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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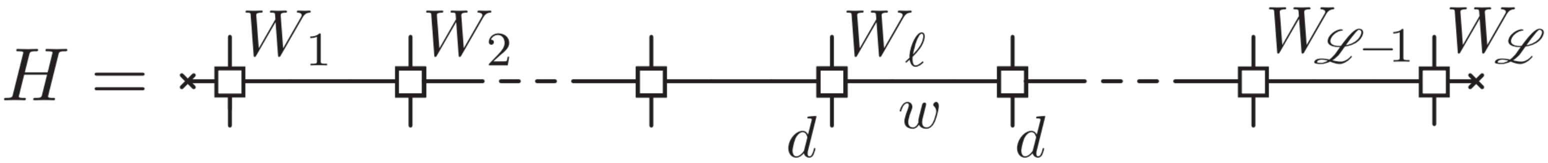
Xingyu Zhang 2023.9.8

MPO and MPS representation

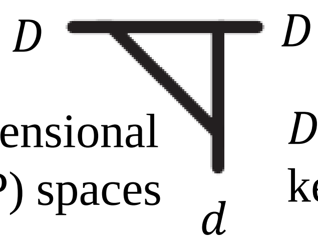
- Hamiltonian expressed by MPO



Exponential growth of physical space d^L

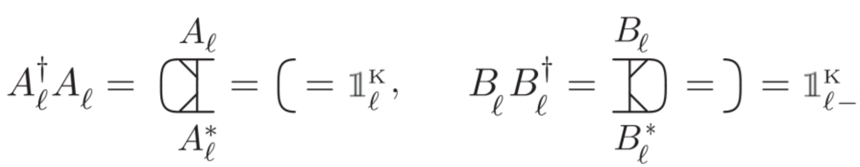
Finite virtual bond dimension w

- Wave function expressed by MPS



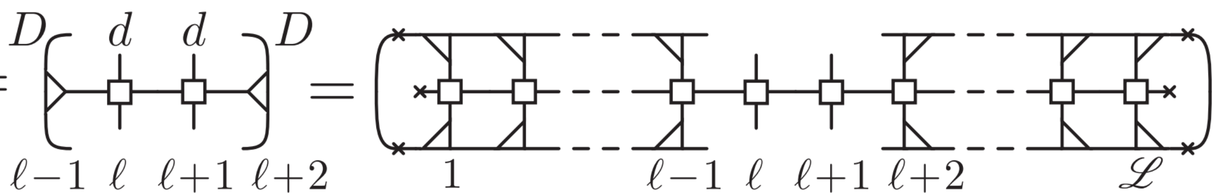
Dd-dimensional parent(P) spaces

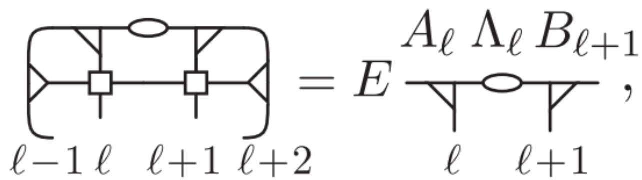
D-dimensional kept(K) spaces



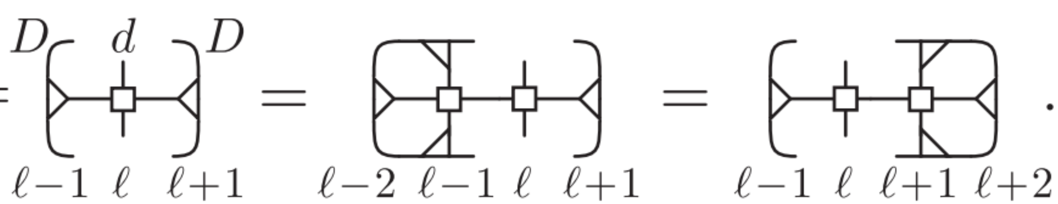
DMRG→Optimize MPS

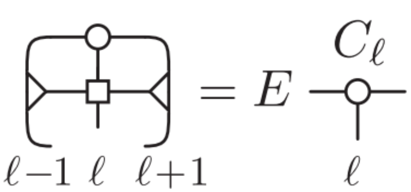
- Two site update

$H_\ell^{2s} =$ 

$(H_\ell^{2s} - E)\psi_\ell^{2s} = 0\,,$ 

- One site update

$H_\ell^{1s} =$ 

$(H_\ell^{1s} - E)\psi_\ell^{1s} = 0\,,$ 

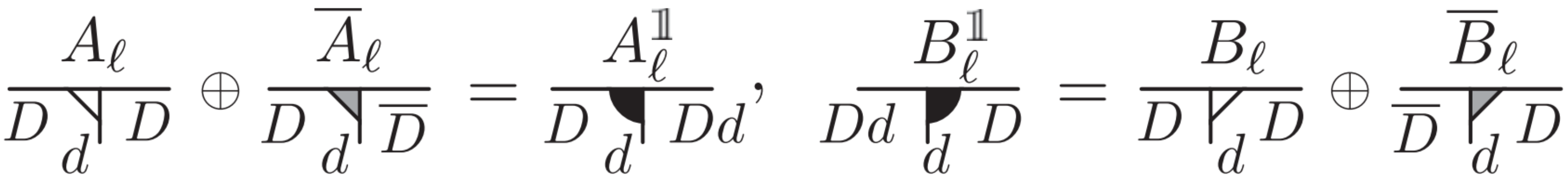
Question

- Two site update
  - increase D
  - redistribute symmetry block
  - $\mathcal{O}(D^3 d^2 w)$
- One site update
  - Kept D
  - $\mathcal{O}(D^3 d w)$
- Q: how to reduce computational cost

  without losing accuracy?

