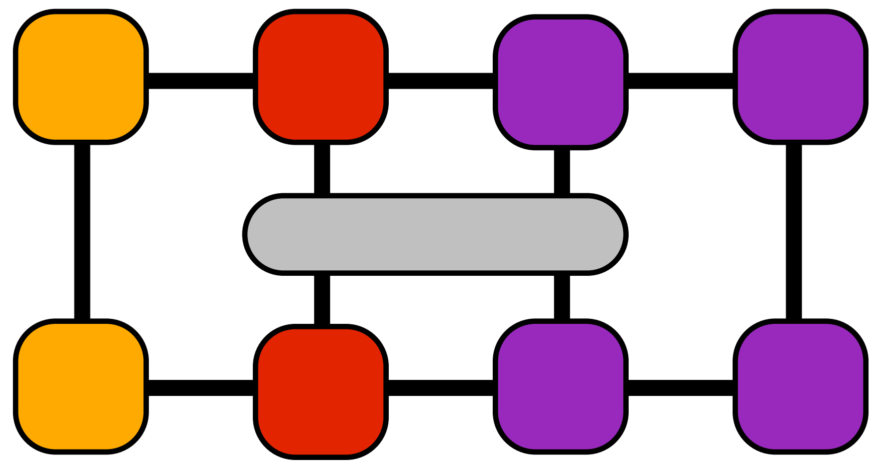
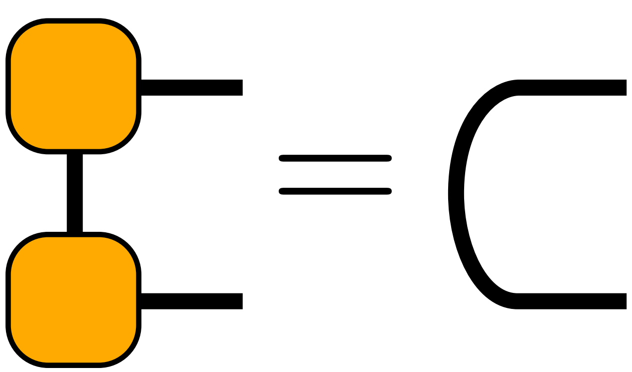
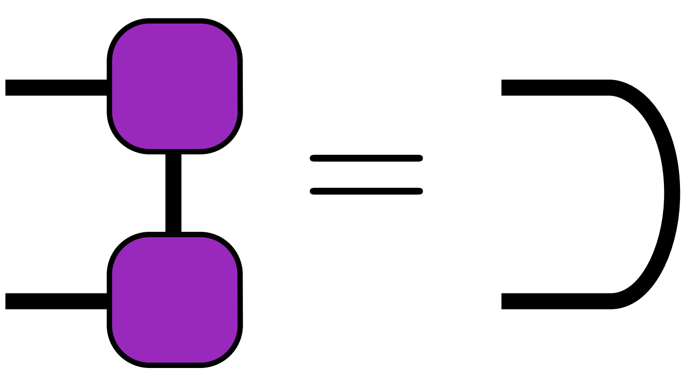
05 Trotter

Just as we can measure one-site operators,
can measure two-site operators



Recall:





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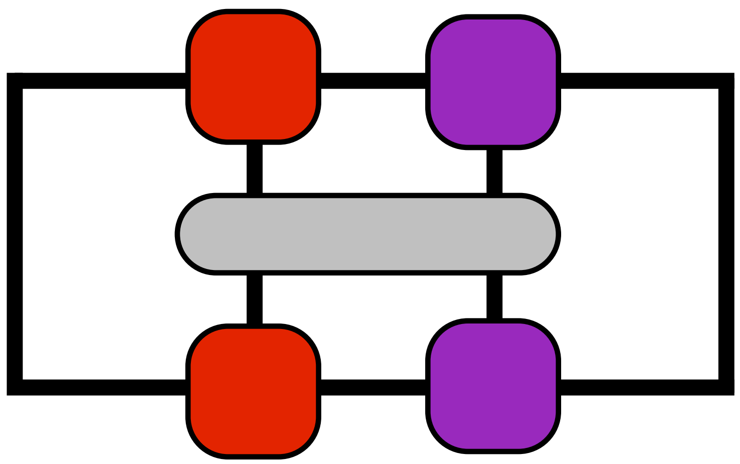

