

CBE DMRG at single-site costs

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Controlled Bond Expansion for Density Matrix Renormalization Group Ground State Search at Single-Site Costs

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MPO and MPS representation

- Hamiltonian expressed by MPO

$$H = * \square^{W_1} \square^{W_2} \cdots \square^{W_\ell} \square^{W_{\ell+1}} \cdots \square^{W_{\mathcal{L}-1}} \square^{W_{\mathcal{L}}} *$$

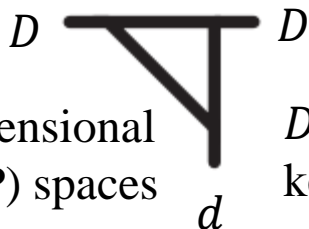
d w d

Exponential growth of physical space d^L Finite virtual bond dimension w

- Wave function expressed by MPS

$$\Psi = * \vee^{A_1} \vee^{A_2} \cdots \vee^{A_\ell} \bigcirc^{\Lambda_\ell} \vee^{B_{\ell+1}} \cdots \vee^{B_{\mathcal{L}-1}} \vee^{B_{\mathcal{L}}} *$$

d D D d



Dd -dimensional
parent(P) spaces

D -dimensional
kept(K) spaces

$$A_\ell^\dagger A_\ell = \bigcap_{A_\ell^*}^{A_\ell} = \left(= \mathbb{1}_\ell^K, \quad B_\ell B_\ell^\dagger = \bigcap_{B_\ell^*}^{B_\ell} = \right) = \mathbb{1}_{\ell-1}^K$$

DMRG→Optimize MPS

- Two site update

$$H_\ell^{2s} = \left[\begin{array}{c} D \\ \text{---} d \quad d \text{---} \\ \ell-1 \quad \ell \quad \ell+1 \quad \ell+2 \end{array} \right]^D = \left(\begin{array}{c} \text{---} \times \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \times \text{---} \\ \times \text{---} \square \text{---} \square \text{---} \square \text{---} \square \text{---} \square \text{---} \square \text{---} \times \\ 1 \quad \ell-1 \quad \ell \quad \ell+1 \quad \ell+2 \quad \mathcal{L} \end{array} \right)$$

$$(H_\ell^{2s} - E)\psi_\ell^{2s} = 0, \quad \left[\text{Diagram: A box with two vertical lines, each containing a square, connected by a horizontal line with a loop on top. The box is labeled with indices $\ell-1, \ell, \ell+1, \ell+2$ at the bottom.} \right] = E \frac{A_\ell \Lambda_\ell B_{\ell+1}}{\text{Diagram: A box with two vertical lines, each containing a square, connected by a horizontal line with a loop on top. The box is labeled with indices $\ell, \ell+1$ at the bottom.}},$$

- One site update

$$H_\ell^{1s} = \overset{D}{\left[\begin{array}{ccc} & d & \\ \diagup & \square & \diagdown \\ \ell-1 & \ell & \ell+1 \end{array} \right]}^D = \left[\begin{array}{cccc} & & & \\ & \diagup & & \diagdown \\ & \square & & \\ & \diagdown & & \diagup \\ \ell-2 & \ell-1 & \ell & \ell+1 \end{array} \right] = \left[\begin{array}{cccc} & & & \\ & & & \\ & \diagdown & & \diagup \\ & \square & & \square \\ & \diagup & & \diagdown \\ \ell-1 & \ell & \ell+1 & \ell+2 \end{array} \right].$$

$$(H_\ell^{1s} - E)\psi_\ell^{1s} = 0, \quad \text{Diagrammatic equation: } \left[\text{triangle} \right]_{\ell-1, \ell, \ell+1} = E \text{ --- } \left[\text{circle} \right]_\ell \text{ --- } C_\ell$$

Question

- Two site update
 - increase D
 - redistribute symmetry block
 - $\mathcal{O}(D^3 d^2 w)$
- One site update
 - Kept D
 - $\mathcal{O}(D^3 dw)$
- Q: how to reduce computational cost without losing accuracy?