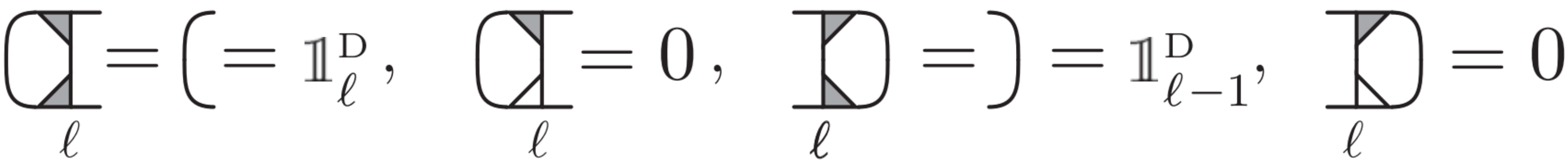
Discarded spaces $\overline{D}$

- Unitary map



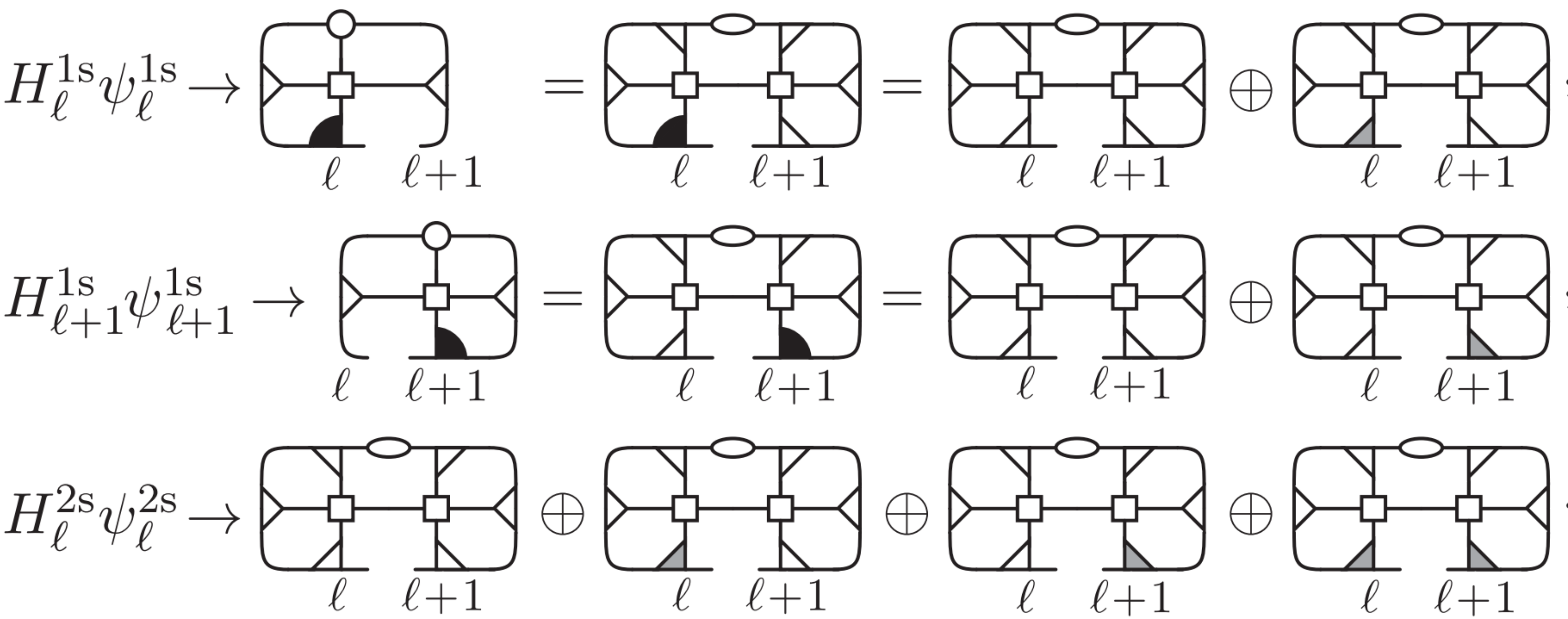
$$\overline{D} = D(d-1)$$

- Orthonormality



- Completeness

Unitary map

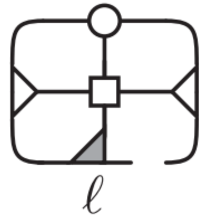


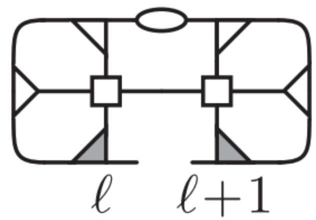
$H_\ell^{1s}\psi_\ell^{1s} \rightarrow$