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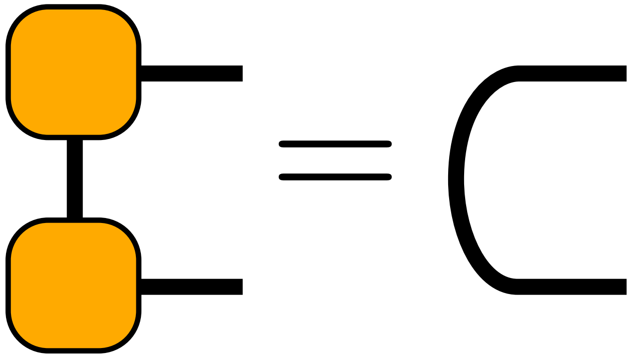
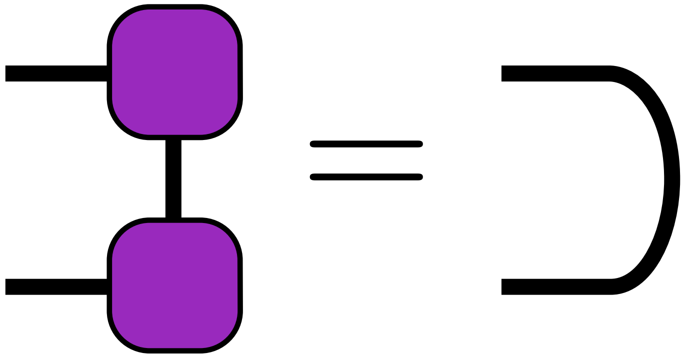
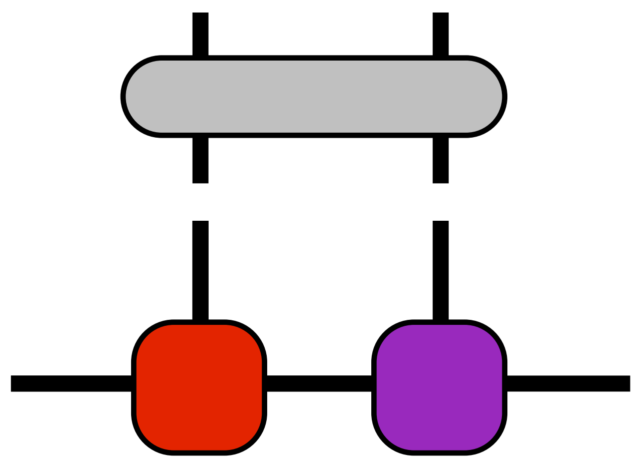




Since two "center" sites have orthogonal environment, ok to apply operators:



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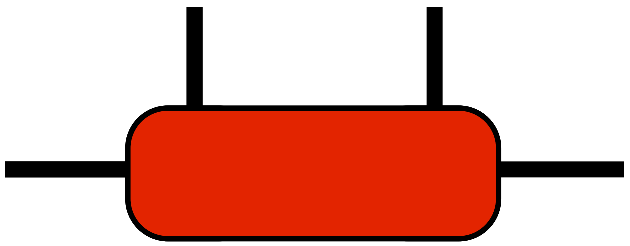

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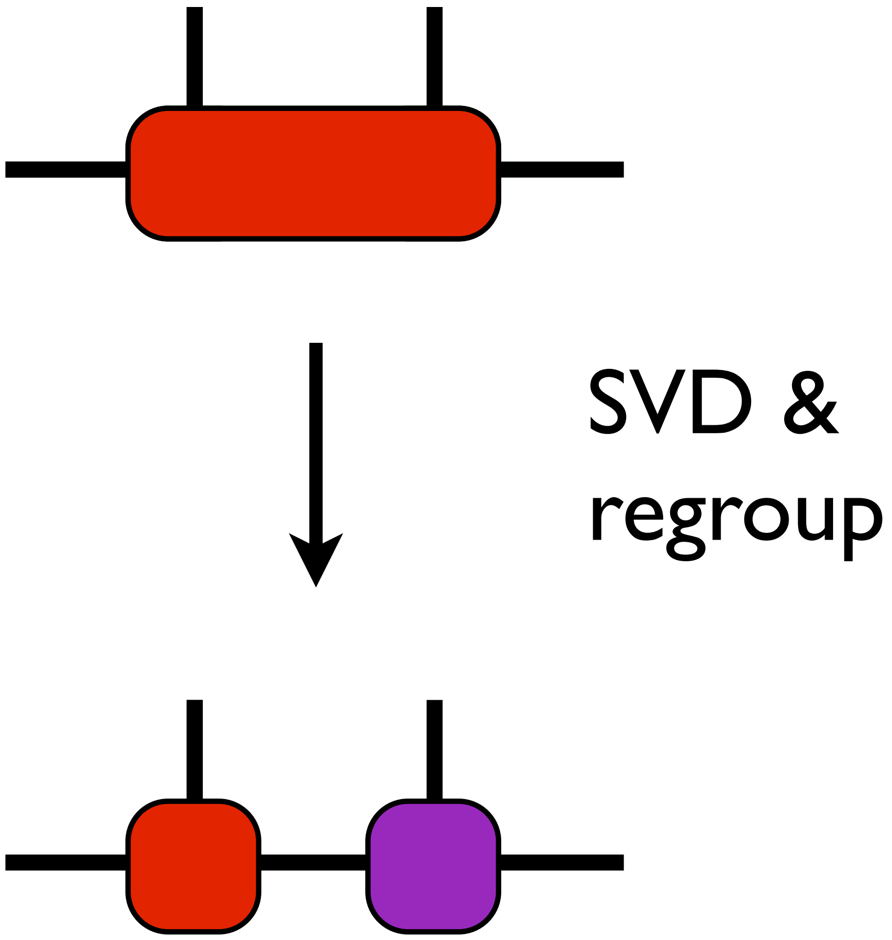
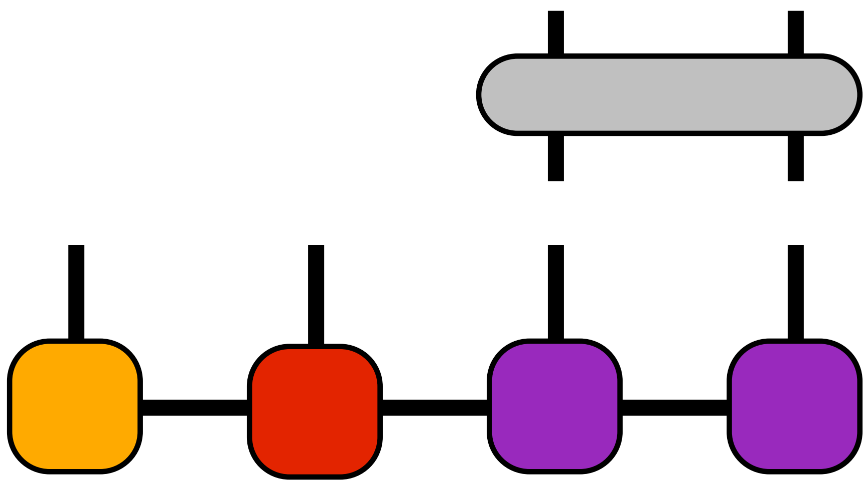


