AD-U1-FPEPS

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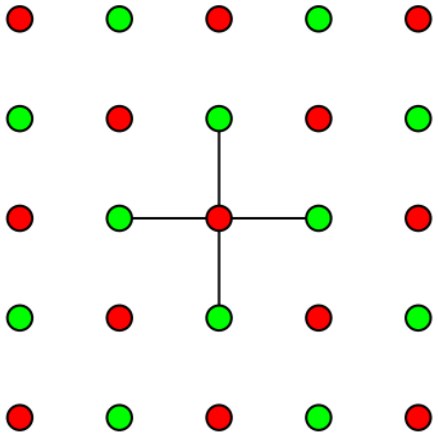
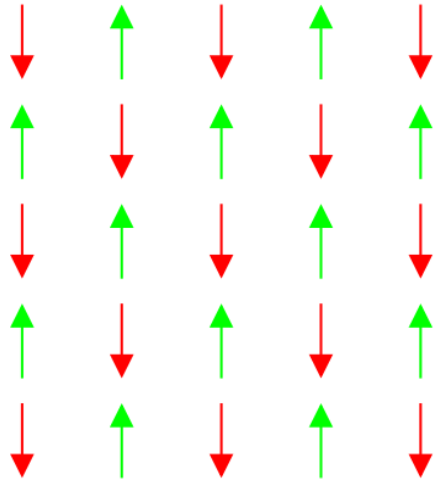
2022.07.22

Hubbard model

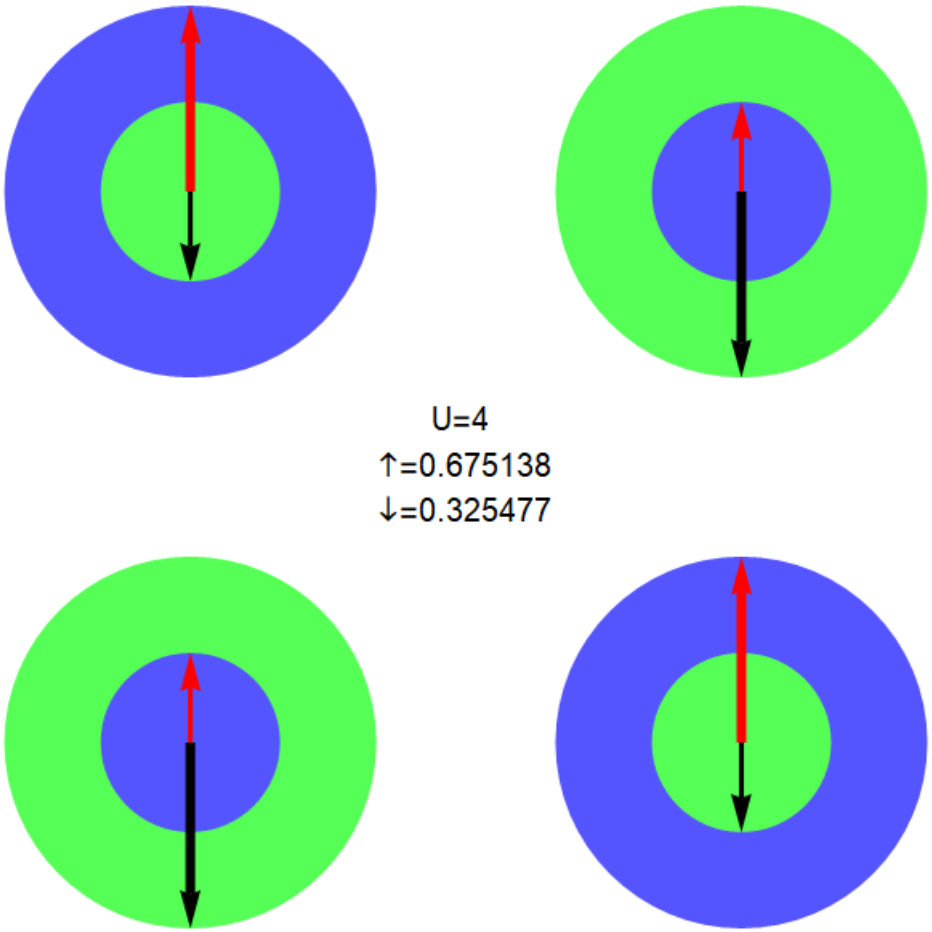
$$\hat{H} = -t \sum_{\langle \mathbf{j},\mathbf{l} \rangle \sigma} \left(c^{\dagger}_{\mathbf{j}\sigma} c_{\mathbf{l}\sigma} + c^{\dagger}_{\mathbf{l}\sigma} c_{\mathbf{j}\sigma} \right) + U \sum_{\mathbf{j}} n_{\mathbf{j}\uparrow} n_{\mathbf{j}\downarrow} - \mu \sum_{\mathbf{j}} (n_{\mathbf{j}\uparrow} + n_{\mathbf{j}\downarrow})$$

