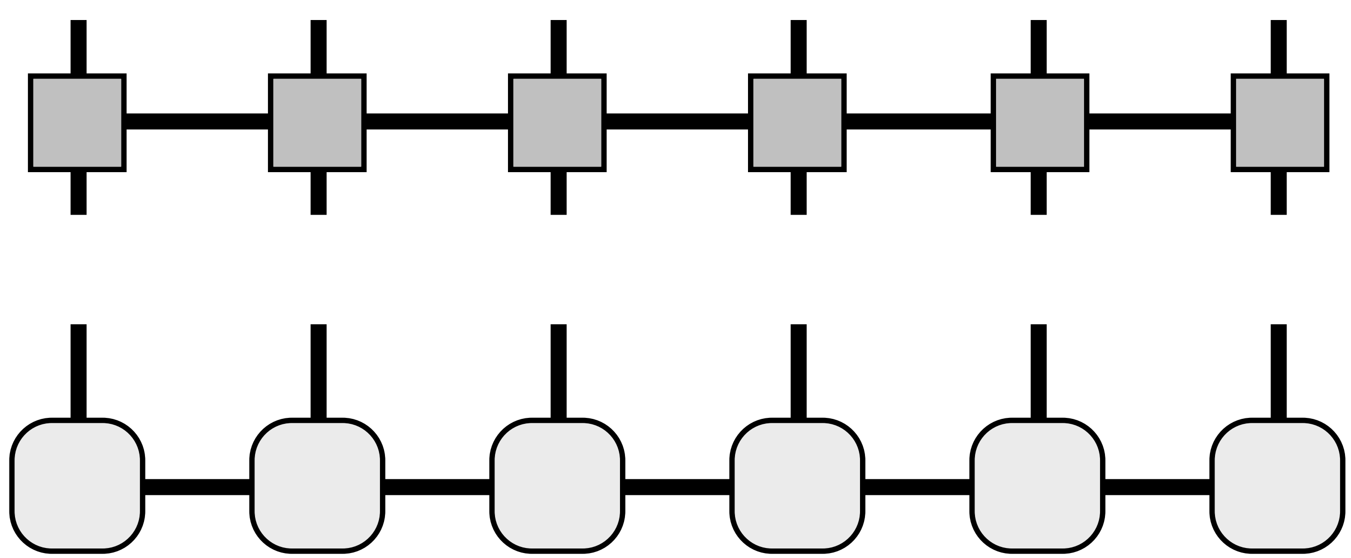
07 DMRG

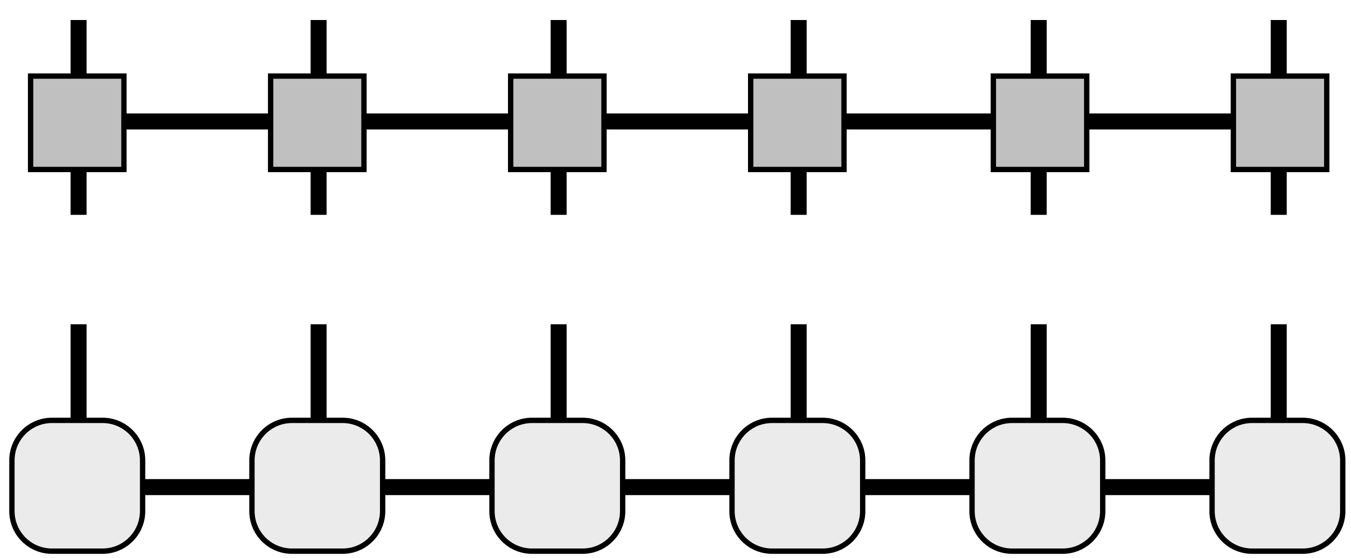
DMRG is the best method for finding ground states of 1d Hamiltonians

Want to solve $H|\Psi\rangle = E|\Psi\rangle$

Think of H as MPO



Important: MPS should be in definite gauge
I.e. most tensors unitary



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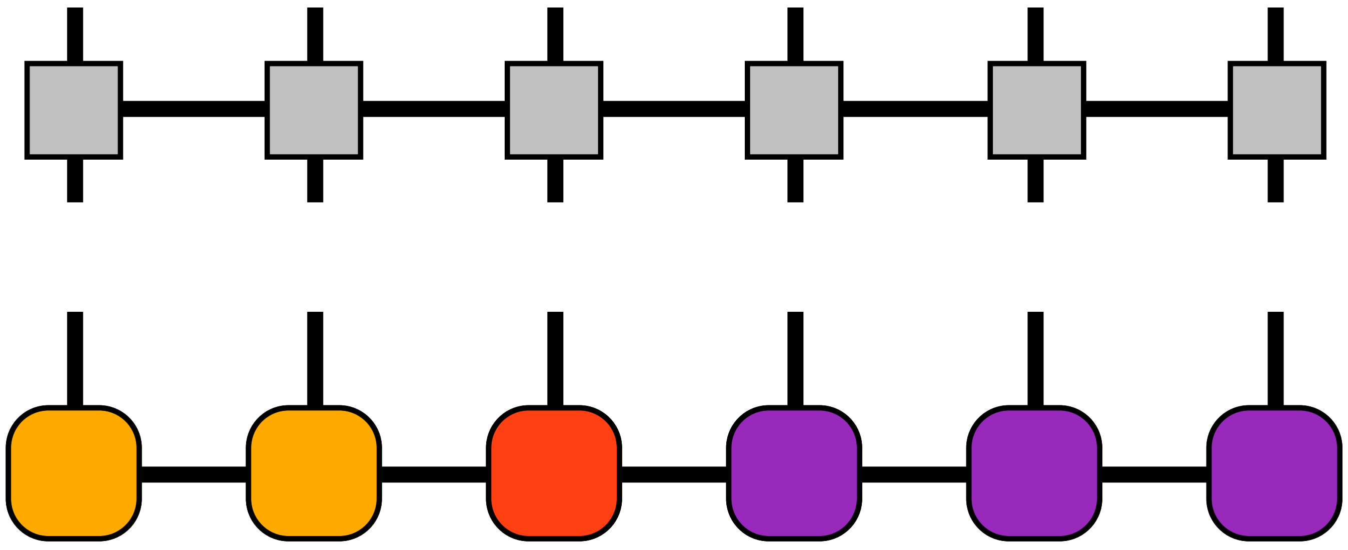
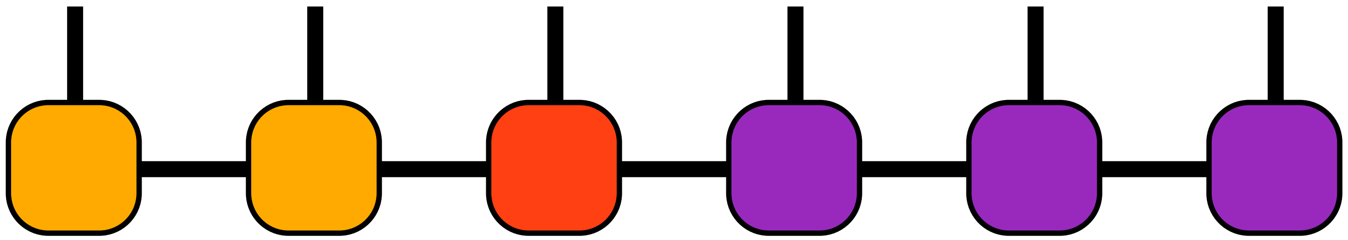


This way, tensors left/right of center define orthonormal bases



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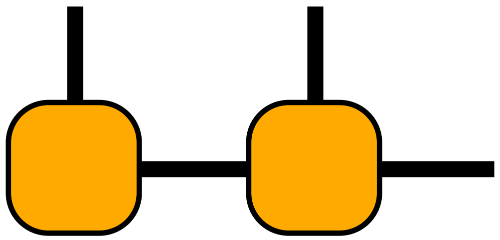