Would NOT be ok on another bond without regauging



Truncating SVD not globally optimal except at orthogonality center

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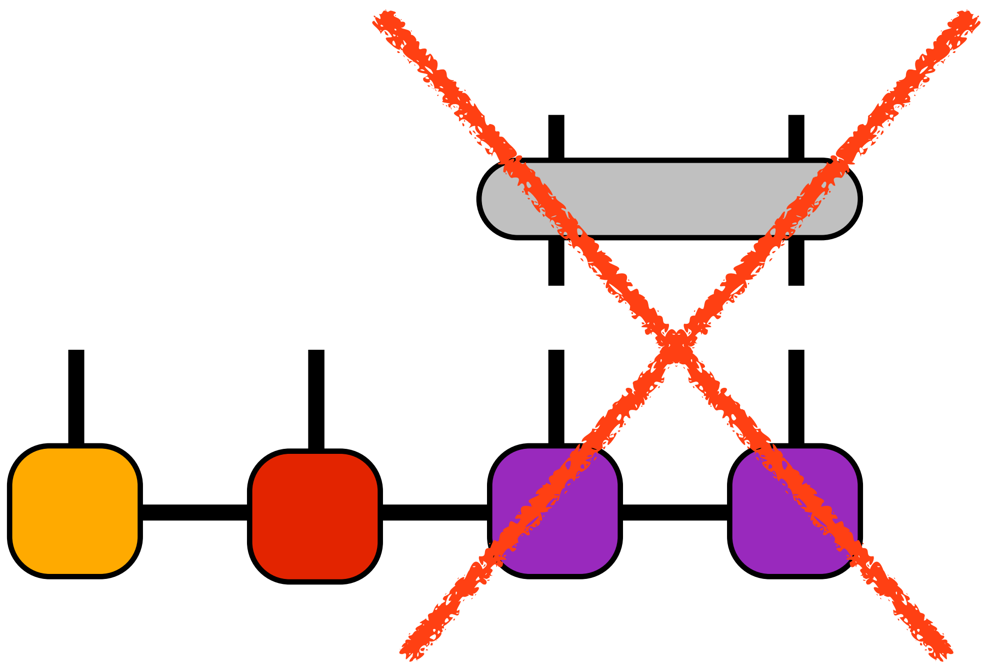

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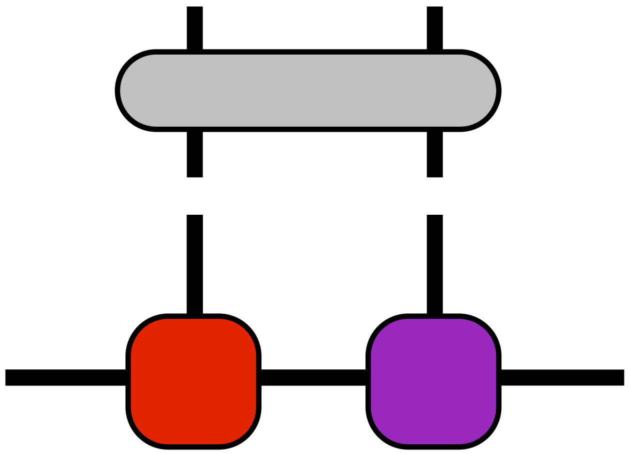
Q: What can we do with this capability?



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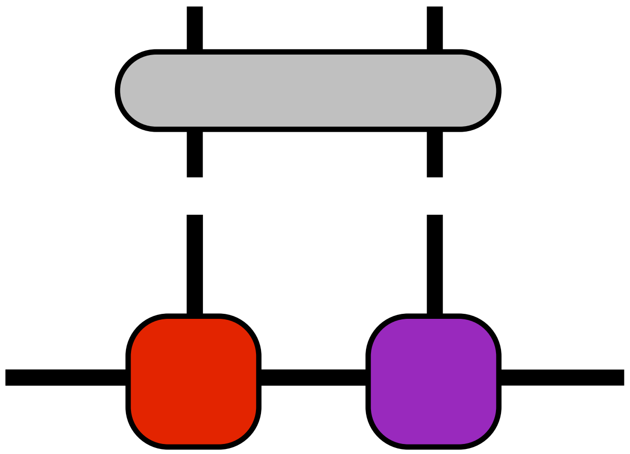