Discarded spaces \bar{D}

- Unitary map

$$\frac{A_\ell}{D \text{ } \text{ } D} \oplus \frac{\overline{A}_\ell}{D \text{ } \text{ } \overline{D}} = \frac{A_\ell^{\mathbb{I}}}{D \text{ } \text{ } Dd}, \quad \frac{B_\ell^{\mathbb{I}}}{Dd \text{ } \text{ } D} = \frac{B_\ell}{D \text{ } \text{ } D} \oplus \frac{\overline{B}_\ell}{\overline{D} \text{ } \text{ } D}$$

$$\overline{D} = D(d-1)$$

- Orthonormality

$$\underbrace{\text{Diagram 1}}_{\ell} = \left(= \mathbb{1}_{\ell}^{\text{D}}, \quad \underbrace{\text{Diagram 2}}_{\ell} = 0, \quad \underbrace{\text{Diagram 3}}_{\ell} = \right) = \mathbb{1}_{\ell-1}^{\text{D}}, \quad \underbrace{\text{Diagram 4}}_{\ell} = 0$$

- Completeness

$$\begin{array}{c} \text{---} \\ | \\ \text{---} \end{array} + \begin{array}{c} \text{---} \\ / \backslash \\ | \\ \text{---} \end{array} = \begin{array}{c} \text{---} \\ | \\ \text{---} \end{array} = \mathbb{I}_\ell^P, \quad \begin{array}{c} \text{---} \\ / \backslash \\ | \\ \text{---} \end{array} + \begin{array}{c} \text{---} \\ \backslash / \\ | \\ \text{---} \end{array} = \begin{array}{c} \text{---} \\ | \\ \text{---} \end{array} = \mathbb{I}_{\ell-1}^P$$

Unitary map

$$\begin{aligned}
 H_\ell^{1s} \psi_\ell^{1s} &\rightarrow \text{Diagram 1} = \text{Diagram 2} = \text{Diagram 3} \oplus \text{Diagram 4} \\
 H_{\ell+1}^{1s} \psi_{\ell+1}^{1s} &\rightarrow \text{Diagram 5} = \text{Diagram 6} = \text{Diagram 7} \oplus \text{Diagram 8} \\
 H_\ell^{2s} \psi_\ell^{2s} &\rightarrow \text{Diagram 9} \oplus \text{Diagram 10} \oplus \text{Diagram 11} \oplus \text{Diagram 12}
 \end{aligned}$$

The diagrams are represented by a grid of 12 boxes, each containing a unitary map diagram. The diagrams are arranged in three rows and four columns. The first row shows the decomposition of $H_\ell^{1s} \psi_\ell^{1s}$ into four terms. The second row shows the decomposition of $H_{\ell+1}^{1s} \psi_{\ell+1}^{1s}$ into two terms. The third row shows the decomposition of $H_\ell^{2s} \psi_\ell^{2s}$ into four terms. The diagrams are labeled with ℓ and $\ell+1$ at the bottom, indicating the indices of the states involved.

Energy variance

- $\Delta_E = \|(H - E)\Psi\|^2$

$$\Delta_E = \Delta_E^{1\perp} + \Delta_E^{2\perp} + \dots$$

$$\Delta_E^{1\perp} = \sum_{\ell=1}^{\mathcal{L}} \left\| \text{Diagram}_1(\ell) \right\|^2, \quad \Delta_E^{2\perp} = \sum_{\ell=1}^{\mathcal{L}-1} \left\| \text{Diagram}_2(\ell, \ell+1) \right\|^2$$

The diagrams represent terms in the energy variance expansion. The first diagram, labeled with index ℓ , shows a single site with a square representing the Hamiltonian H and a circle representing the energy E . The second diagram, labeled with indices ℓ and $\ell+1$, shows two sites with squares representing H and a circle representing E .

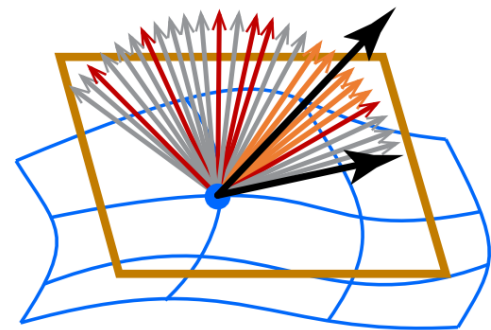
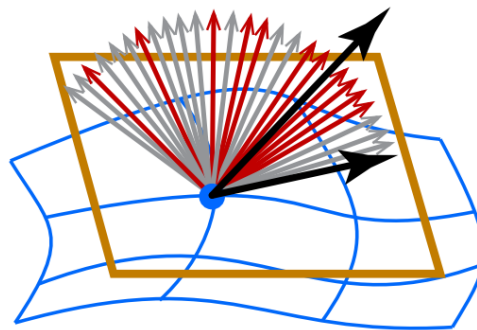
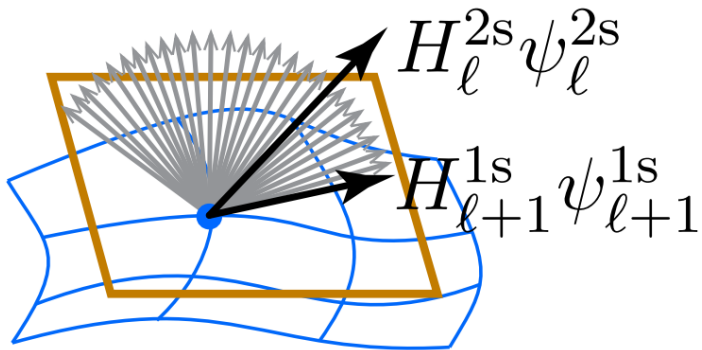
- 1s DMRG minimizes only $\Delta_E^{1\perp}$, 2s minimizes $\Delta_E^{1\perp}$ and $\Delta_E^{2\perp}$