- $\mu = \frac{U}{2}$, Particle-hole symmetry

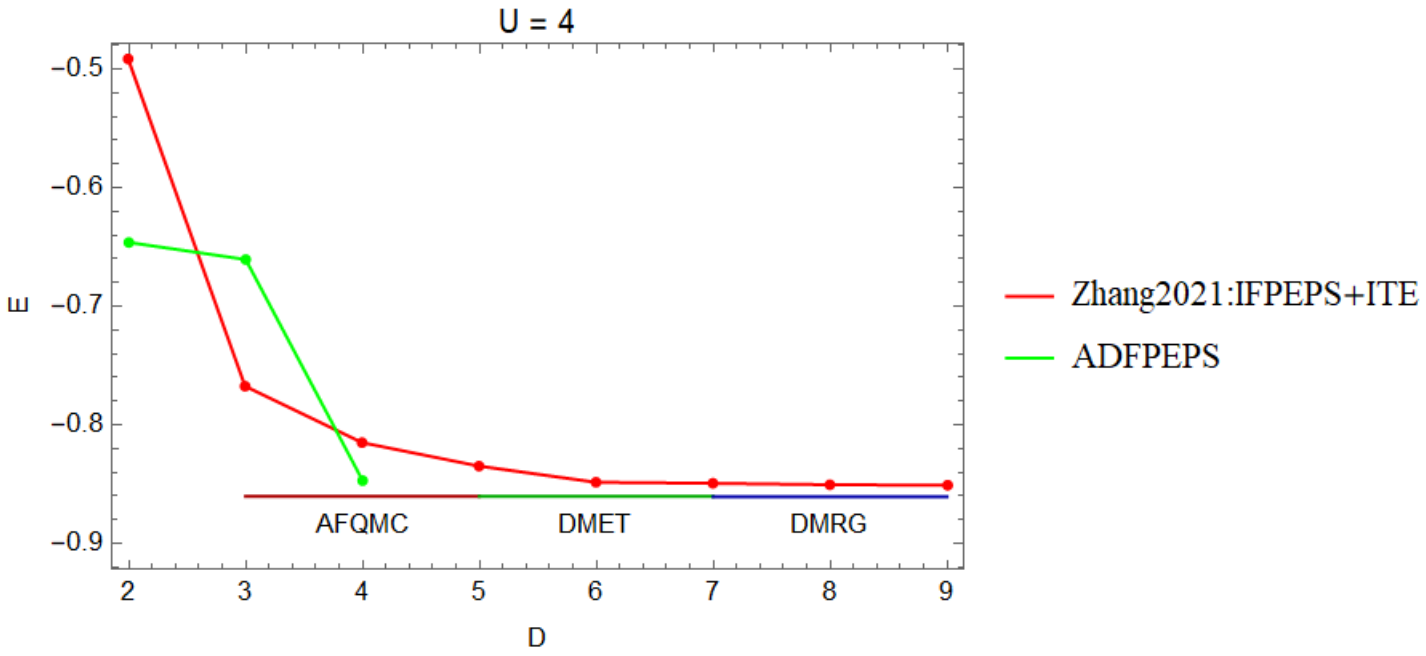




U=4 half-filled



U=4 half-filled

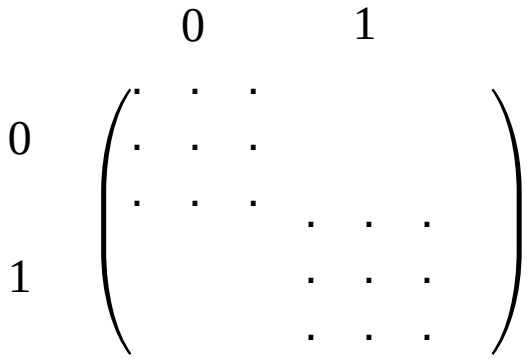


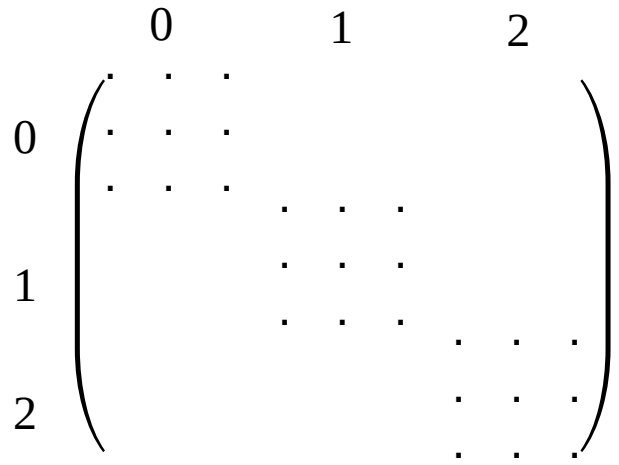
- $D = 2,4$ is lower, but $D = 3$ is higher in contrast with ITE
- AD optimization is not stable at end (maybe for insufficient χ)
- 0.02 higher than other method, may need large D
- $D \geq 6$ is hard to achieve without symmetry for large memory usage