A: For short-ranged Hamiltonians, can time evolve

Trick is to use Trotter decomposition

Useful for Hamiltonians of the form

$$H = H_1 + H_2 + H_3 + \dots$$

For example

$$H = \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1}$$

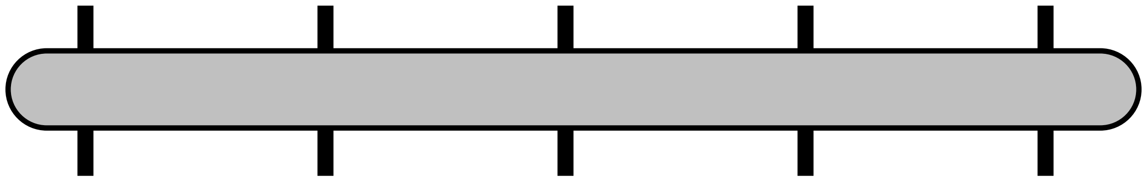
$$= (\mathbf{S}_1 \cdot \mathbf{S}_2) + (\mathbf{S}_2 \cdot \mathbf{S}_3) + (\mathbf{S}_3 \cdot \mathbf{S}_4)$$

For a small time step τ

$$e^{-\tau H} \simeq e^{-\tau H_1/2} e^{-\tau H_2/2} e^{-\tau H_3/2} \ldots$$

$$\cdots e^{-\tau H_3/2} e^{-\tau H_2/2} e^{-\tau H_1/2} + \mathcal{O}(\tau^3)$$

Diagramatically,



$$\simeq$$

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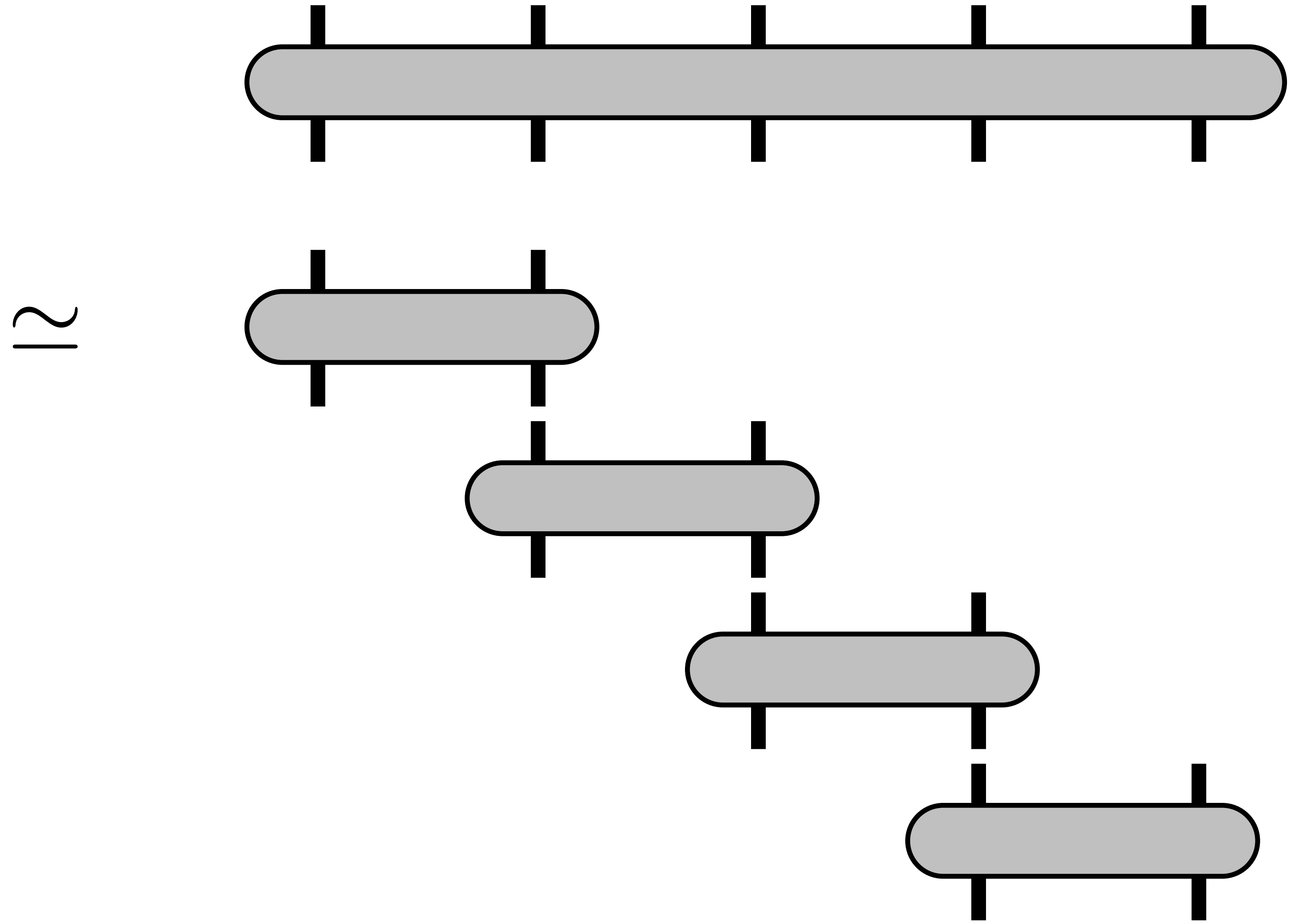