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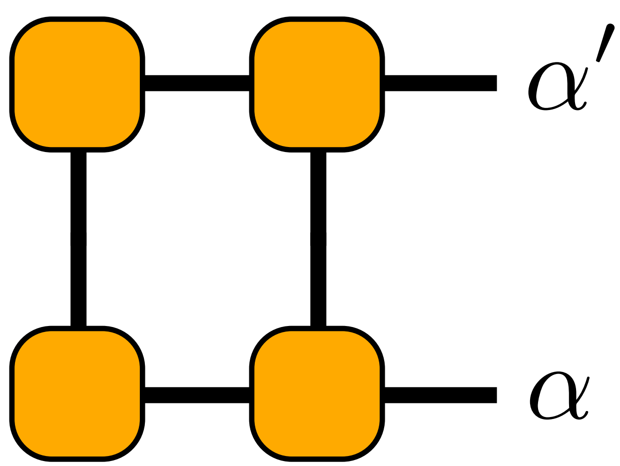
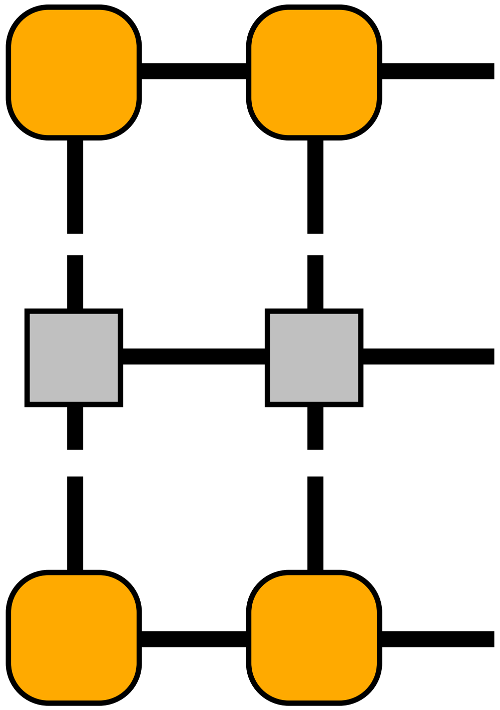


$$= \delta_{\alpha}^{\alpha'}$$

Can project Hamiltonian into this basis



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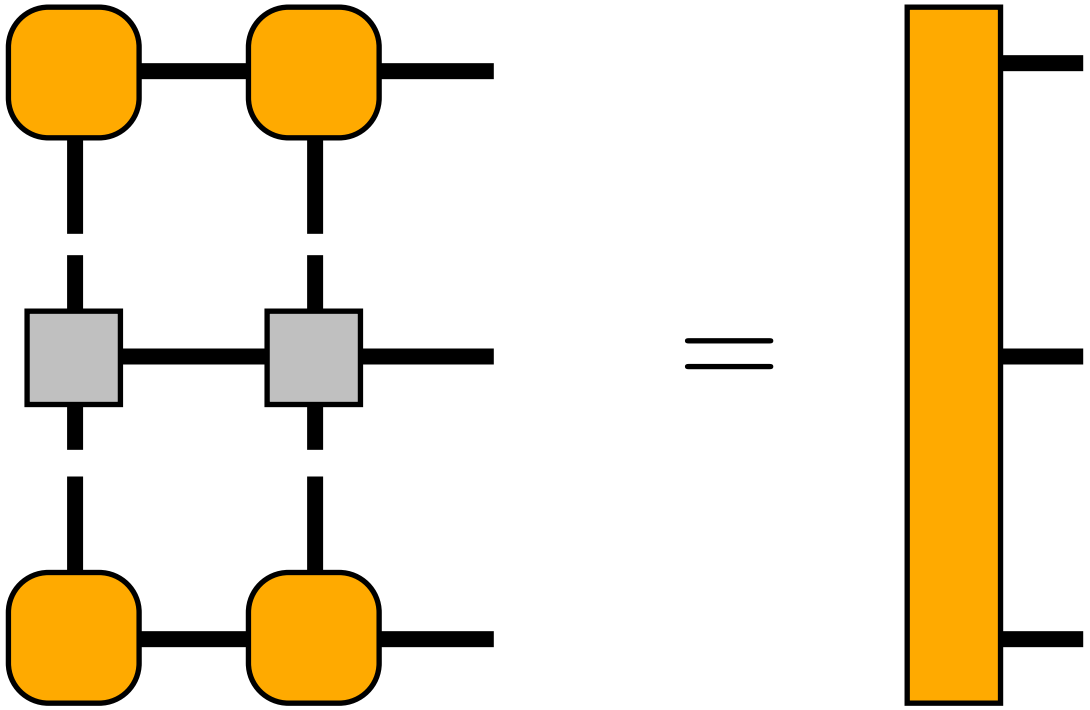
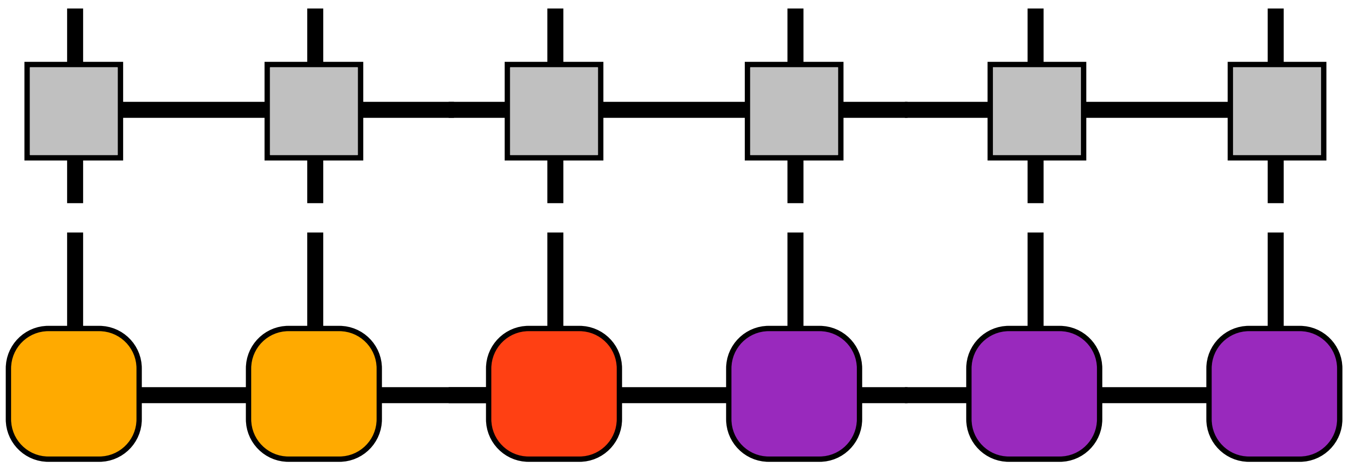


Doing the same on the right gives



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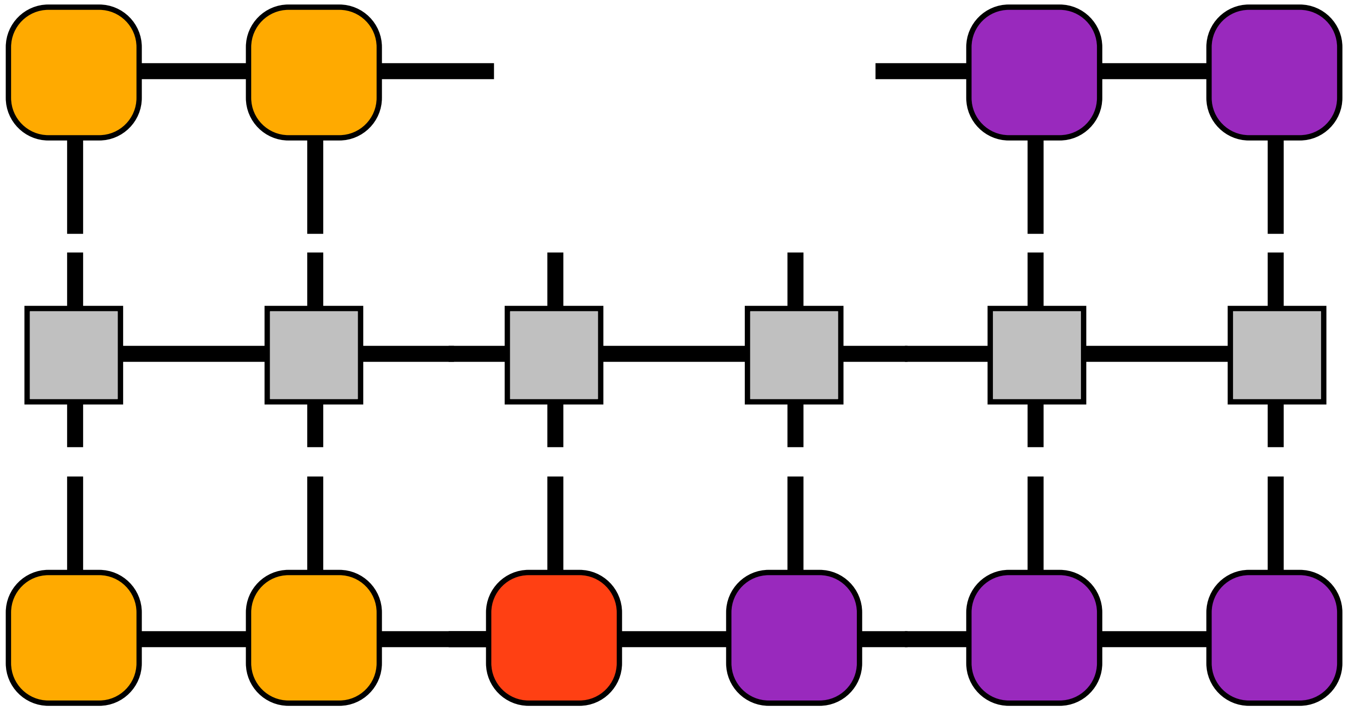