$H_{\ell+1}^{1s}\psi_{\ell+1}^{1s} \rightarrow$
$H_\ell^{2s}\psi_\ell^{2s} \rightarrow$
ℓ $\ell+1$

Energy variance

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

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

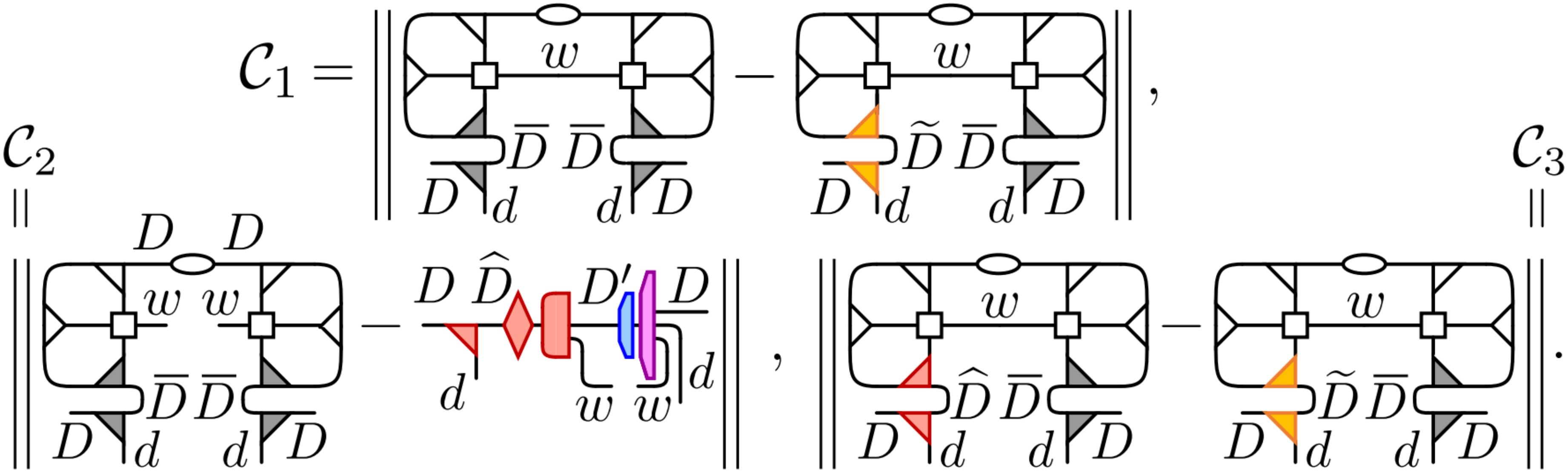
$$\Delta_E^{1\perp} = \sum_{\ell=1}^{\mathscr{L}} \Bigg\|$$


