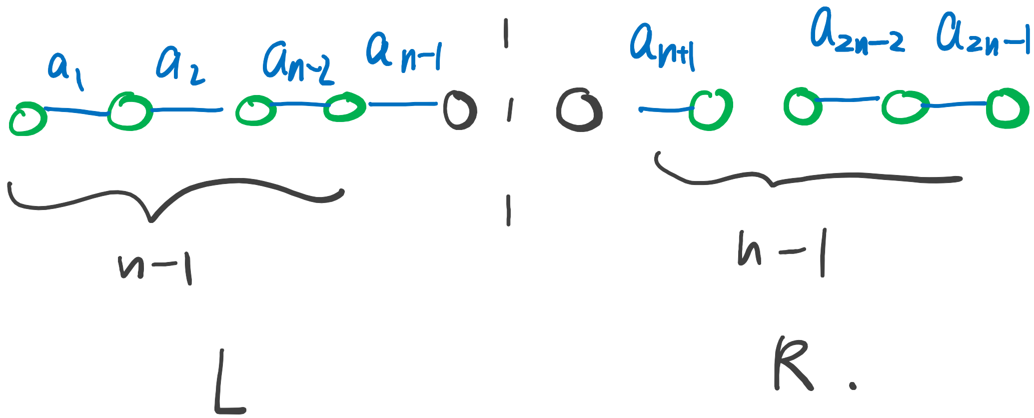
$$\langle \phi^{R(3)}_{\beta} | \phi^{R(3)}_{\beta'} \rangle = \underbrace{\sum_{s_3} \left(B_3(s_3)\, B_3^{*}(s_3) \right)_{\beta,\beta'} = \delta_{\beta\beta'}}_{\text{orthogonality of } U, V.} .$$

(ex.er) $$|\psi\rangle = \sum_{\alpha\beta} C_{\alpha\beta} \, | \phi^{L(2)}_{\alpha} \, \phi^{R(3)}_{\beta} \rangle$$

$$= \sum_{s_1,\cdots s_4} A_1(s_1)\, A_2(s_2)\, C \, B_3(s_3)\, B_4(s_4)$$

$$C_{\alpha\beta} = \sigma_k \, \delta_{\alpha k} \, \delta_{\beta k} .$$

2n sites



$$|\phi^{L(n-1)}_{\alpha}\rangle \qquad |\phi^{R(n+2)}_{\beta}\rangle$$ given. orthogonal.

$$\alpha = 1, \cdots, a_{n-1} \qquad \beta = 1, \cdots, a_{n+1}$$

$$|\tilde{\phi}^{L(n)}_{\tilde{\alpha}}\rangle = |\phi^{L(n-1)}_{\alpha}\rangle \otimes |s_n\rangle \quad , \quad \tilde{\alpha} = (\alpha, s_n)$$

$$|\tilde{\phi}^{R(n+1)}_{\tilde{\beta}}\rangle = |s_{n+1}\rangle \otimes |\phi^{R(n+2)}_{\beta}\rangle \quad \tilde{\beta} = (s_{n+1}, \beta).$$

$$\sum_{\tilde{\alpha}'\tilde{\beta}'} \langle \tilde{\phi}^{L(n)}_{\tilde{\alpha}} \tilde{\phi}^{R(n+1)}_{\tilde{\beta}} | H | \tilde{\phi}^{L(n)}_{\tilde{\alpha}'} \tilde{\phi}^{R(n+1)}_{\tilde{\beta}'} \rangle \tilde{C}_{\tilde{\alpha}'\tilde{\beta}'}$$

$$= \tilde{C}_{\tilde{\alpha}'\tilde{\beta}'} E$$

$$\tilde{C}_{\tilde{\alpha}\tilde{\beta}} \simeq \sum_{K} U_{\tilde{\alpha}K} \sigma_K V^*_{\tilde{\beta}K} \quad , \; K=1, \cdots, m$$

$$(A_n(S_n))_{\alpha', K} = U_{(\alpha', S_n), K}$$

$$(B_{n+1}(S_{n+1}))_{K, \beta'} = \overline{V}_{(S_{n+1}, \beta'), K}$$

$$\sum_{S_n} (A_n(S_n))^* (A_n(S_n)) = U^* U = I_m$$

$$\sum_{s_{n+1}} \left(B_{n+1}(s_{n+1})\right)\left(B_{n+1}(s_{n+1})\right)^{*} = V^{*}V = I_m .$$