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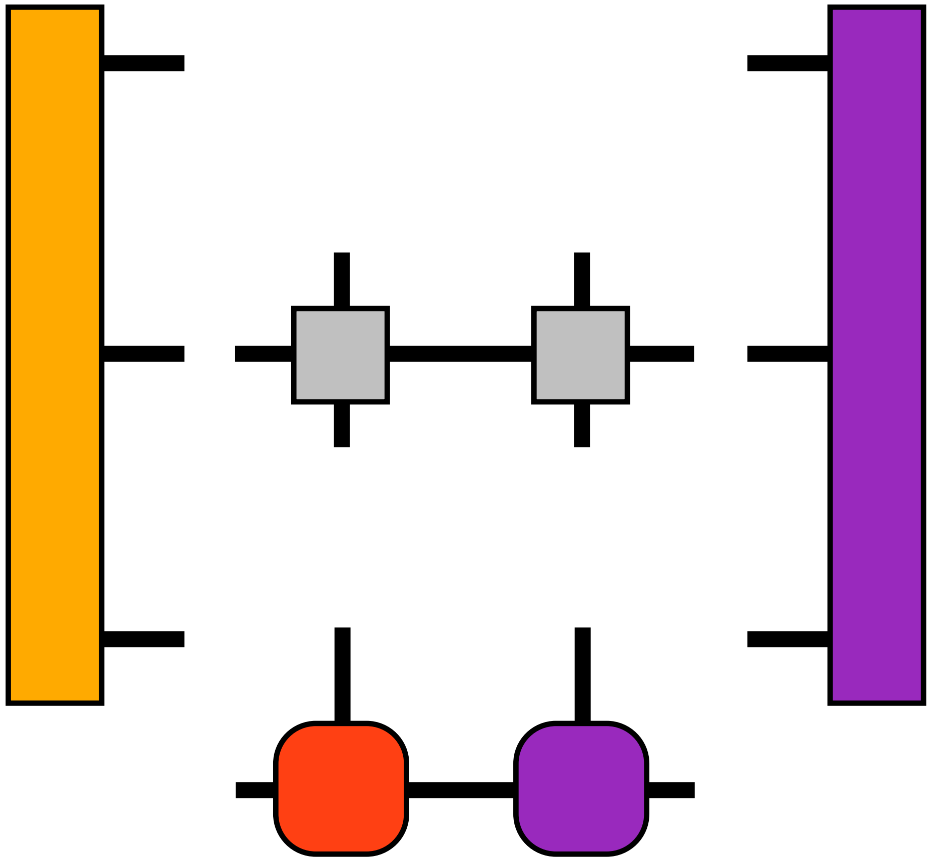
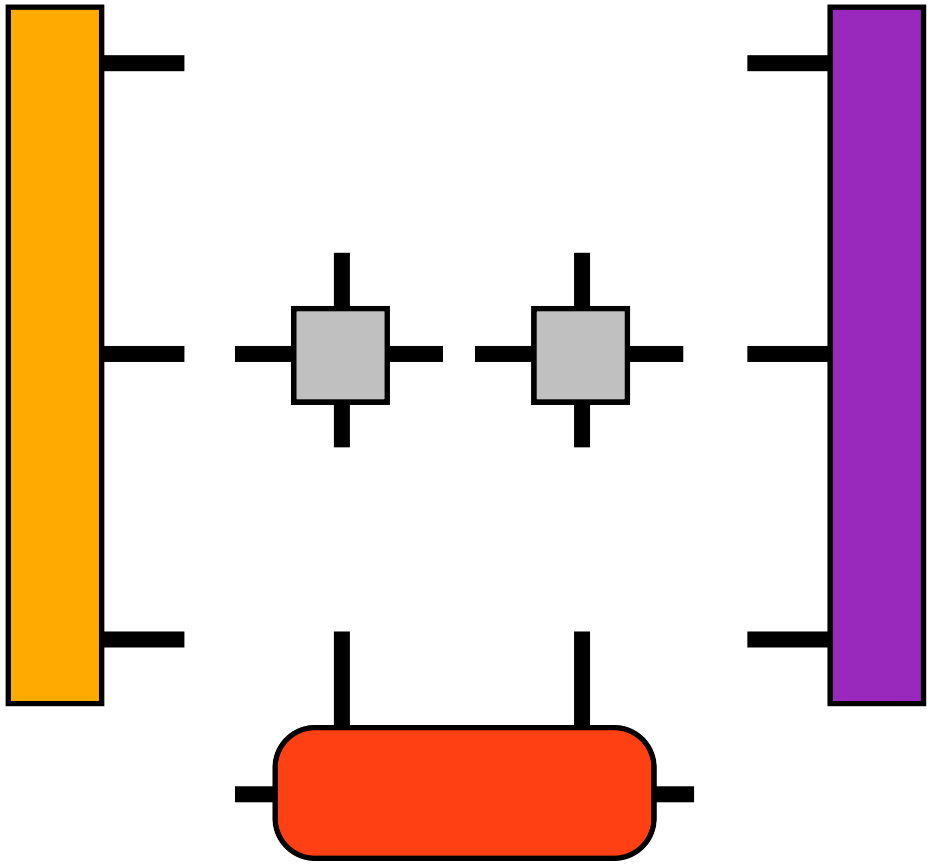


$$\tilde{H}|\tilde{\Psi}\rangle = \tilde{E}|\tilde{\Psi}\rangle$$

Can efficiently multiply effective $\tilde{H}$ times $|\tilde{\Psi}\rangle$

Order important!