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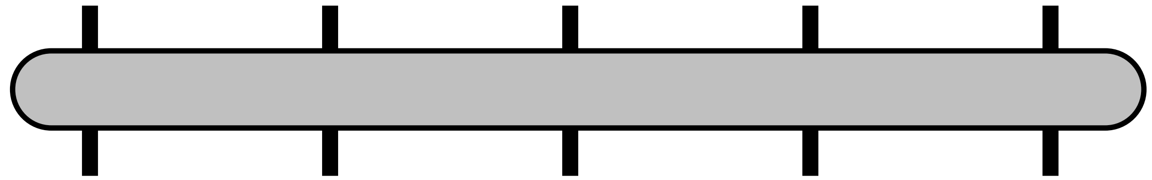

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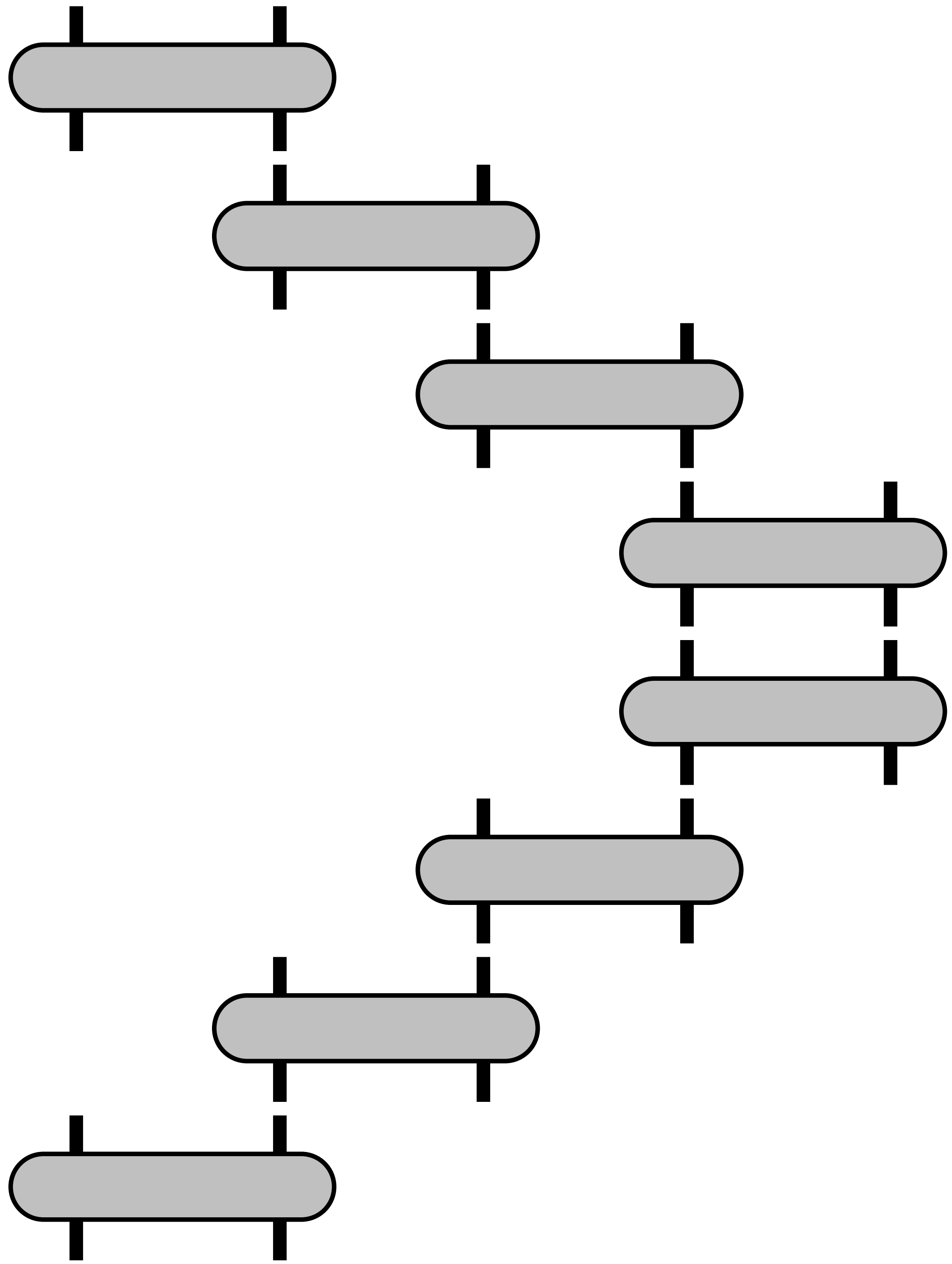
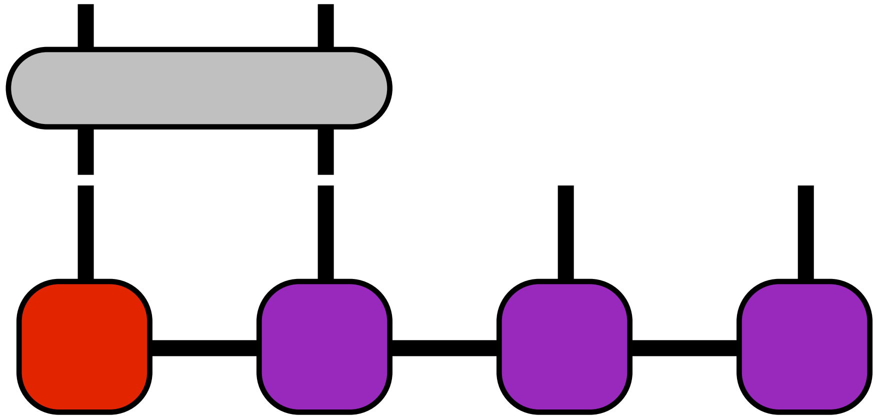