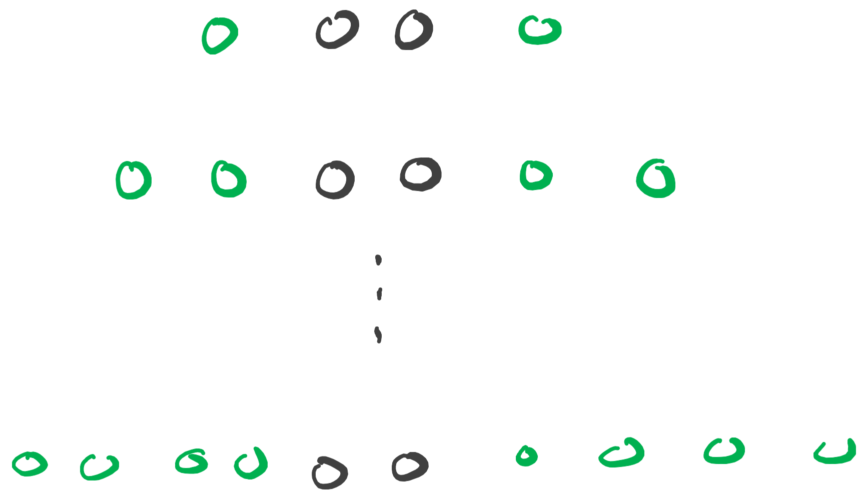
$$|\phi^{L(n)}_{\alpha}\rangle = \sum_{\alpha'}\sum_{s_n} \left(A_n(s_n)\right)_{\alpha',\alpha} |\phi^{L(n-1)}_{\alpha'}\rangle \otimes |s_n\rangle$$

$$|\phi^{R(n+1)}_{\beta}\rangle = \sum_{\beta'}\sum_{s_{n+1}} \left(B_n(s_{n+1})\right)_{\beta,\beta'} |s_{n+1}\rangle \otimes |\phi^{R(n+2)}_{\beta'}\rangle$$

$$\langle \phi^{L(n)}_{\alpha} | \phi^{L(n)}_{\alpha'}\rangle = \delta_{\alpha\alpha'}$$

$$\langle \phi^{R(n+1)}_{\beta} | \phi^{R(n+1)}_{\beta'}\rangle = \delta_{\beta\beta'}$$

Infinite system DMRG



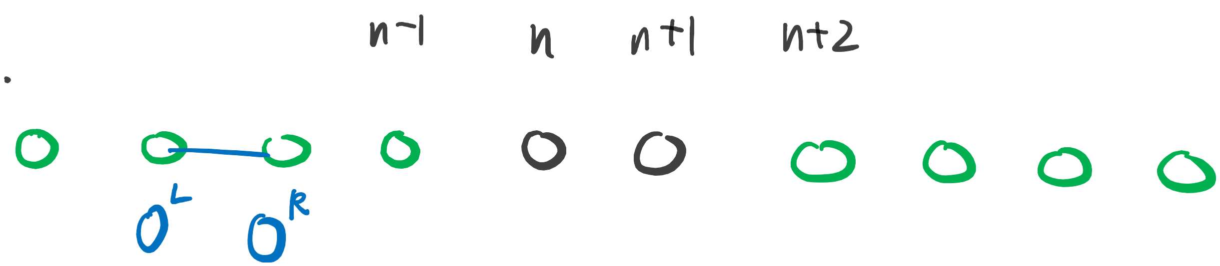
Efficient computation of

$$\langle \phi^{L(n)}_{\alpha'} \, \phi^{R(n+1)}_{\tilde{\beta}'} \, | \, H \, | \, \tilde{\phi}^{L(n)}_{\tilde{\alpha}} \, \tilde{\phi}^{R(n+1)}_{\tilde{\beta}} \rangle .$$

$$H = \sum_{i=1}^{2n-1} \vec{S}_i \cdot \vec{S}_{i+1}$$

$$=: \sum_{i=1}^{2n-1} O_{L,i} \, O_{R,i}$$

Case 1.