Controlled bond expansion


$$C_1 = \left\| \begin{array}{c} \text{Diagram 1} \\ \text{Diagram 2} \end{array} \right\|, \quad C_2 = \left\| \begin{array}{c} \text{Diagram 3} - \text{Diagram 4} \\ \text{Diagram 5} \end{array} \right\|, \quad C_3 = \left\| \begin{array}{c} \text{Diagram 6} - \text{Diagram 7} \end{array} \right\|.$$

The diagrams are Feynman-like diagrams representing interactions between sites. They include labels w , \bar{D} , d , \hat{D} , D , D' , and \tilde{D} . Diagram 1 and 2 are for C_1 . Diagram 3 and 4 are for C_2 , with Diagram 4 containing a red diamond and a blue rectangle. Diagram 6 and 7 are for C_3 .

$$H_\ell^{2s} \psi_\ell^{2s} \xrightarrow{A_\ell^\dagger} H_{\ell+1}^{1s} \psi_{\ell+1}^{1s}$$



CBE update step

I. Compute $\tilde{A}_\ell^{\text{tr}}$ () using shrewd selection

II. Expand bond dimension $D \rightarrow D + \tilde{D}$

$$\frac{A_\ell}{D \underset{d}{\downarrow} D} \oplus \frac{\tilde{A}_\ell^{\text{tr}}}{D \underset{d}{\downarrow} \tilde{D}} = \frac{A_\ell^{\text{ex}}}{D \underset{d}{\downarrow} (D + \tilde{D})} \xrightarrow{C_{\ell+1}^{\text{ex},i}} \frac{C_{\ell+1}}{D \underset{d}{\downarrow} D} = \text{diagram of } C_{\ell+1}$$