Apply to MPS as follows:



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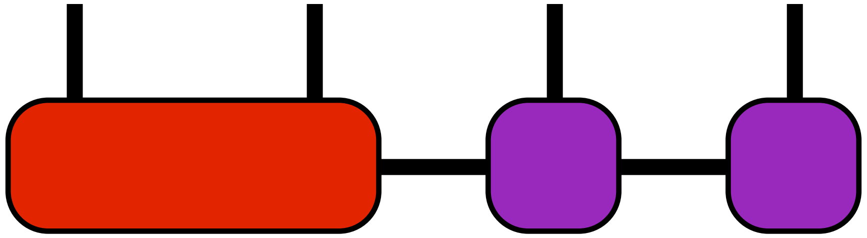

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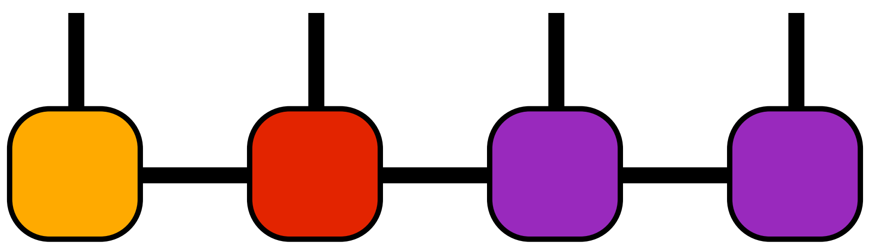

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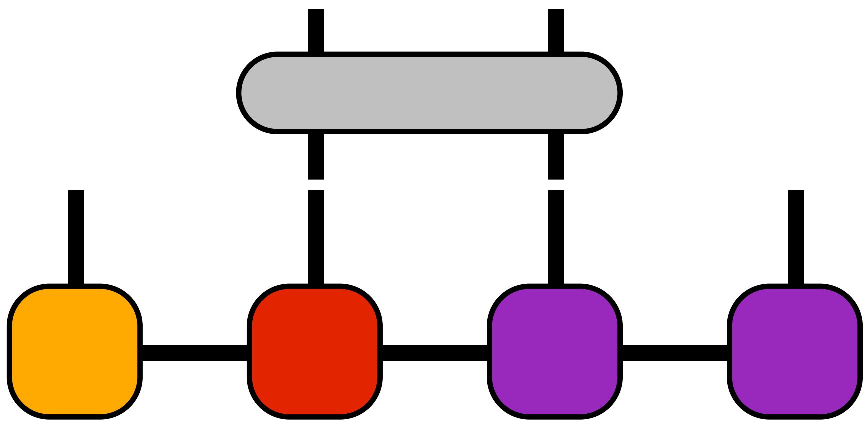

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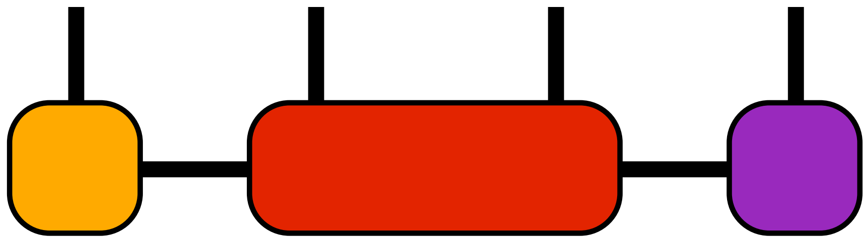

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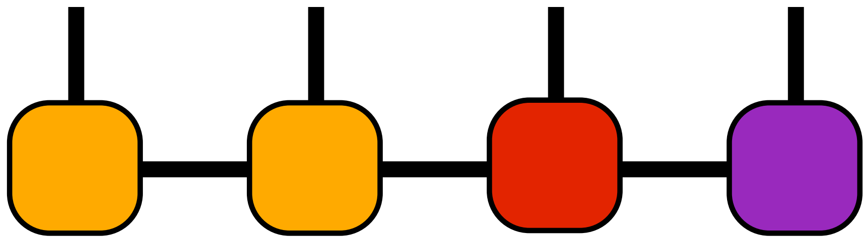

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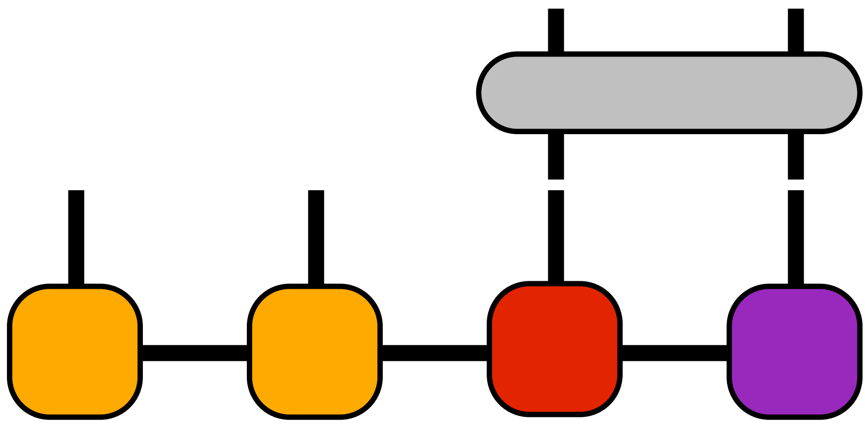