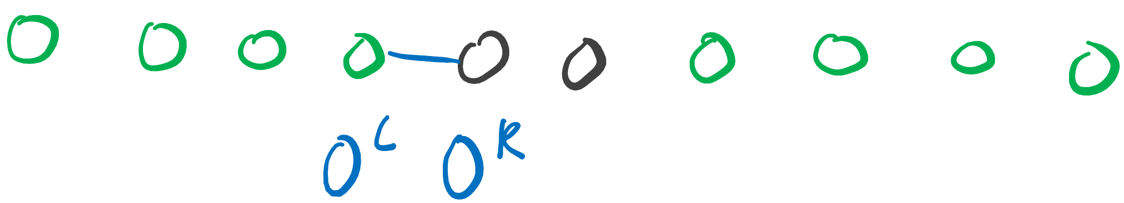


$$(\star)\quad \langle \tilde{\phi}^{L(n)}_{\tilde{\alpha}'}, \tilde{\phi}^{R(n+1)}_{\tilde{\beta}'} \,|\, O^L O^R \,|\, \tilde{\phi}^{L(n)}_{\tilde{\alpha}} \, \tilde{\phi}^{R(n+1)}_{\tilde{\beta}} \rangle$$

$$= \delta_{\tilde{\beta}'\tilde{\beta}} \, \delta_{s_n' s_n} \langle \phi^{L(n-1)}_{\alpha'} \,|\, O^L O^R \,|\, \phi^{L(n-1)}_{\alpha} \rangle .$$

reuse $\quad \langle O^L O^R \rangle^{L(n-1)}_{\alpha'\alpha}$

Case 2.

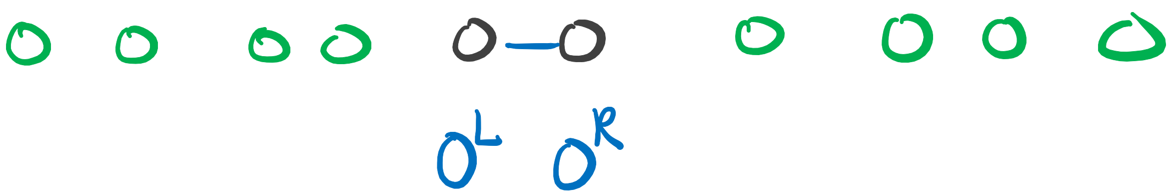


$$\langle \tilde\phi^{L(n)}_{\tilde\alpha'} \tilde\phi^{R(n+1)}_{\tilde\beta'} | O^L O^R | \tilde\phi^{L(n)}_{\tilde\alpha} \tilde\phi^{R(n+1)}_{\tilde\beta} \rangle$$

$$= \underbrace{\langle \phi^{L(n-1)}_{\alpha'} | O^L | \phi^{L(n-1)}_{\alpha} \rangle}_{\text{reuse}} \underbrace{\langle S_n' | O^R | S_n \rangle}_{\text{direct compute}} \delta_{\tilde\beta'\tilde\beta}$$

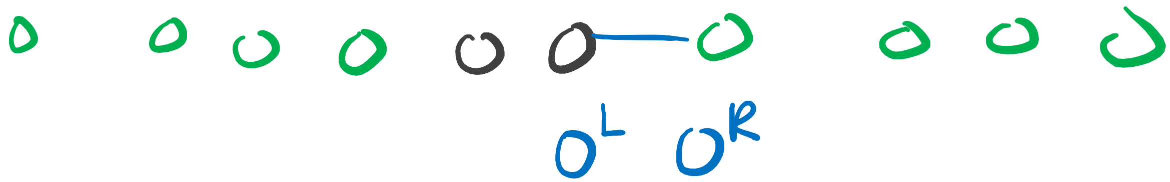
$$\langle O^L \rangle^{L(n-1)}_{\alpha'\alpha}$$

Case 3.



$$(\star) = \langle S_n' | O^L | S_n \rangle \langle S_{n+1}' | O^R | S_{n+1} \rangle \delta_{\alpha'\alpha} \delta_{\beta'\beta}$$

Case 4.



Same case 2

Same case 1.