$$\Bigg\|^2, \quad \Delta_E^{2\perp} = \sum_{\ell=1}^{\mathscr{L}-1} \Bigg\|$$


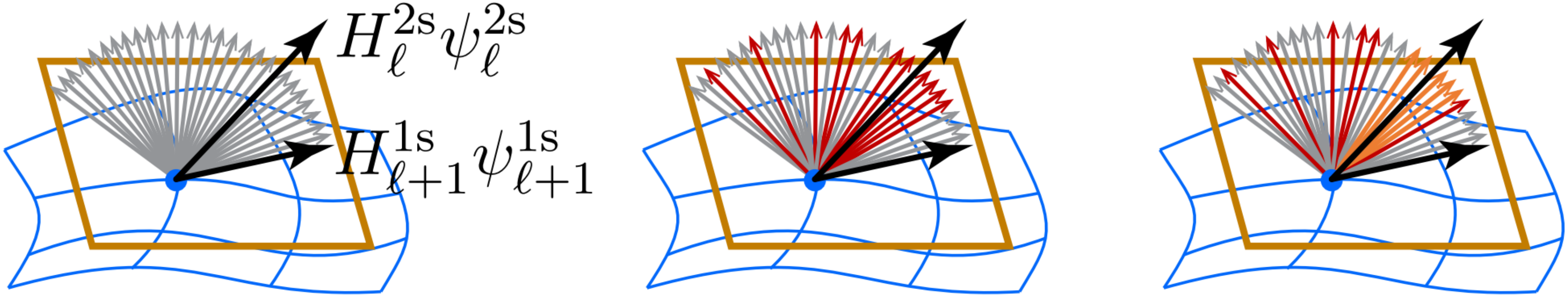
$$\Bigg\|^2$$

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

Controlled bond expansion



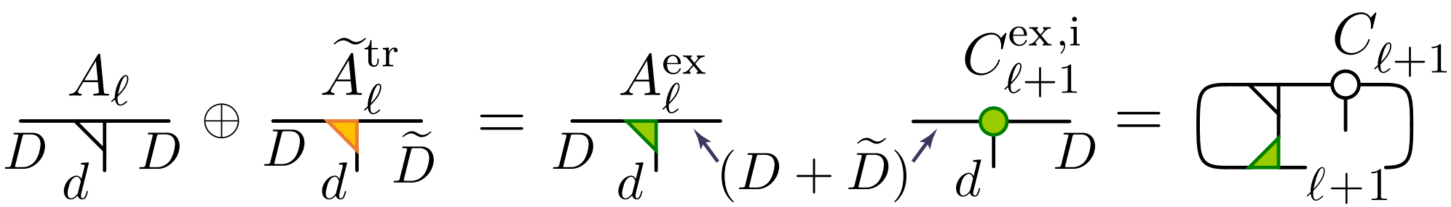
$$H_\ell^{2s}\psi_\ell^{2s} \overset{A_\ell^\dagger}{\mapsto} H_{\ell+1}^{1s}\psi_{\ell+1}^{1s}$$