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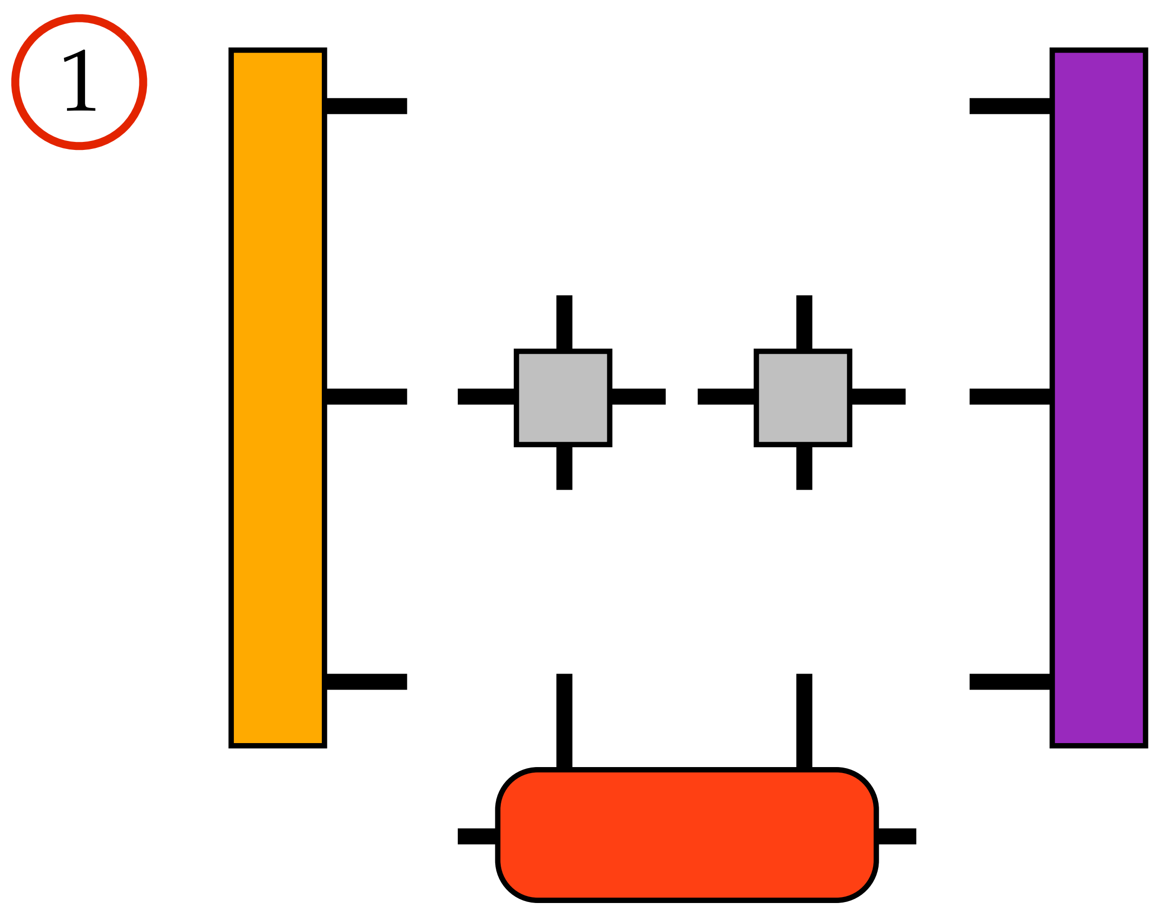
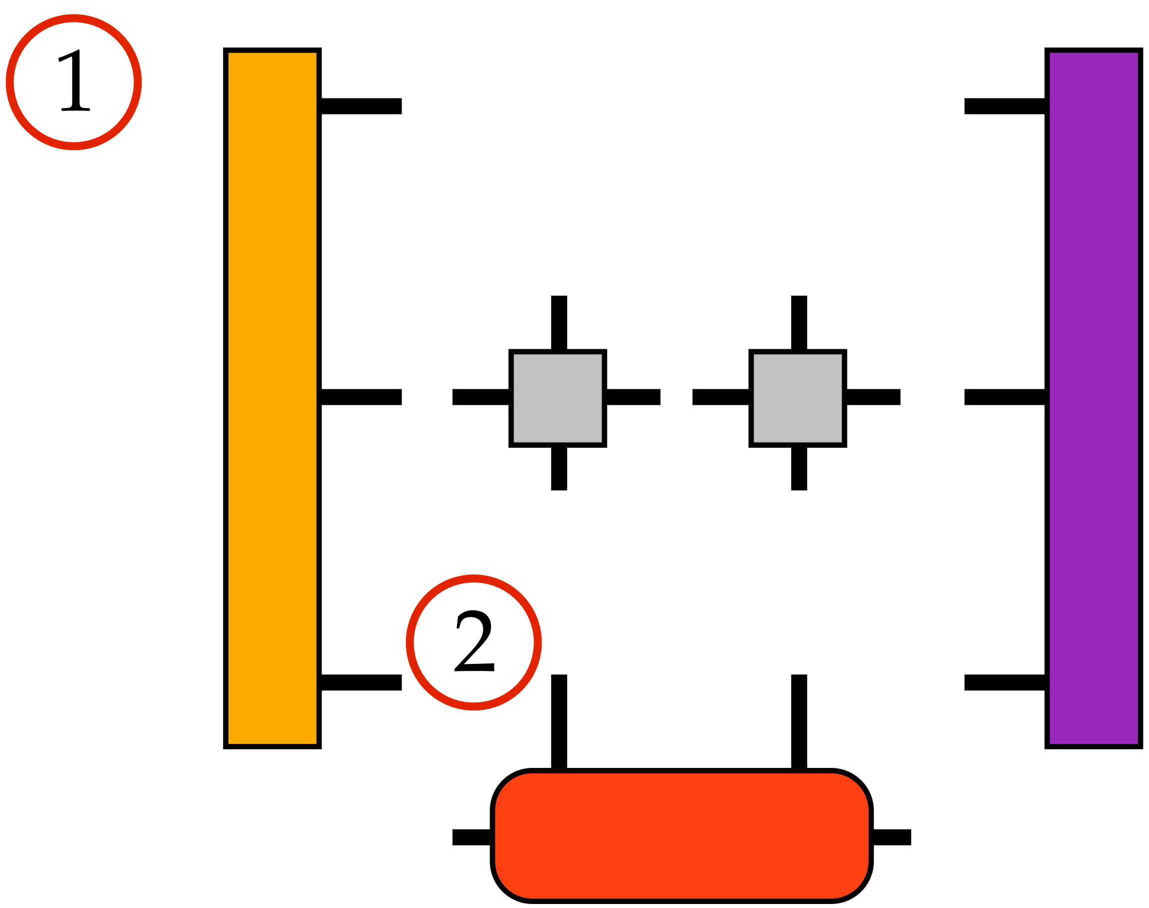


Can efficiently multiply effective $\tilde{H}$ times $|\tilde{\Psi}\rangle$

Order important!

$2 \sim m^3$

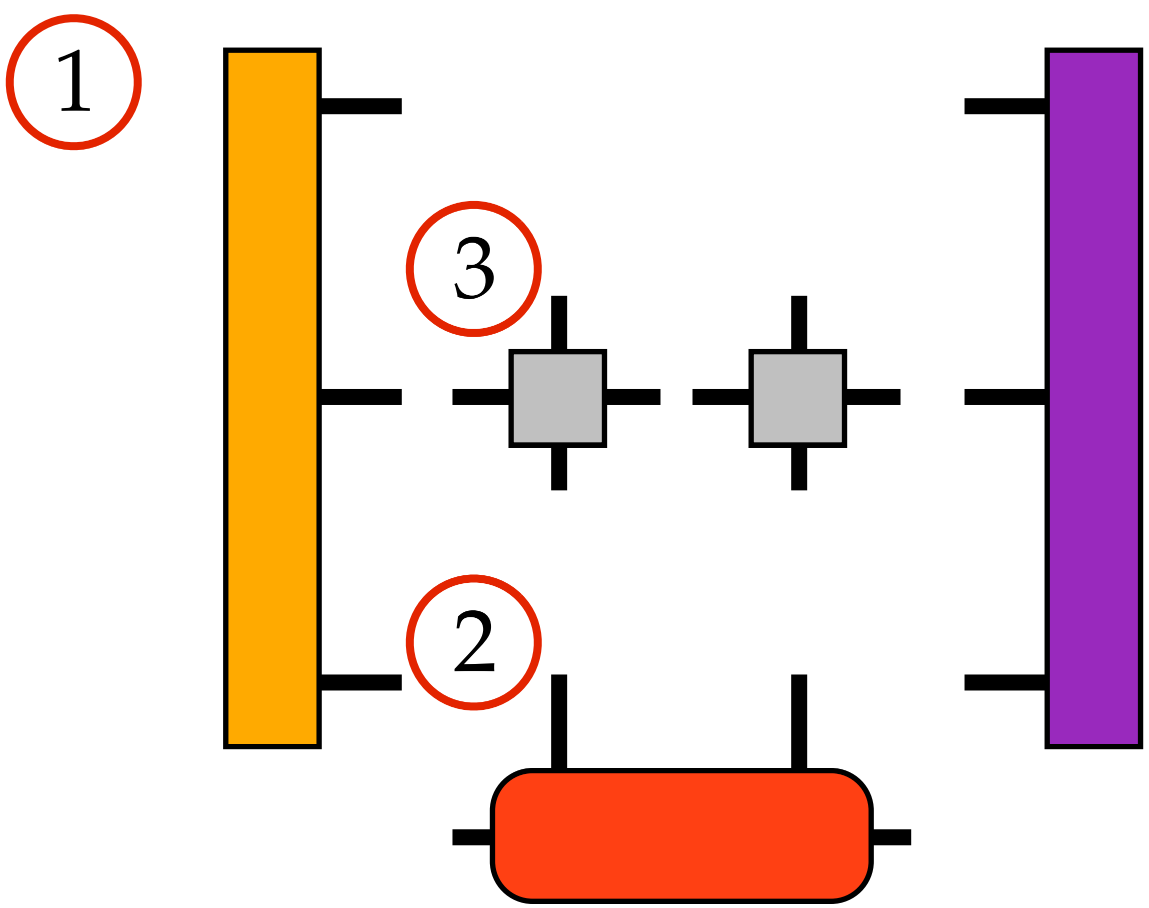


Can efficiently multiply effective $\tilde{H}$ times $|\tilde{\Psi}\rangle$

Order important!

$2 \sim m^3$

$3 \sim m^2$



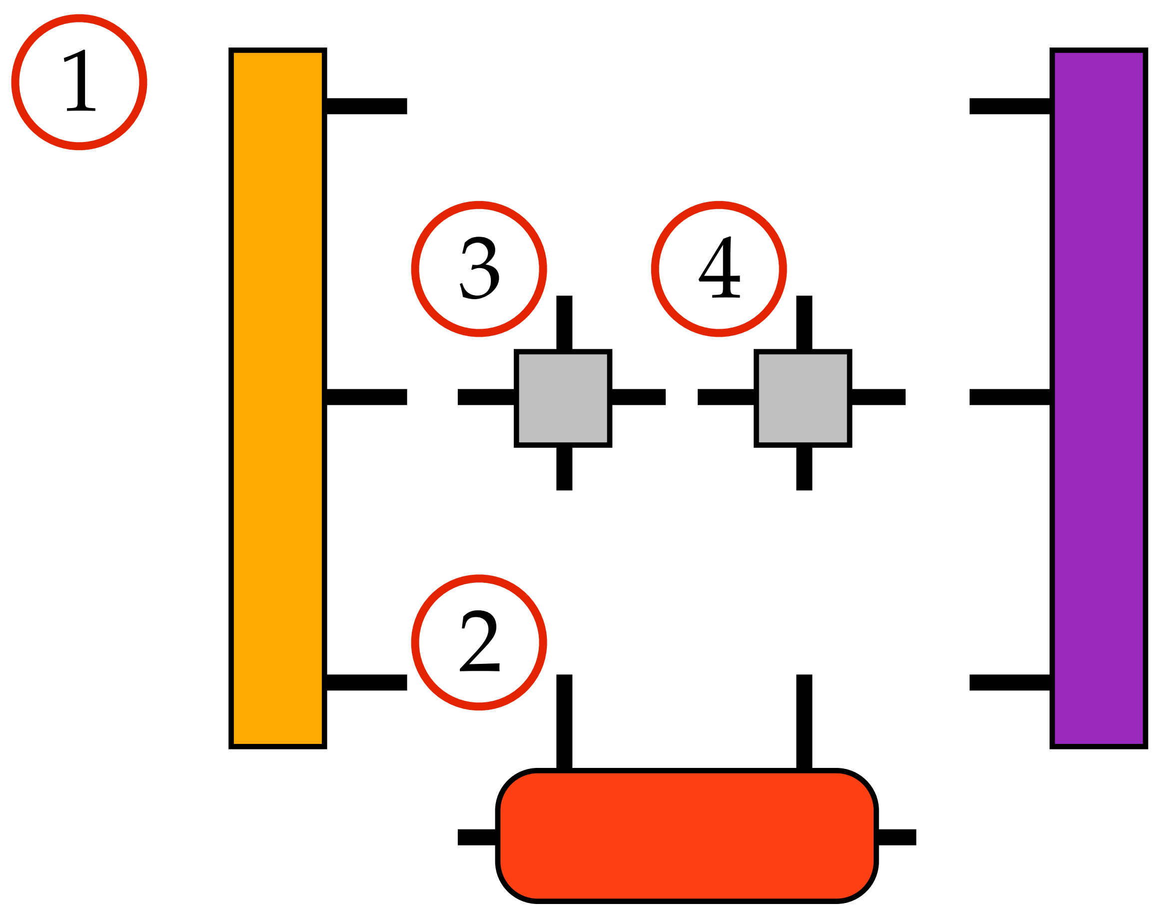
Can efficiently multiply effective $\tilde{H}$ times $|\tilde{\Psi}\rangle$