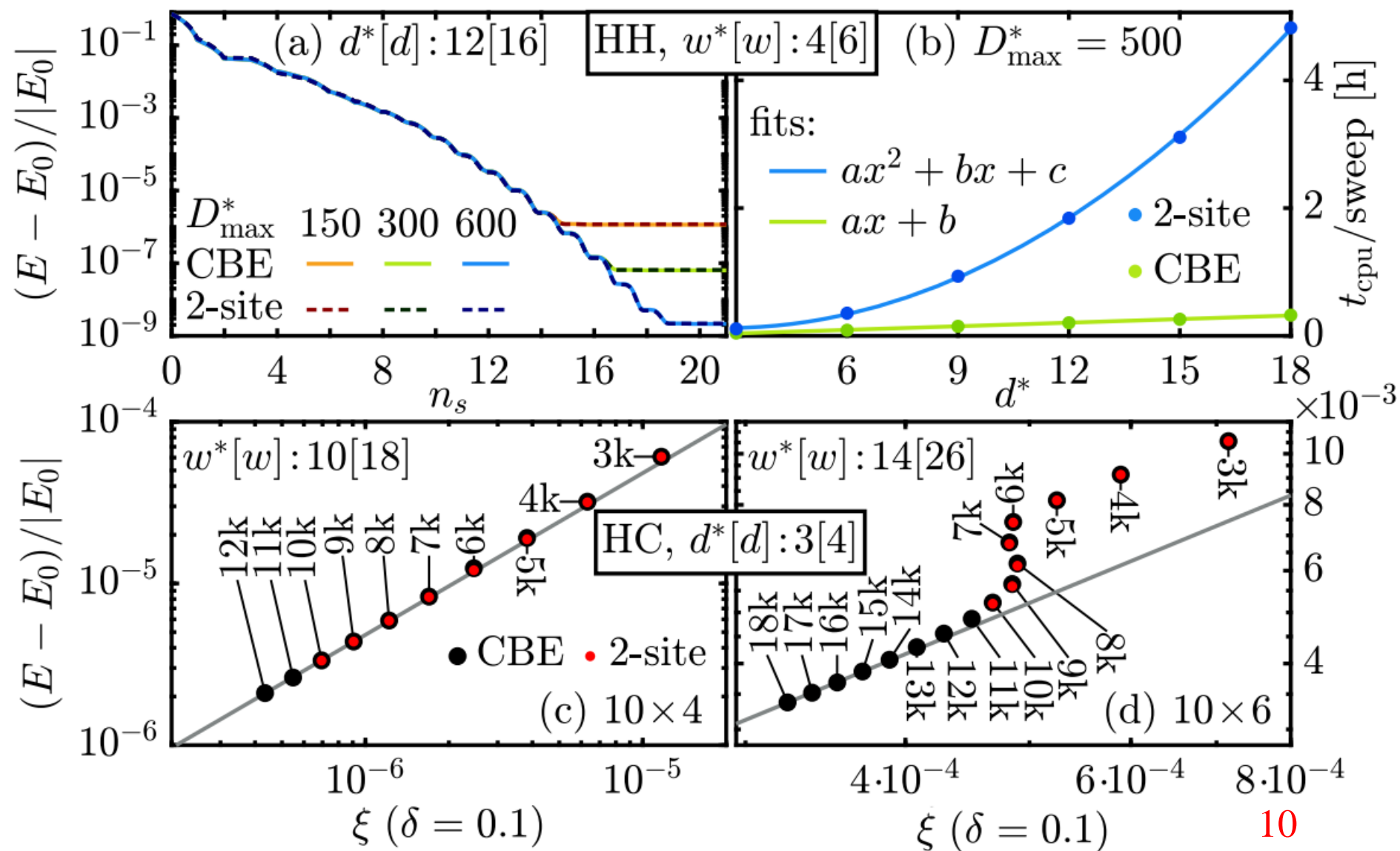
The diagram for $C_{\ell+1}$ shows a square with a vertical line in the center. The left half of the square is shaded green, and the right half is white. The top and bottom edges are labeled $\ell+1$.

III. Update $C_{\ell+1}^{\text{ex}}$ using $H_{\ell+1}^{\text{ls},\text{ex}} = \text{diagram of } H_{\ell+1}^{\text{ls},\text{ex}} = {}^{D+\tilde{D}} \left[\text{diagram of } H_{\ell+1}^{\text{ls},\text{ex}} \right]^D$

The diagram for $H_{\ell+1}^{\text{ls},\text{ex}}$ shows a square with a vertical line in the center. The left half of the square is shaded green, and the right half is white. The top and bottom edges are labeled $\ell+1$.

IV. Shift isometry center and truncate $D + \tilde{D} \rightarrow D$

result



Why $\overline{A}_\ell \nabla \rightarrow \widehat{A}_\ell^{\text{pr}} \nabla$?