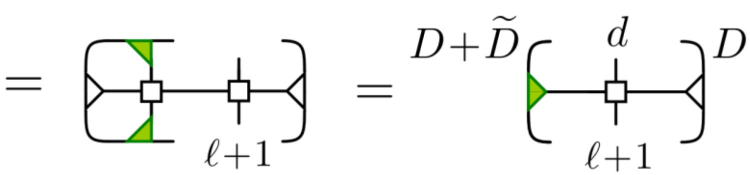
CBE update step

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

II. Expand bond dimension $D \to D + \widetilde{D}$

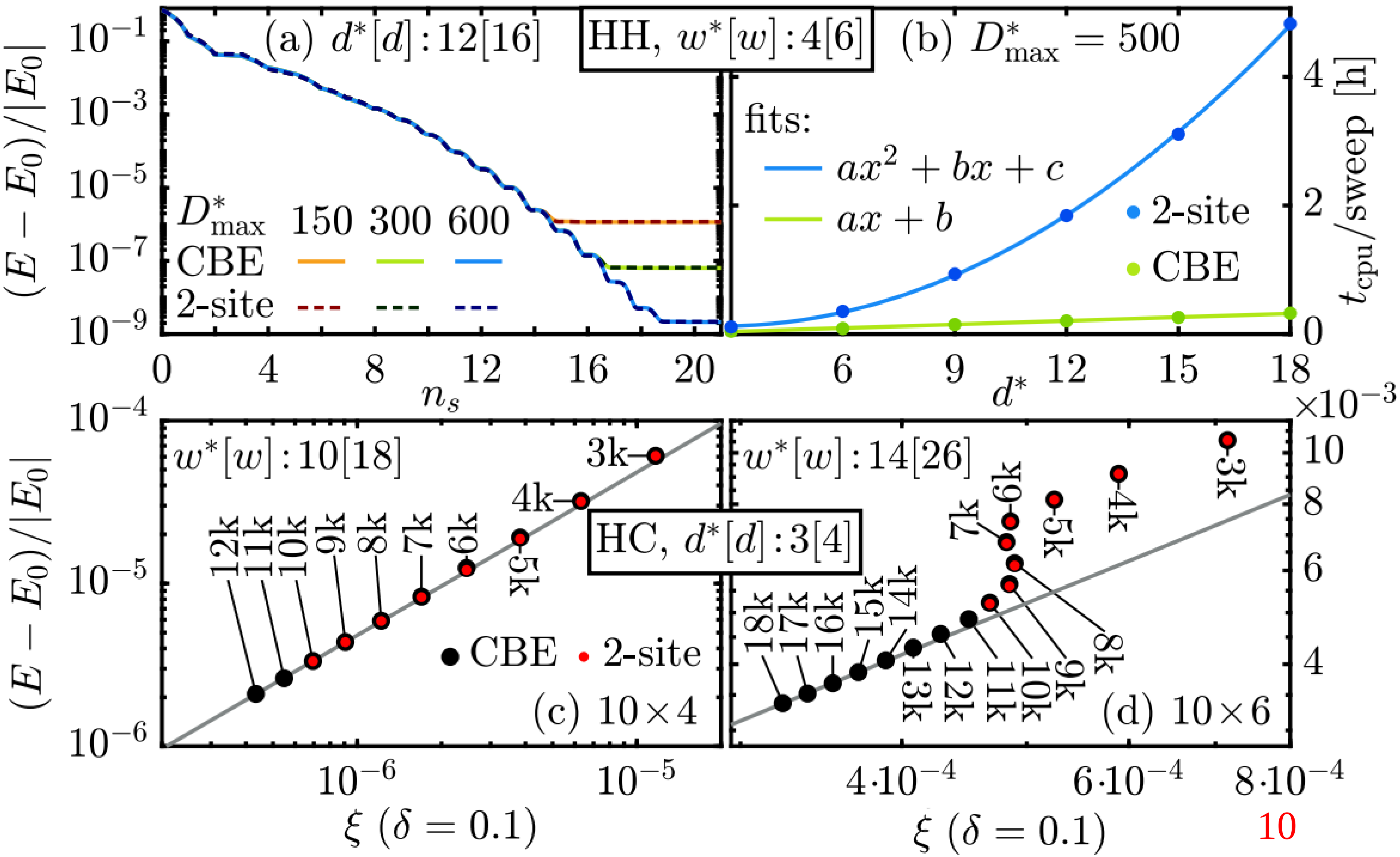


III. Update $C^{\mathrm{ex}}_{\ell+1}$ using $H^{\mathrm{1s,ex}}_{\ell+1} =$



IV. Shift isometry center and truncate $D + \widetilde{D} \to D$

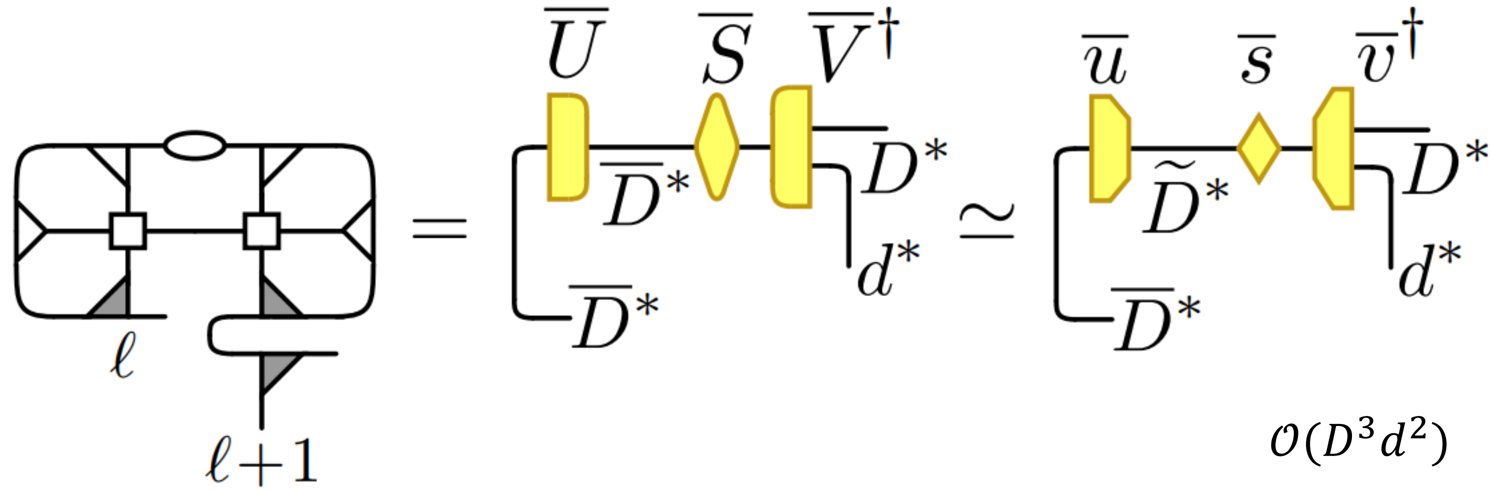
result