Order important!

$2 \sim m^3$

$3 \sim m^2$

$4 \sim m^2$



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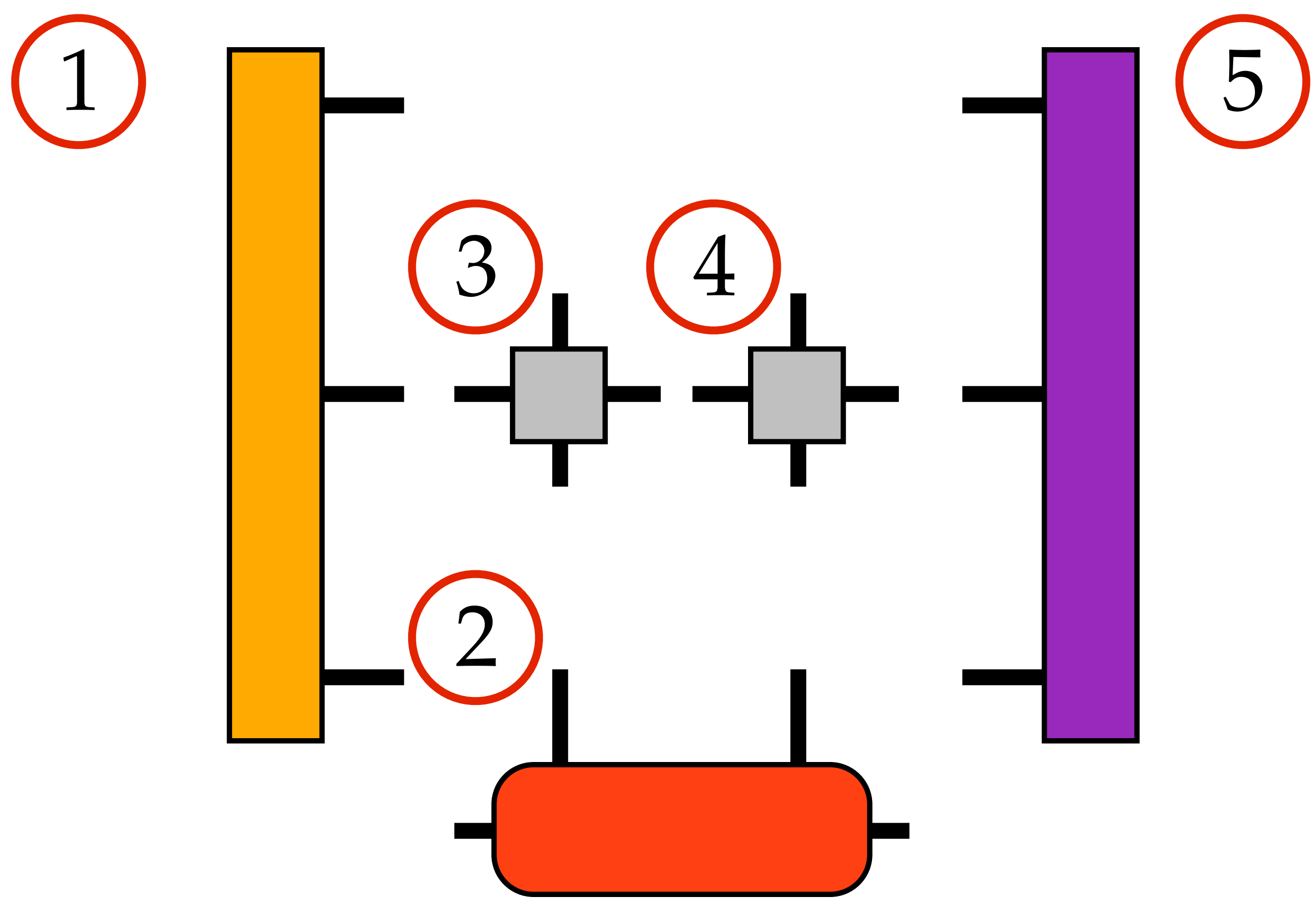


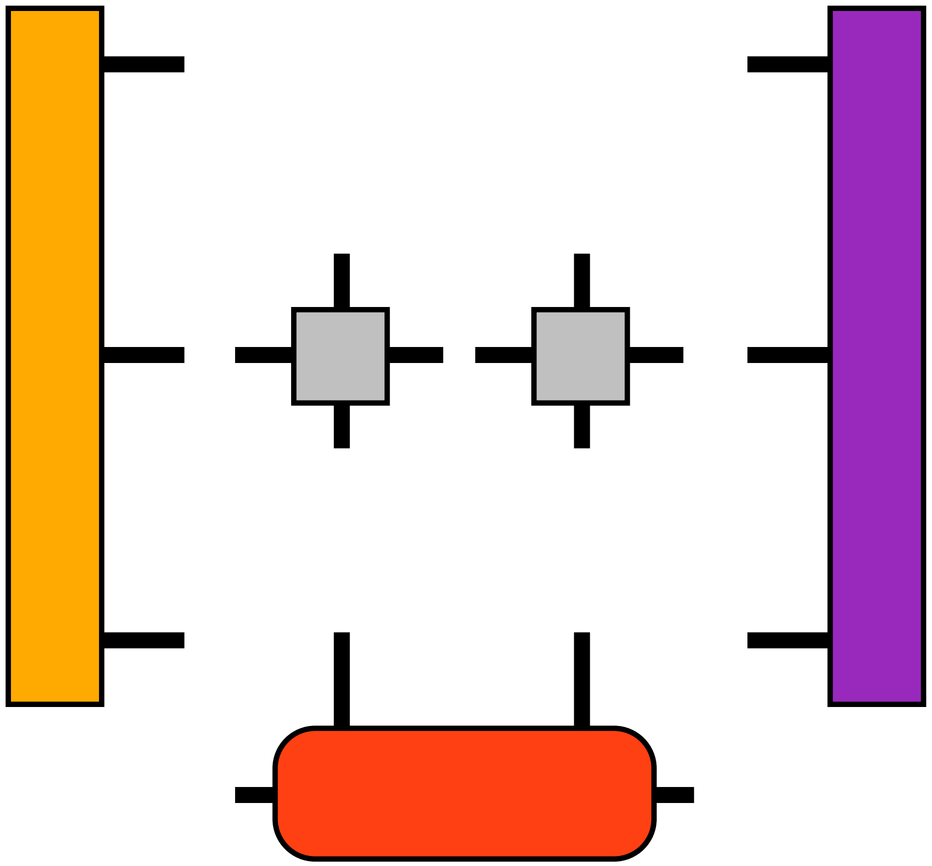
$2 \sim m^3$

$3 \sim m^2$

$4 \sim m^2$

$5 \sim m^3$

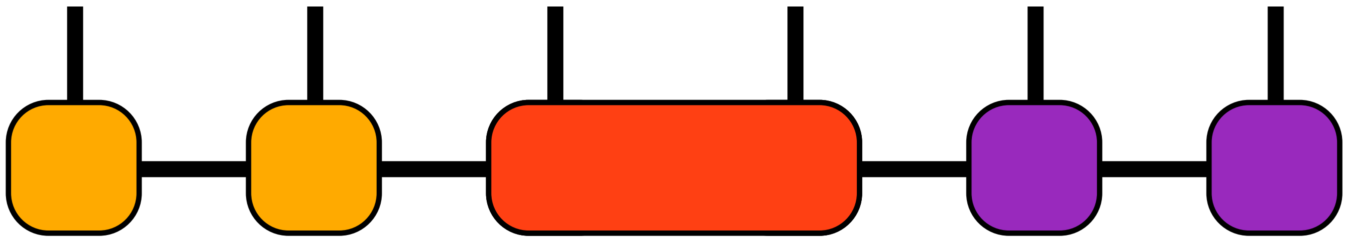
Use Lanczos/Davidson to solve
(sparse matrix eigensolver)