Update basis. $\langle O^L \rangle \to \langle s_n' | O^L | s_n \rangle$

$$\langle O^L O^R \rangle^{L(n-1)}_{\alpha'\alpha} \delta_{s_n' s_n} \longrightarrow \langle O^L O^R \rangle^{L(n)}$$

1. $\langle O^L O^R \rangle^{L(n)} = U^* \left(\langle O^L O^R \rangle^{L(n-1)} \otimes I_2 \right) U$

2. $\langle O^L \rangle^{L(n)} = U^* \left(I_{a_{n-1}} \otimes \langle O^L \rangle \right) U.$

4. $\langle O^R \rangle^{R(n+1)} = V^* \left(\langle O^R \rangle \otimes I_{a_{n+2}} \right) V$

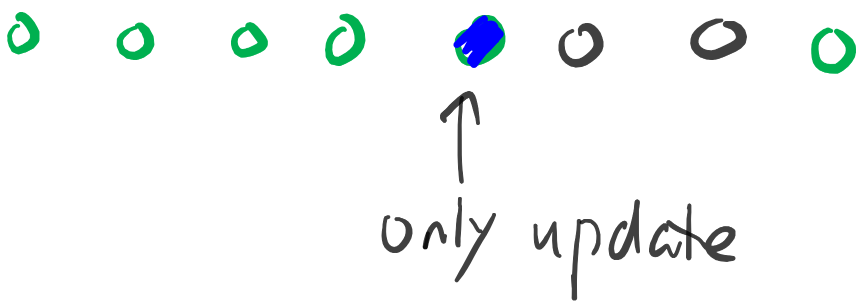
5. $\langle O^L O^R \rangle^{R(n+1)} = V^* \left(I_2 \otimes \langle O^L O^R \rangle^{R(n+2)} \right) V$

3. intact.

Finite system DMRG.

sweeping

right sweep



then left sweep.

fermionic system.

$$H = -t \sum_{i=1}^{N-1} \sum_{\sigma} \left(c_{i\sigma}^{\dagger} c_{i+1\sigma} + h.c. \right) + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow}.$$

Jordan-Wigner transformation.

$1\uparrow$	$1\downarrow$	$2\uparrow$	$2\downarrow$	$\cdots$	$N\uparrow$	$N\downarrow$		fermions
1	2	3				$2N$.		spins.

$$c_{i\uparrow}^{\dagger} = Z^{(i-1), \leftarrow} \otimes \left(A^{\dagger} \otimes I \right) \otimes I^{(i+1), \rightarrow}$$

$$Z^{j,\leftarrow} = \underbrace{Z \otimes Z \otimes \cdots \otimes Z}_{2j}$$

$$\underline{I}^{j,\rightarrow} = \underbrace{\underline{I} \otimes \cdots \otimes \underline{I}}_{2(N-j+1)}$$

$$C_{i\downarrow}^{\dagger} = Z^{(i-1),\leftarrow} \otimes (\underline{I} \otimes A^{\dagger}) \otimes \underline{I}^{i+1,\rightarrow} .$$

$C_{i\uparrow}$, $C_{i\downarrow}$ similar.

$$c^\dagger_{i\uparrow}\, c_{i+1\uparrow} = \left(Z^{i-1,\leftarrow} \otimes (A^\dagger \otimes I) \otimes (I \otimes I) \otimes I^{i+2,\rightarrow}\right)$$

$$\left(Z^{i-1,\leftarrow} \otimes (Z \otimes Z) \otimes (A \otimes I) \otimes I^{i+2,\rightarrow}\right)$$

$$= I^{i-1,\leftarrow} \otimes \underbrace{(A^\dagger Z \otimes Z)}_{O^L} \otimes \underbrace{(A \otimes I)}_{O^R.} \otimes I^{i+2,\rightarrow}$$

$$c^\dagger_{i+1,\uparrow}\, c_{i,\uparrow} = I^{i-1,\leftarrow} \otimes \underbrace{(ZA \otimes Z)}_{O^L} \otimes \underbrace{(A^\dagger \otimes I)}_{O^R} \otimes I^{i+2,\rightarrow}$$

Similar for other terms.

Use previous alg. Note distinction between left and right side

($Z \otimes Z$ always on the left)