$D = 4$ $3 - 4h$
$D = 5$ $24h$

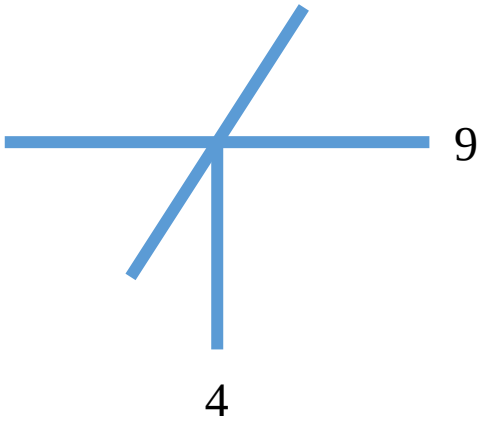
U1-tensor block division

- $Z2 \rightarrow U1$





- iPEPS

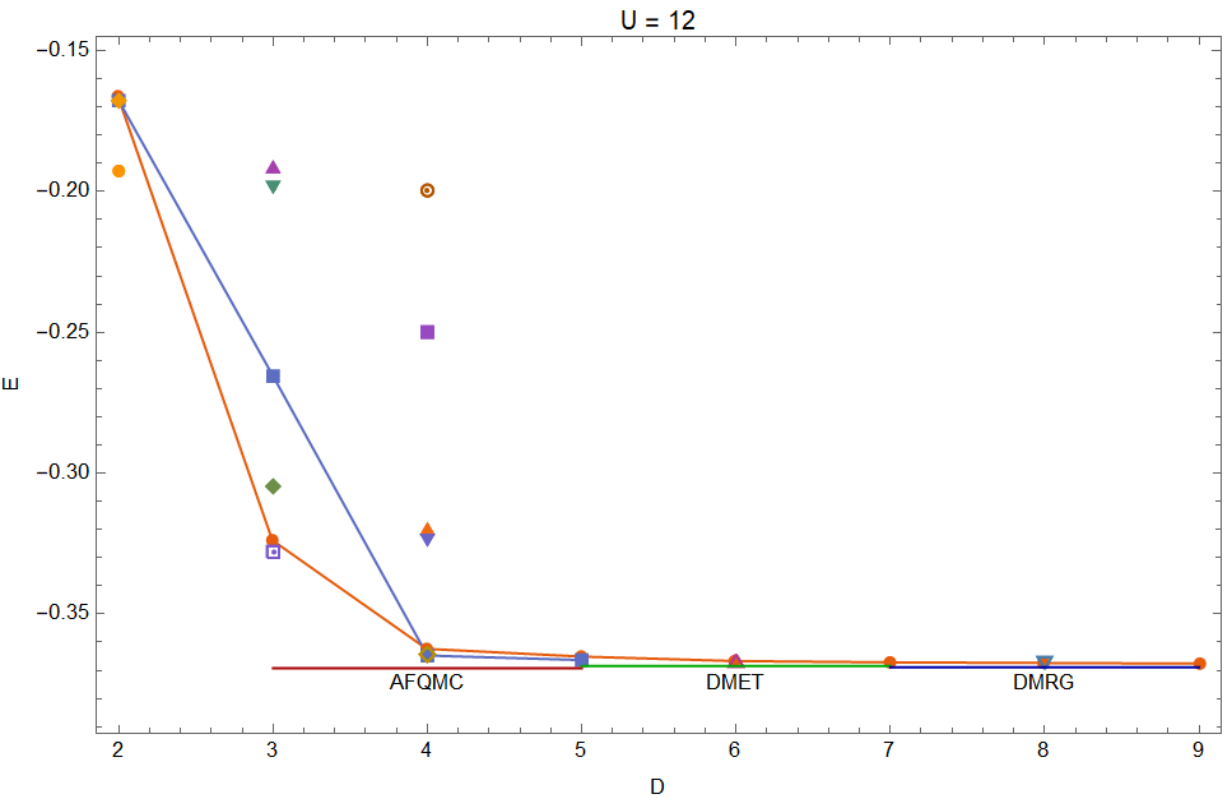


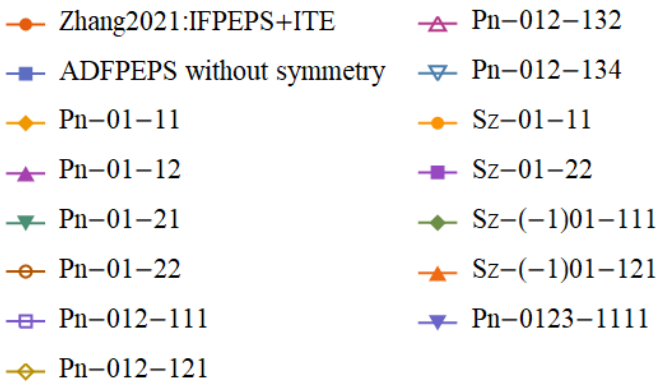
state	Sz	Pn
0	0	0
↑	+1	1
↓	−1	1
↑↓	0	2

$$\begin{array}{rl} & \begin{array}{cccc} 0 & 1 & 2 & 3 \end{array} \\ 9 = & 3 + 3 + 3 \\ = & 1 + 4 + 3 + 1 \end{array}$$

Physical bond division is decided by Hamiltonian, but virtual bond division is arbitrary.