Noack, Manmana, AIP Conf. Proc. **789**, 93 (2005)

Now, with improved wavefunction,
shift orthogonality center
(using SVD)

Important to truncate to m singular values
("number of states kept" in DMRG)



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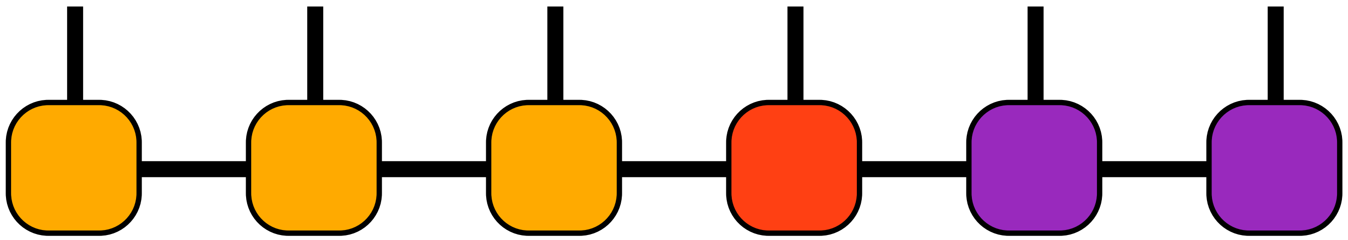
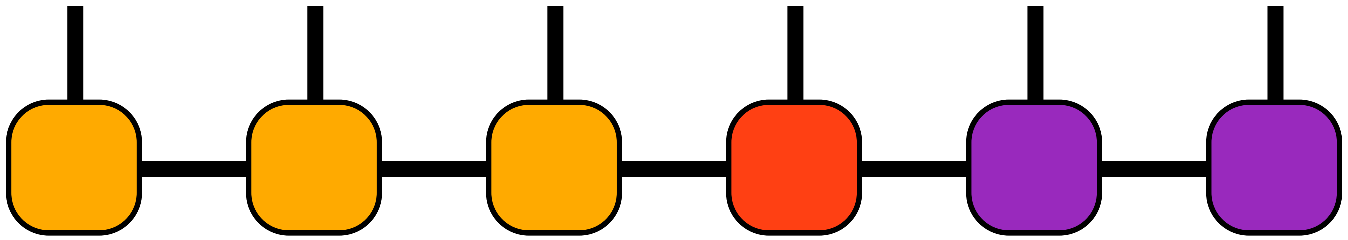


Grow projected Hamiltonian



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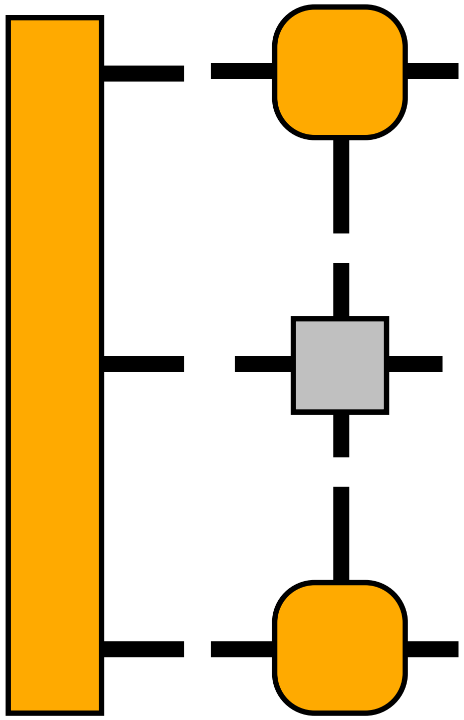

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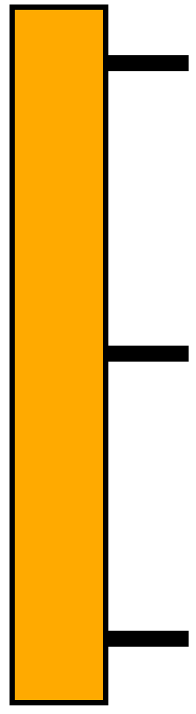
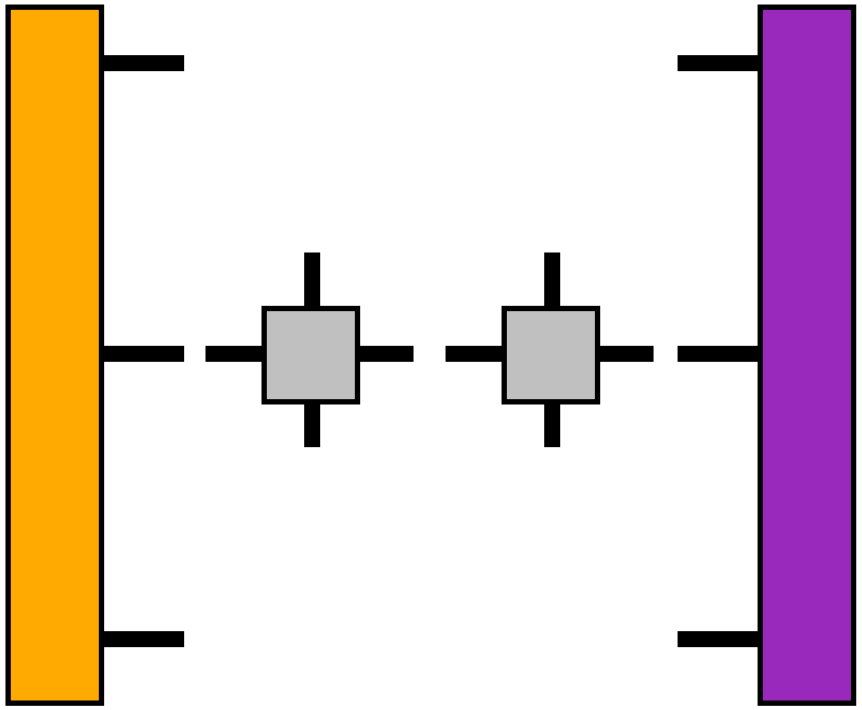
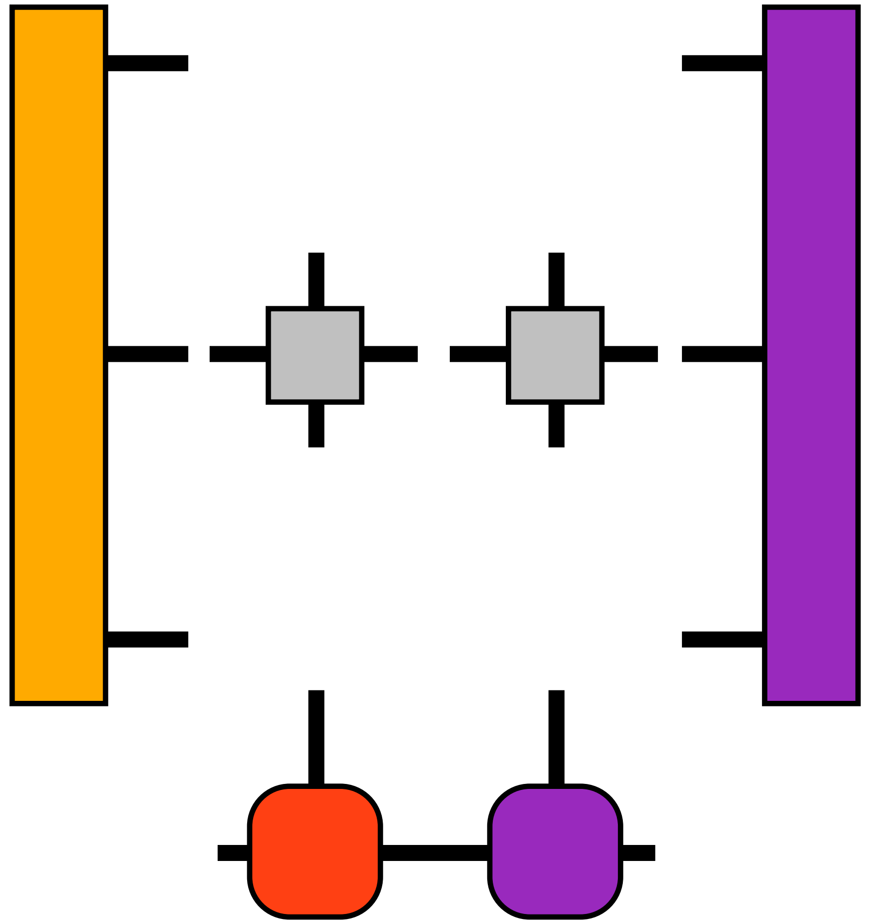