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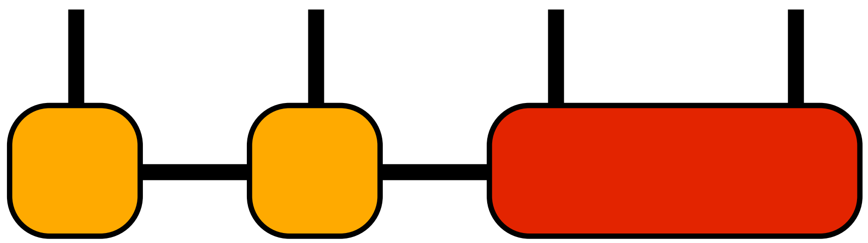

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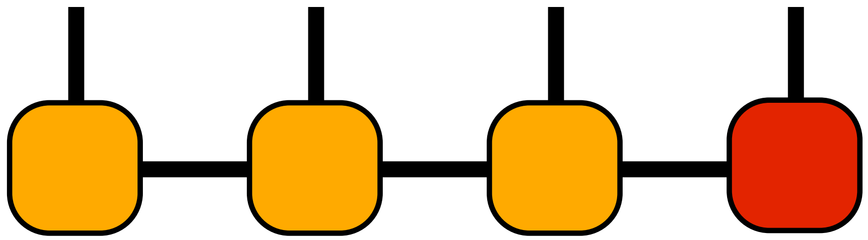

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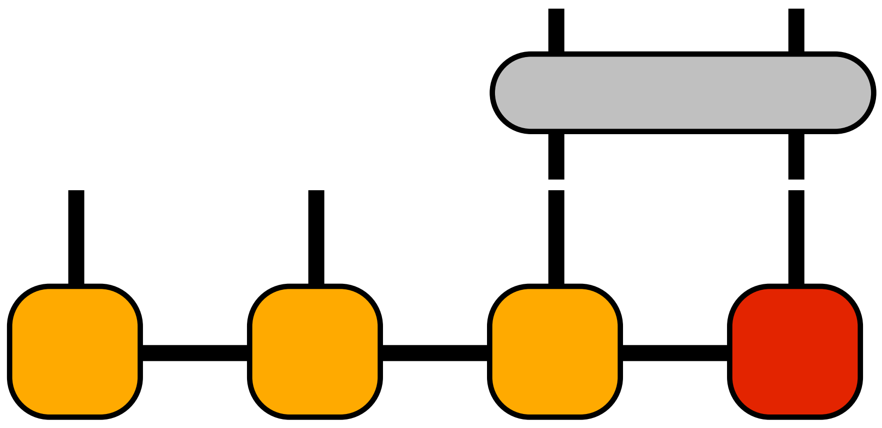

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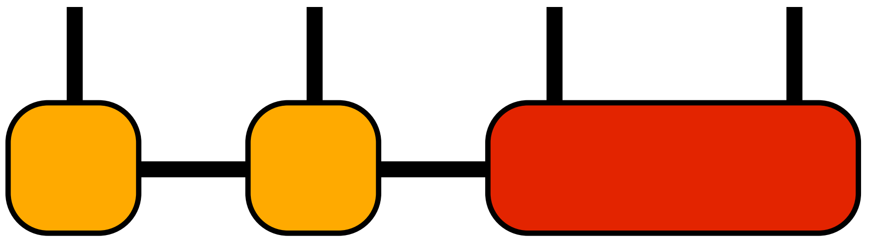

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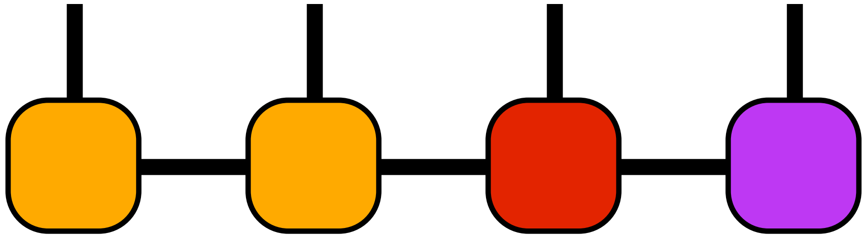

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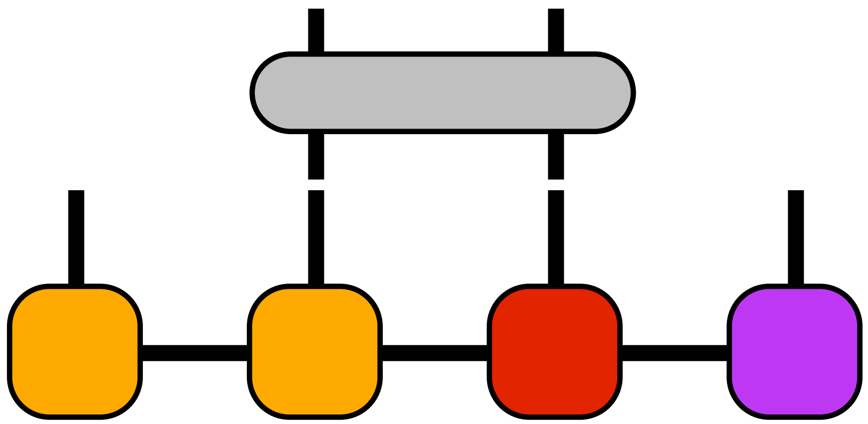