U=12 half-filled use U1-symmetry





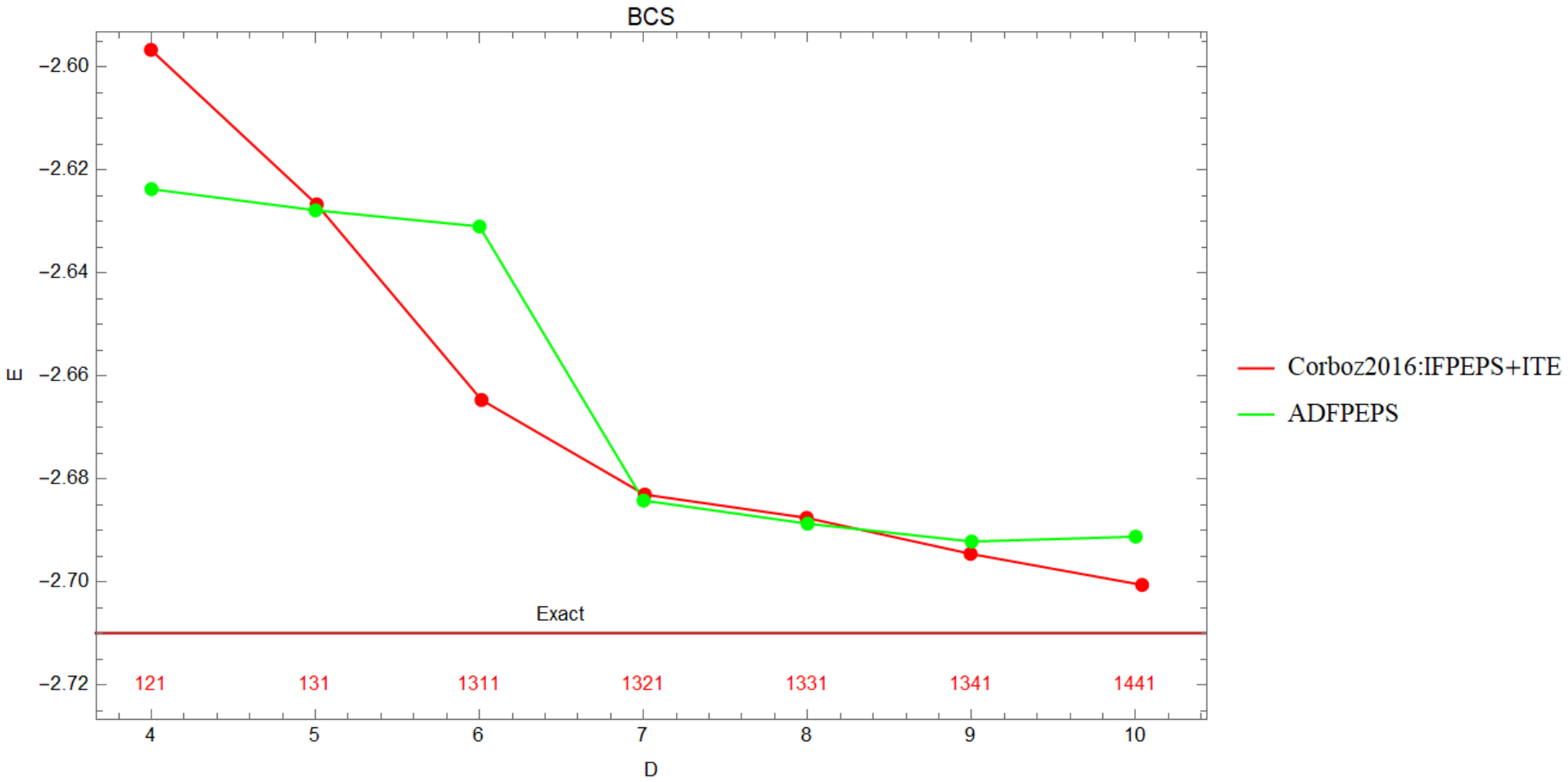
D=8 3.5days

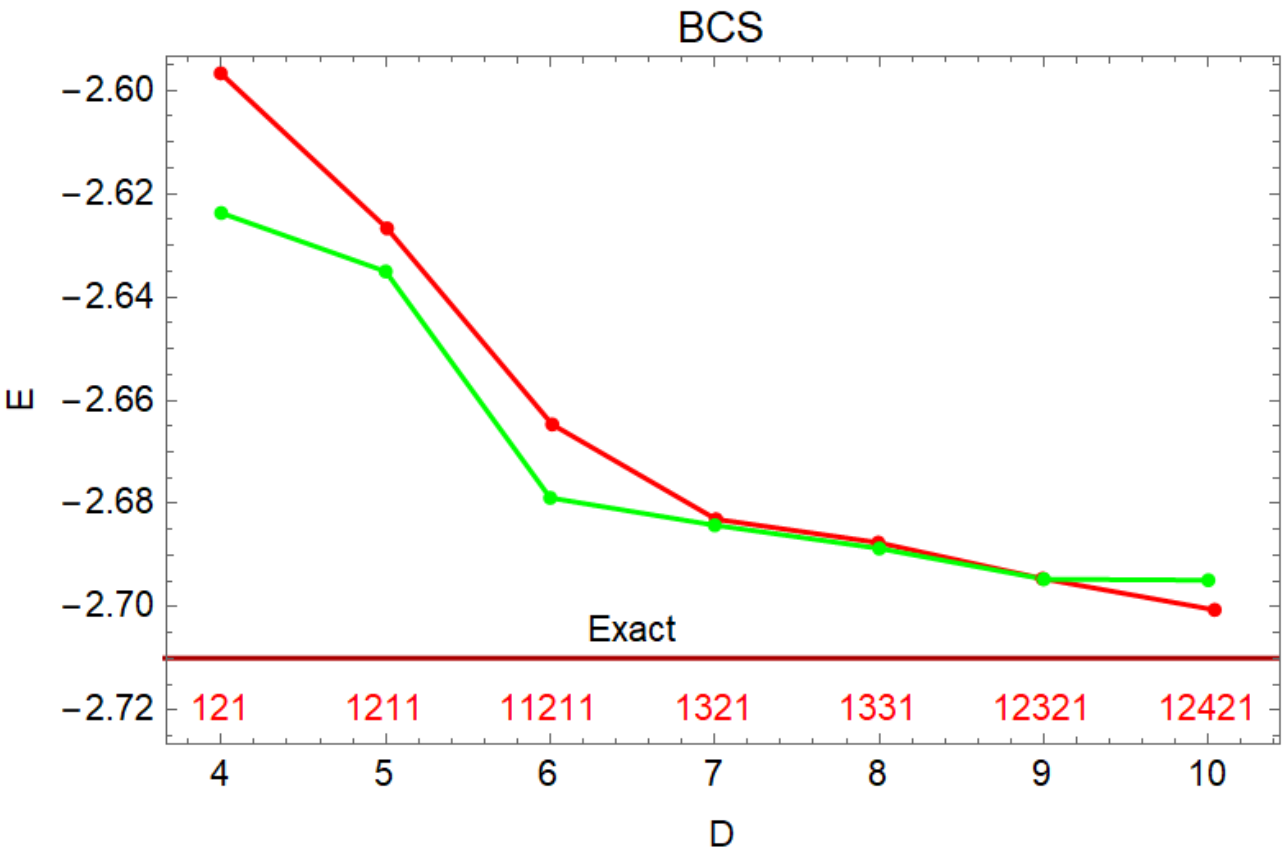
More division is better than bigger dimension

Bogoliubov-de Gennes (BdG)

$$\hat{H} = -t \sum_{\langle i,j,\sigma \rangle} (\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \text{H.c.