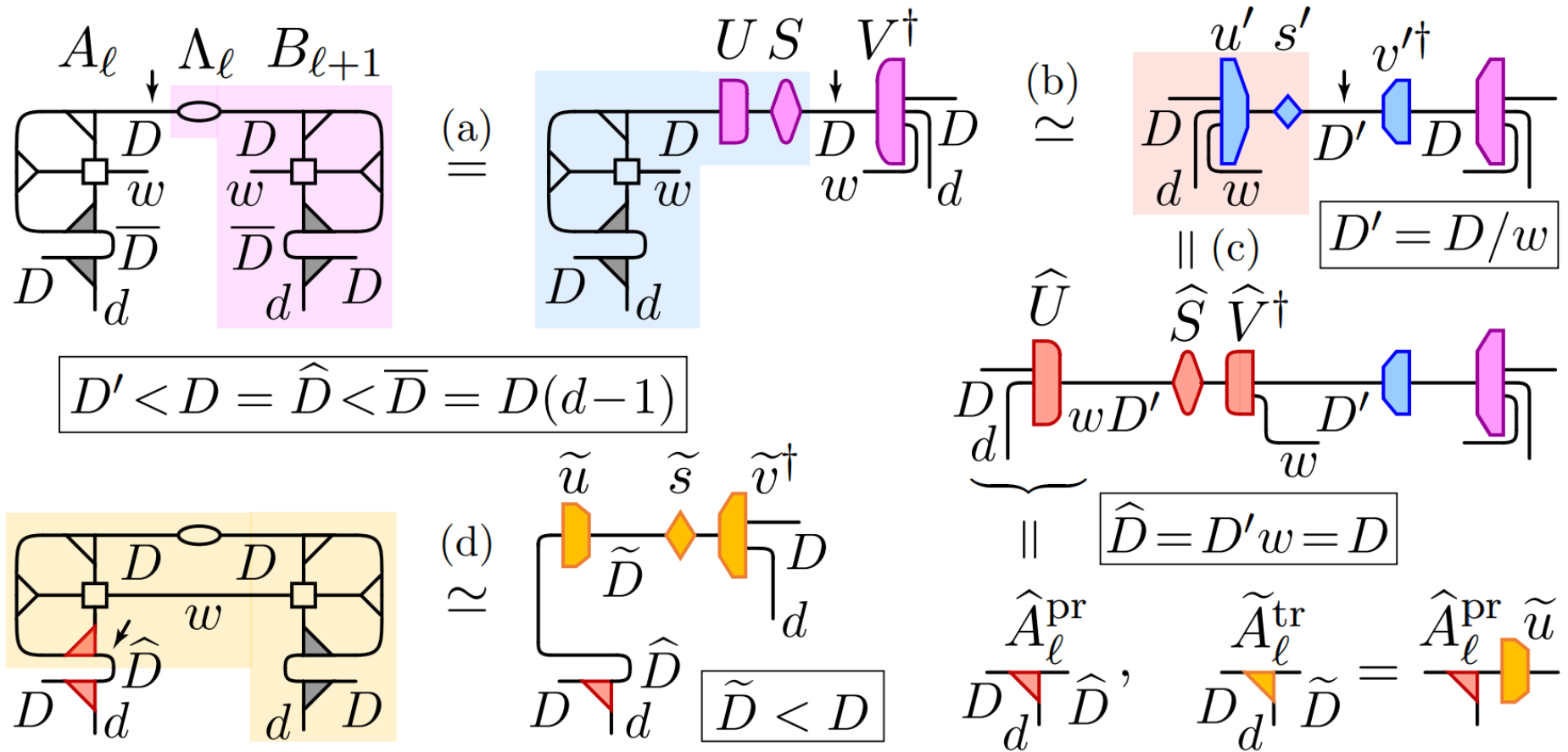
$$\overline{M}^{\text{full}} = \text{Diagram} = \begin{array}{c} \overline{U} \quad \overline{S} \quad \overline{V}^\dagger \\ \text{[Circuit with yellow components]} \\ \overline{D}^* \quad d^* \end{array} \simeq \begin{array}{c} \overline{u} \quad \overline{s} \quad \overline{v}^\dagger \\ \text{[Circuit with yellow components]} \\ \widetilde{D}^* \quad D^* \quad d^* \end{array} \quad \mathcal{O}(D^3 d^2)$$

The diagram for $\overline{M}^{\text{full}}$ shows a circuit with a loop containing a square and a triangle, and a vertical branch with a triangle. The loop is labeled ℓ and the branch is labeled $\ell+1$. The circuit is then represented by a series of components: a yellow rectangle labeled \overline{U} , a yellow diamond labeled \overline{S} , and a yellow rectangle labeled \overline{V}^\dagger . The input is \overline{D}^* and the output is d^* . This is then approximated by a similar circuit with components \overline{u} , \overline{s} , and \overline{v}^\dagger , and a \widetilde{D}^* component, with a complexity of $\mathcal{O}(D^3 d^2)$.