(a) $d^*[d]:12[16]$
HH, $w^*[w]:4[6]$
(b) $D^*_{\max} = 500$
$(E-E_0)/|E_0|$
$D^*_{\max}$ 150 300 600
CBE
2-site
n_s
fits:
ax^2+bx+c
$ax+b$
2-site
CBE
$t_{\rm cpu}$/sweep [h]
d^*
$w^*[w]:10[18]$
HC, $d^*[d]:3[4]$
$w^*[w]:14[26]$
CBE
2-site
(c) 10×4
(d) 10×6
$\xi\ (\delta=0.1)$
$\times10^{-3}$

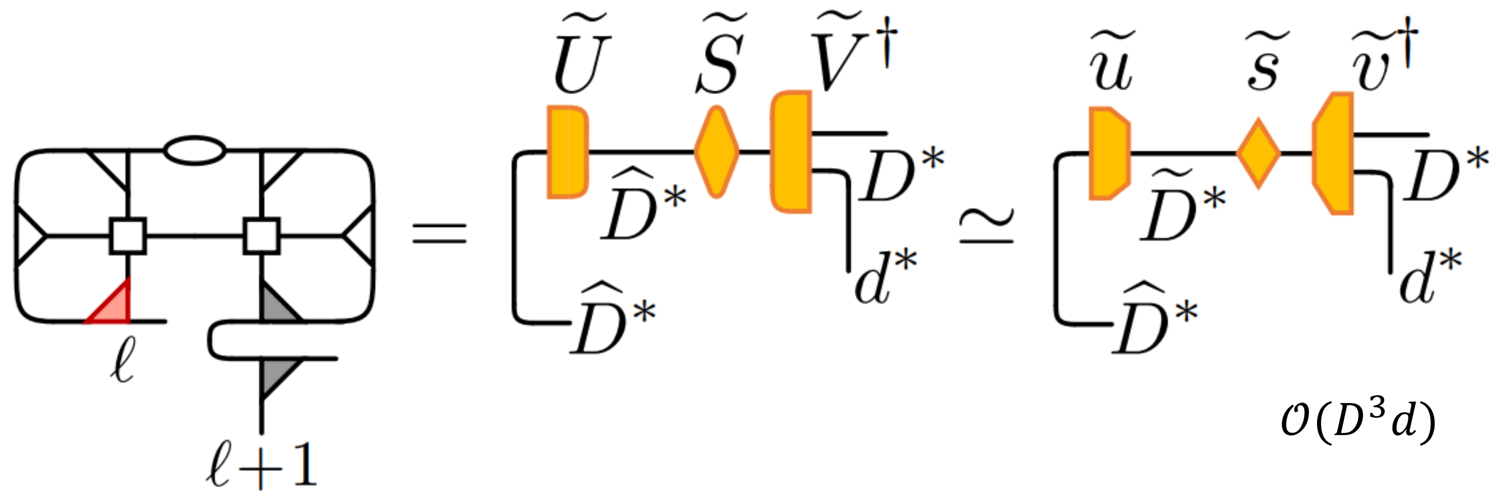
Why $\overline{A}_\ell \rightarrow \widehat{A}^{\mathrm{pr}}_\ell$?