}) + \sum_{\langle \text{i,j} \rangle} \gamma_{\text{ij}} (\hat{\text{c}}^{\dagger}_{\text{i}\uparrow} \hat{\text{c}}^{\dagger}_{\text{j}\downarrow} - \hat{\text{c}}^{\dagger}_{\text{i}\downarrow} \hat{\text{c}}^{\dagger}_{\text{j}\uparrow} + \text{H.c.})$$

- Can be exact solved by diagonalized
- Only need 1×1 cell


BCS
−2.60
−2.62
−2.64
−2.66
−2.68
−2.70
−2.72
E
Exact
121
131
1311
1321
1331
1341
1441
4
5
6
7
8
9
10
D
Corboz2016:IFPEPS+ITE
ADFPEPS



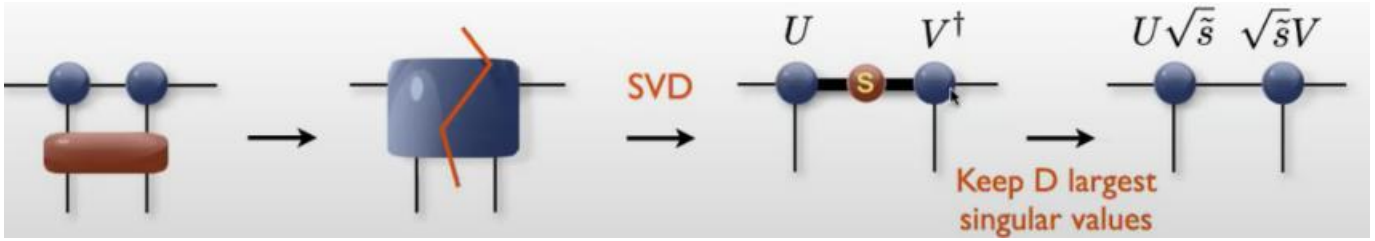
Corboz2016:IFPEPS+ITE

ADFPEPS

4 division 12h
5 division 35h
6 division 1 week

- Small division converges quickly, more division is better but hard to achieve
- Difficulty for fermion model is ability expression rather than ability of optimization
- For large D, the difficulty is how to divide the U1 block