Grow projected Hamiltonian

Recover older projected Hamiltonian saved in memory



Iterating leads to sweeping procedure

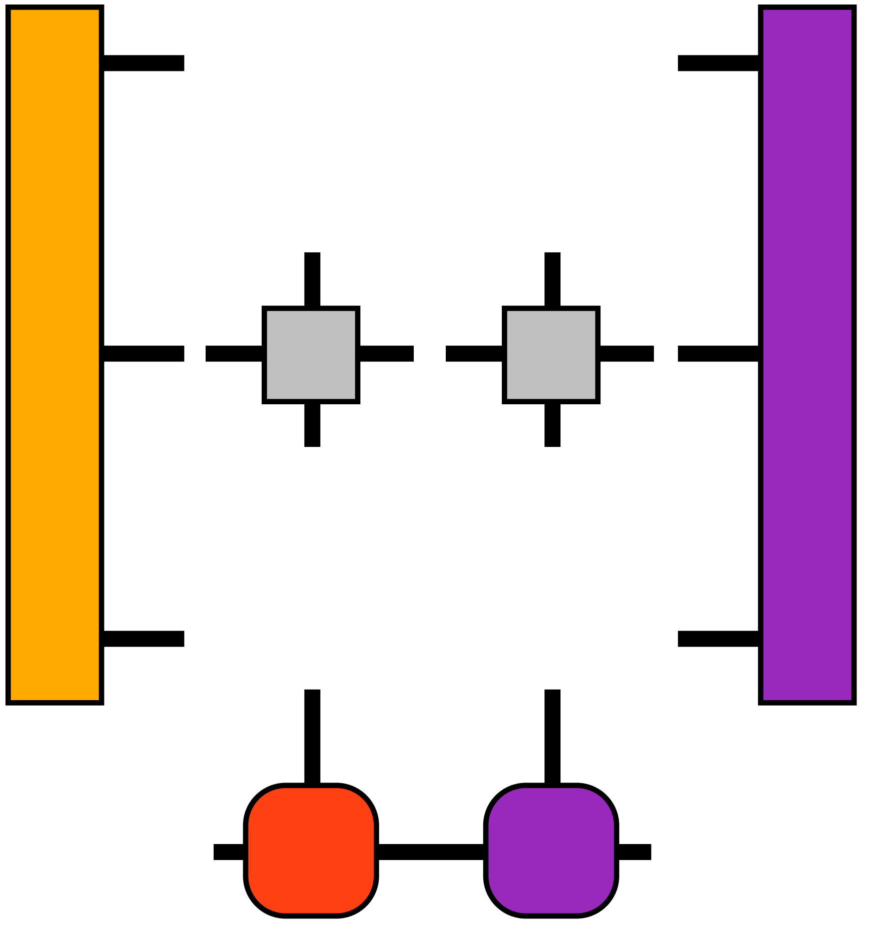


Iterating leads to sweeping procedure

I. Solve eigenproblem

II. SVD wavefunction

III. Grow effective H



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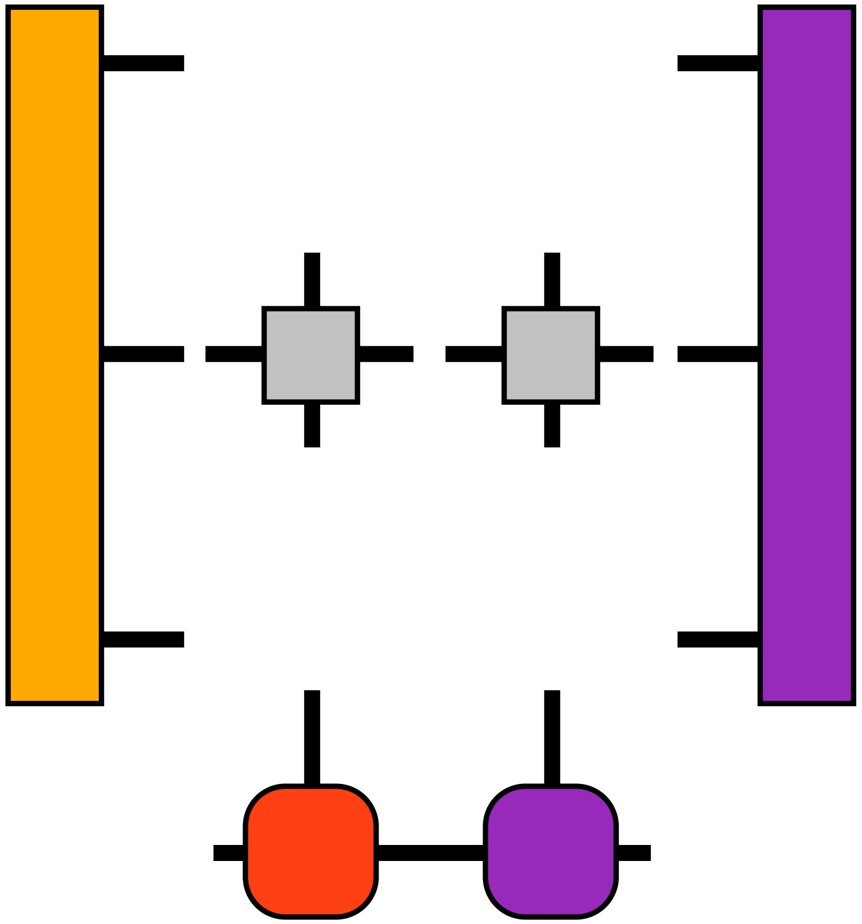

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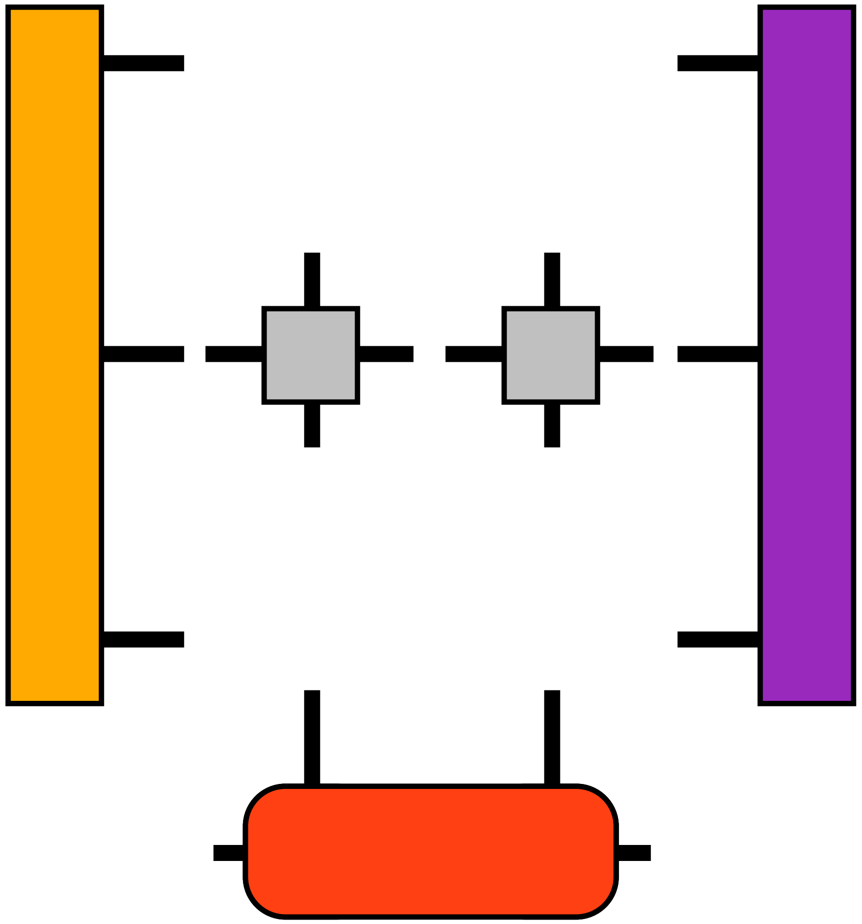

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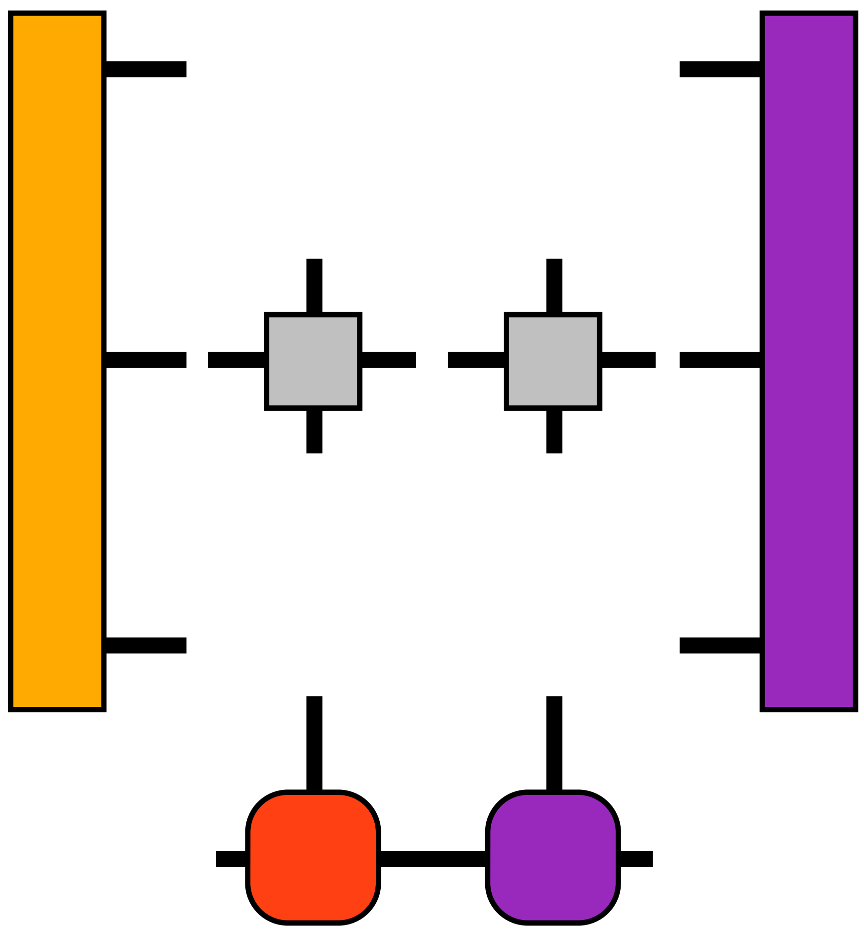