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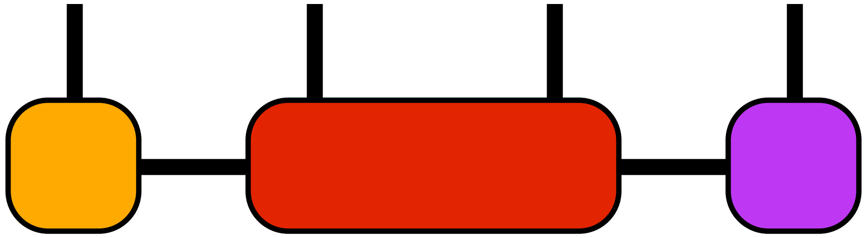

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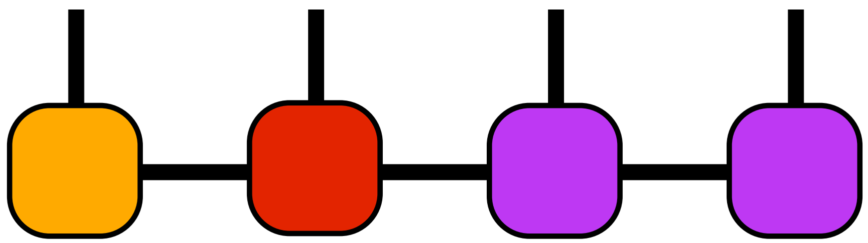

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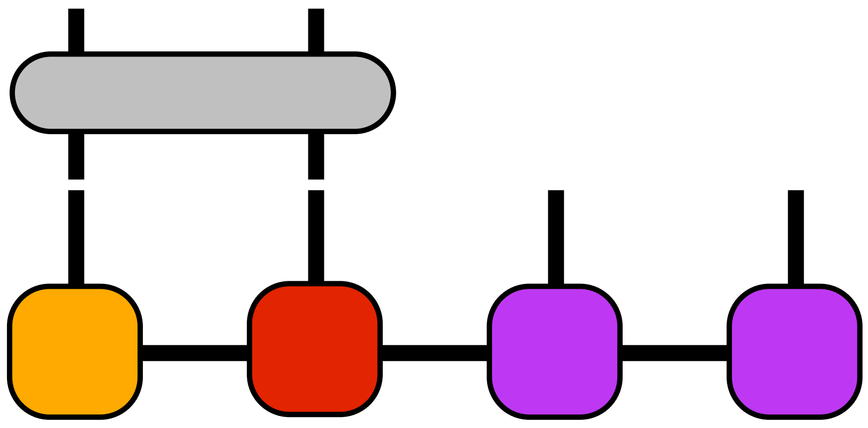

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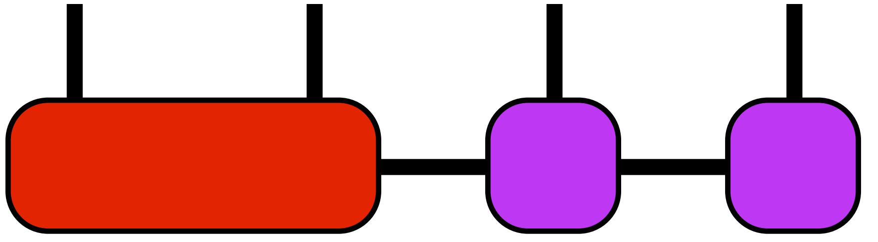

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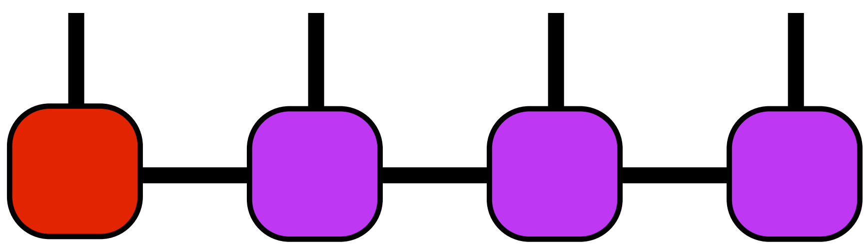

Interesting applications: $$|\psi'\rangle = e^{-\tau H}|\psi\rangle$$

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If τ real (imaginary time evolution), enough steps will give **ground state**

If τ imaginary, evolve in real time, study **dynamics** [1]

Evolving through imaginary time $\beta/2 = 1/(2T)$ simulates **finite temperature** [2]

[1] White, Feiguin PRL **93**, 076401 (2004)

[2] White PRL **102**, 190601 (2009)

We'll implement time evolution for the Heisenberg chain

`<library folder>/tutorial/05_gates`

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

2. Apply the gate G to the MPS bond tensor AA.
   The gate G can be multiplied times AA as if it's an ITensor.

3. Reset the prime level back to zero using AA's
   `.noprime()` class method.

3. Try increasing the total time "ttotal" to imaginary time evolve
   toward the ground state.
   (Exact energy for 20 sites: $E_0 = -8.6824733317$)