divide the U1 block use SVD



$$A = \begin{pmatrix} \cdot & \cdot & \cdot & & & & & & \\ \cdot & \cdot & \cdot & & & & & & \\ \cdot & \cdot & \cdot & & & & & & \\ & & & \cdot & \cdot & \cdot & & & \\ & & & \cdot & \cdot & \cdot & & & \\ & & & \cdot & \cdot & \cdot & & & \\ & & & & & & \cdot & \cdot & \cdot \\ & & & & & & \cdot & \cdot & \cdot \\ & & & & & & \cdot & \cdot & \cdot \end{pmatrix} \times \begin{pmatrix} \cdot & & & & & & & & \\ & \cdot & & & & & & & \\ & & \cdot & & & & & & \\ & & & \cdot & & & & & \\ & & & & \cdot & & & & \\ & & & & & \cdot & & & \\ & & & & & & \cdot & & \\ & & & & & & & \cdot & \\ & & & & & & & & \cdot \end{pmatrix} \times \begin{pmatrix} \cdot & \cdot & \cdot & & & & & & \\ \cdot & \cdot & \cdot & & & & & & \\ \cdot & \cdot & \cdot & & & & & & \\ & & & \cdot & \cdot & \cdot & & & \\ & & & \cdot & \cdot & \cdot & & & \\ & & & \cdot & \cdot & \cdot & & & \\ & & & & & & \cdot & \cdot & \cdot \\ & & & & & & \cdot & \cdot & \cdot \\ & & & & & & \cdot & \cdot & \cdot \end{pmatrix}$$

U S $V^\dagger$

- Merge two legs of U1 tensor will increase number of blocks.
- Sort S from different blocks, keep largest D value may decrease number of blocks.
- So after split to origin leg, block would be divided differently from original one.

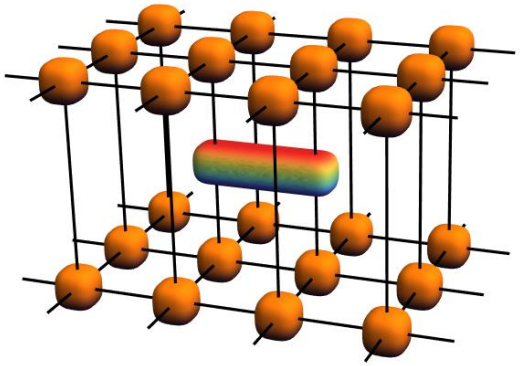
Open question

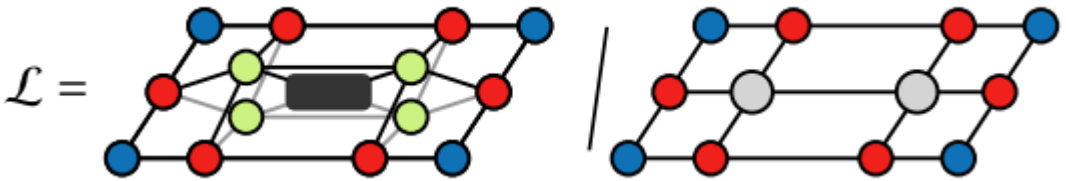
- Optimize U1 iPEPS block with AD
- Divide U1 boundary MPS block in VUMPS
- Optimize U1 code for large D with more division blocks