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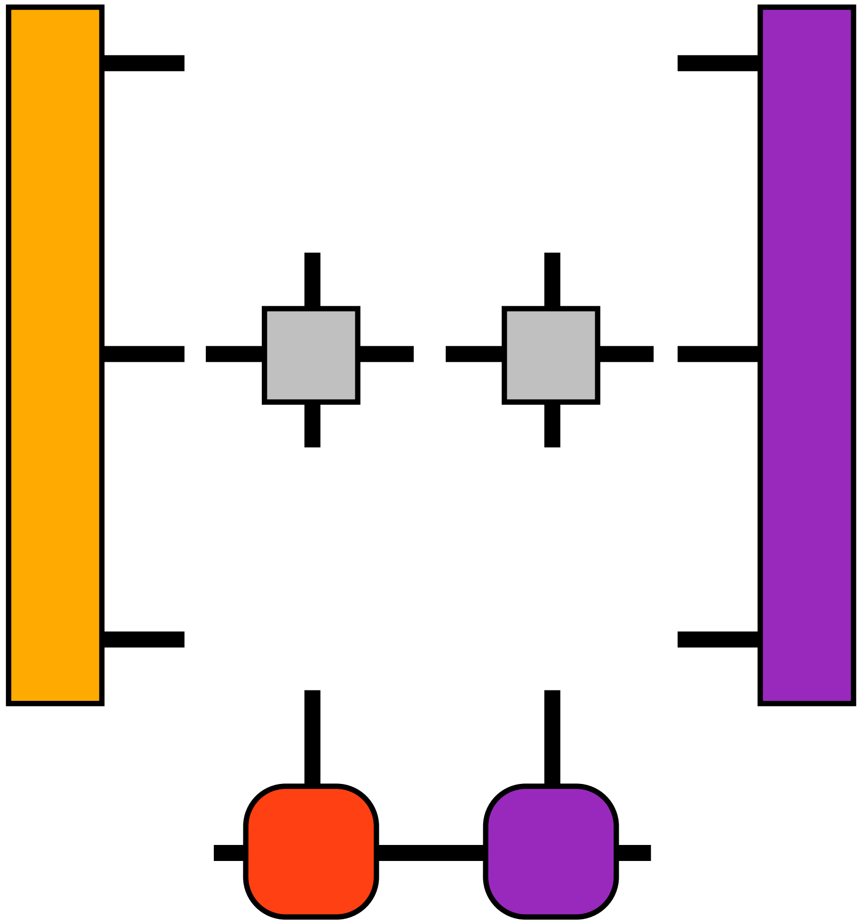

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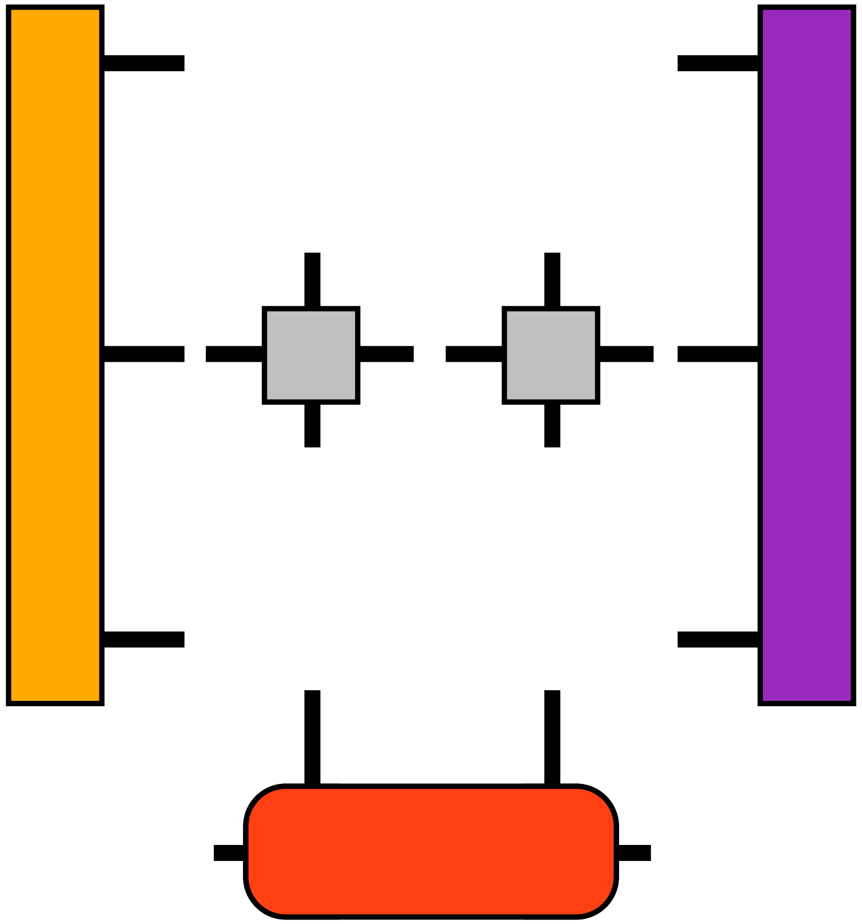

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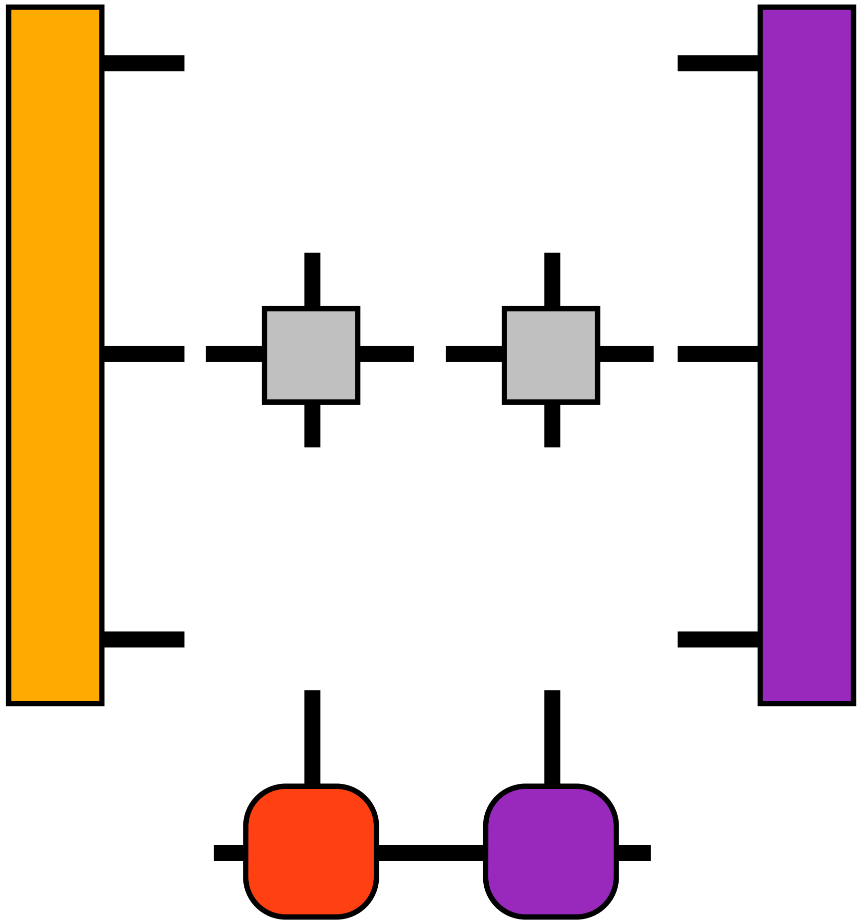

We'll implement a key missing step of the DMRG algorithm

`<library folder>/tutorial/06_DMRG`

1. Read through **`dmrg.cc`**; compile; and run

2. SVD the two-site tensor phi into factors A, D, B
   The last argument to svd should be "opts" to pass through parameters controlling truncation:

```
svd(phi, ... , opts);
```

3. Multiply the singular-value tensor D back into A or B as appropriate to shift orthogonality center of MPS.

4. Add code to print out the energy at each step (or even to measure other local operators).