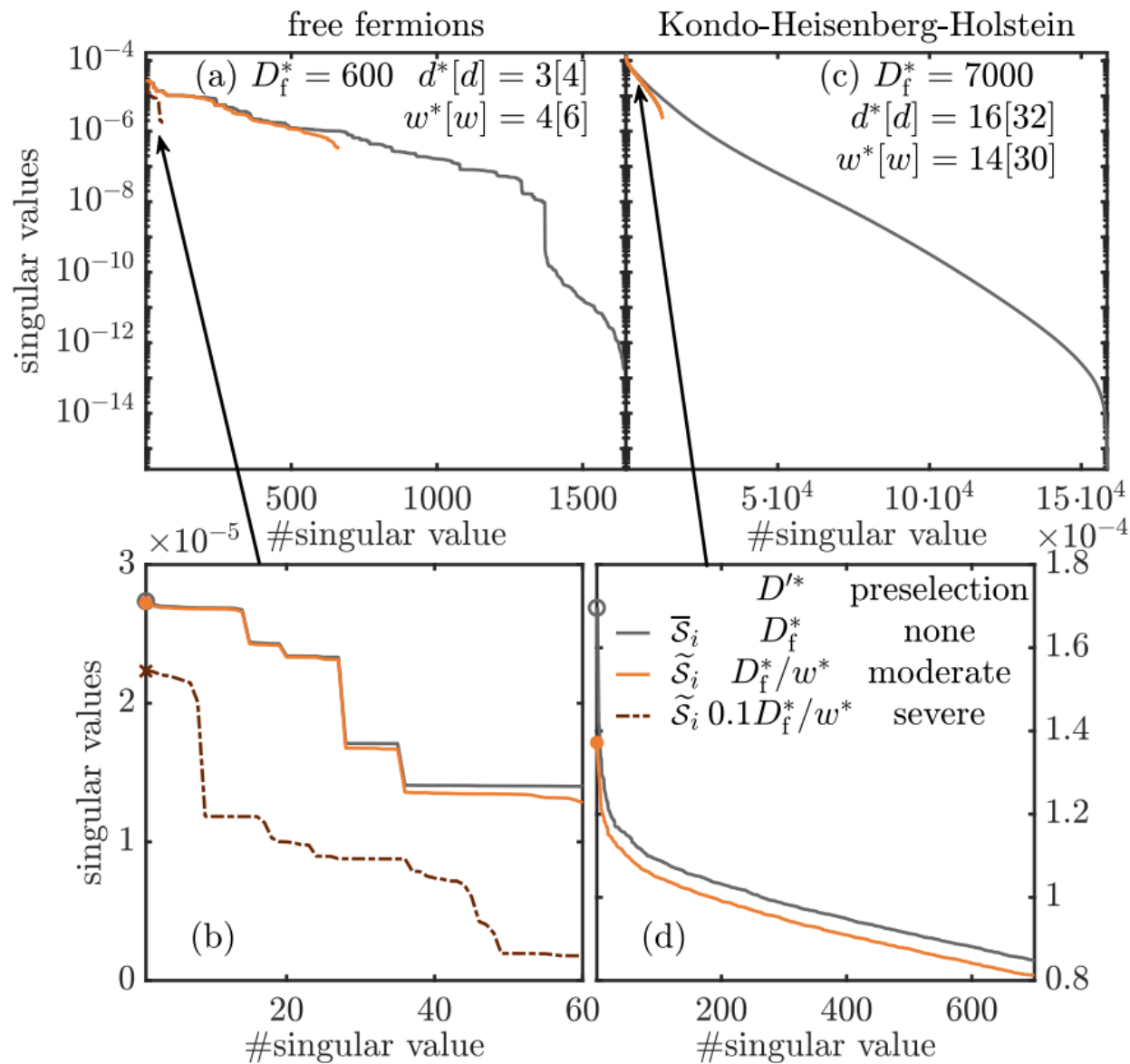
$$\widehat{M}^{\text{pr}} = \text{Diagram} = \begin{array}{c} \widetilde{U} \quad \widetilde{S} \quad \widetilde{V}^\dagger \\ \text{[Circuit with orange components]} \\ \widehat{D}^* \quad D^* \quad d^* \end{array} \simeq \begin{array}{c} \widetilde{u} \quad \widetilde{s} \quad \widetilde{v}^\dagger \\ \text{[Circuit with orange components]} \\ \widetilde{D}^* \quad D^* \quad d^* \end{array} \quad \mathcal{O}(D^3 d)$$

The diagram for \widehat{M}^{pr} is similar to the one for $\overline{M}^{\text{full}}$, but the triangle in the loop is red. The circuit is then represented by a series of components: an orange rectangle labeled \widetilde{U} , an orange diamond labeled \widetilde{S} , and an orange rectangle labeled \widetilde{V}^\dagger . The input is \widehat{D}^* and the output is d^* . This is then approximated by a similar circuit with components \widetilde{u} , \widetilde{s} , and \widetilde{v}^\dagger , and a \widetilde{D}^* component, with a complexity of $\mathcal{O}(D^3 d)$.

shrewd selection



$\bar{S}(\text{---}\text{---})$ and $\tilde{S}(\text{---}\text{---})$



comments

- Is such shrewd selection the only one? Is it optimal?
- Can we expand to more than two site update?
- How to apply it to PEPS update?