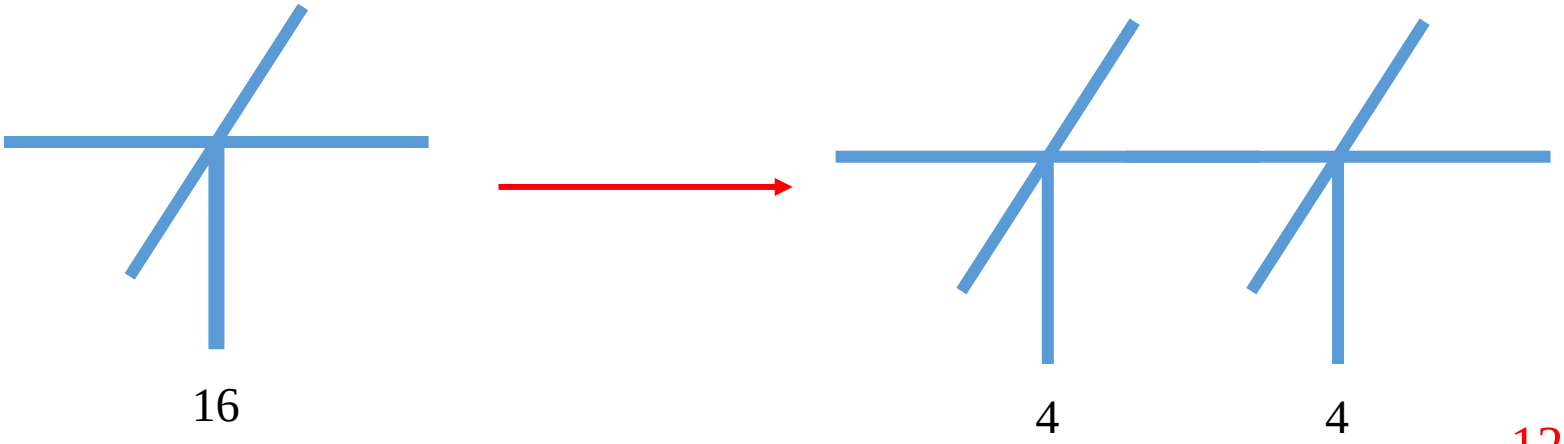
- Momentum space tensor network for fermion?

Optimize U1 iPEPS block with AD

- Merge two iPEPS → ansatz: two-site iPEPS

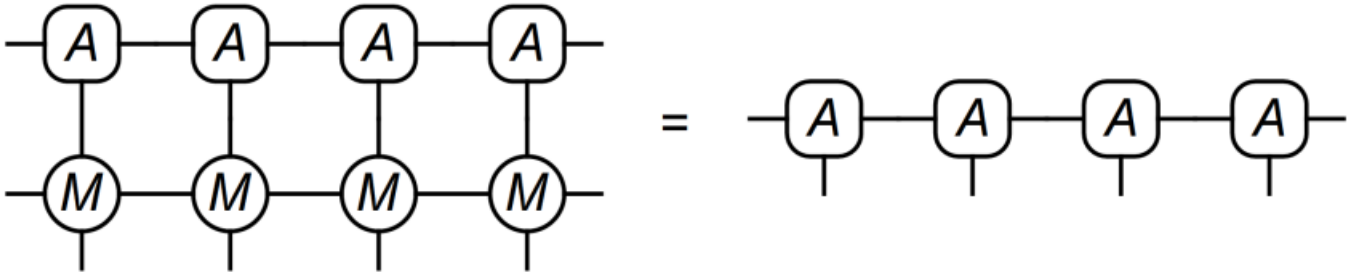


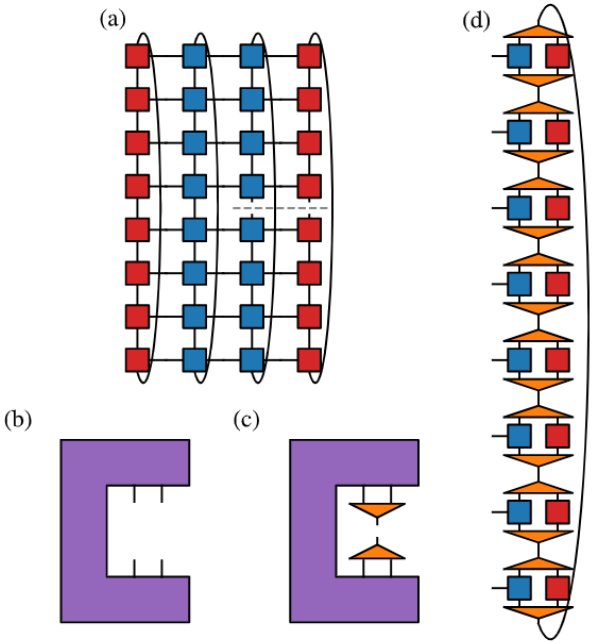




Divide U1 MPS block in VUMPS

- Last step TEBD





- Easy to realize but increased computation cost

  3-leg FL,FR→4-leg FL,FR

- use this trick after one AD Optimization

Thank you for listening!

Q&A?