$\overline{M}^{\mathrm{full}} =$



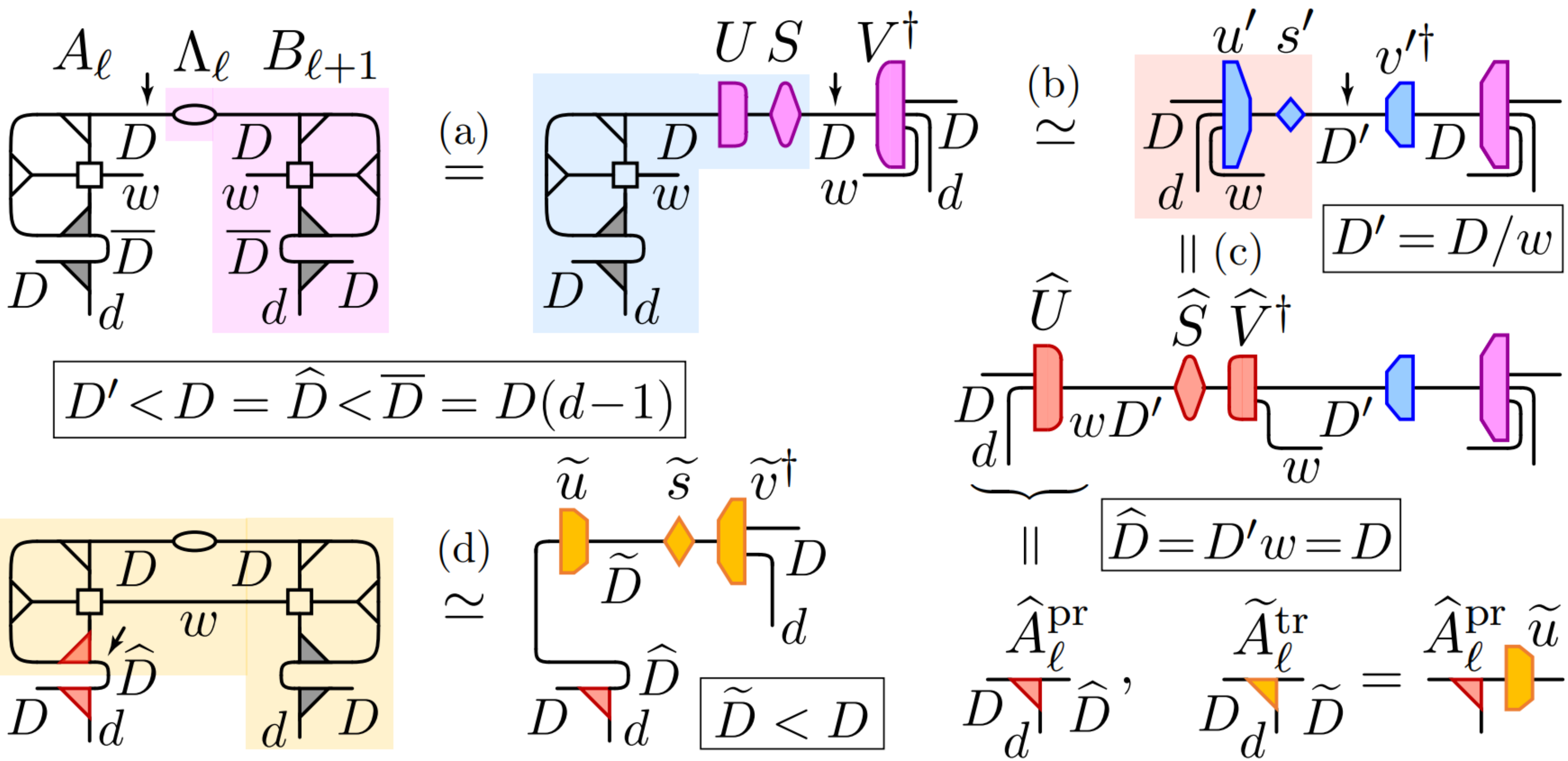
$\mathcal{O}(D^3 d^2)$

$\widehat{M}^{\mathrm{pr}} =$

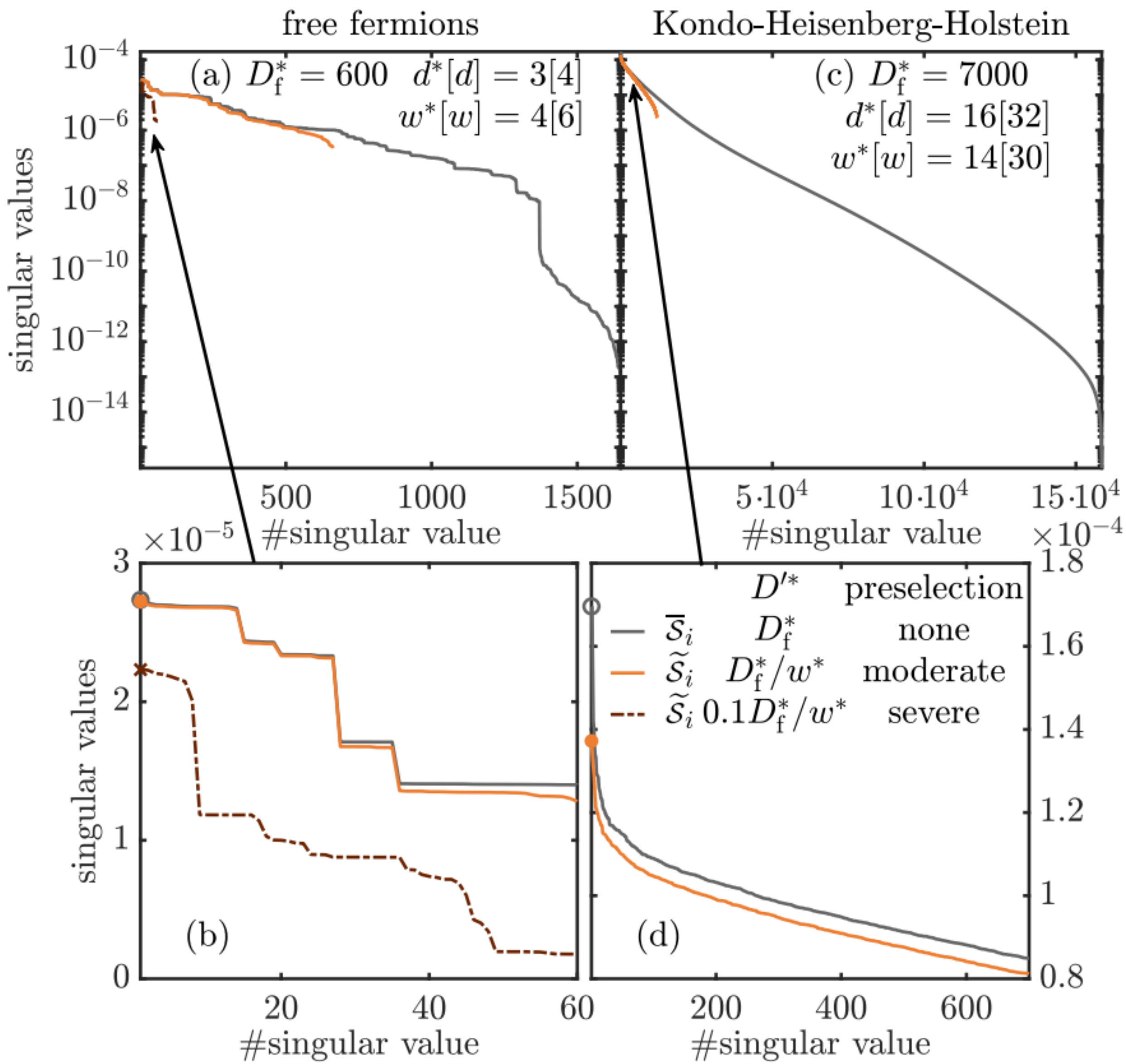


$\mathcal{O}(D^3 d)$

shrewd selection



$\overline{S}$(◆) and $\widetilde{S}$(◆)



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?