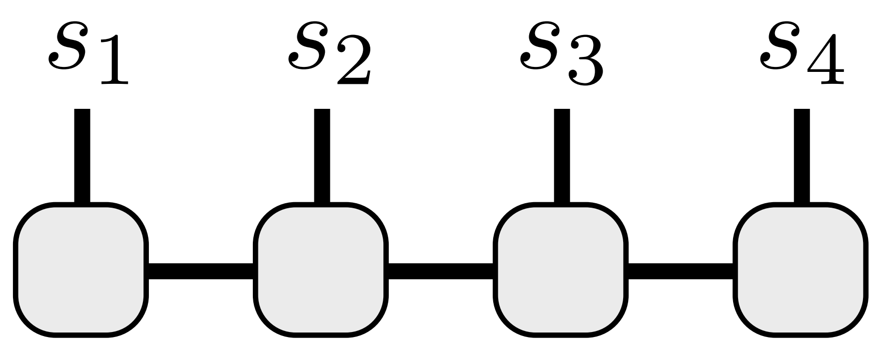
04 Four

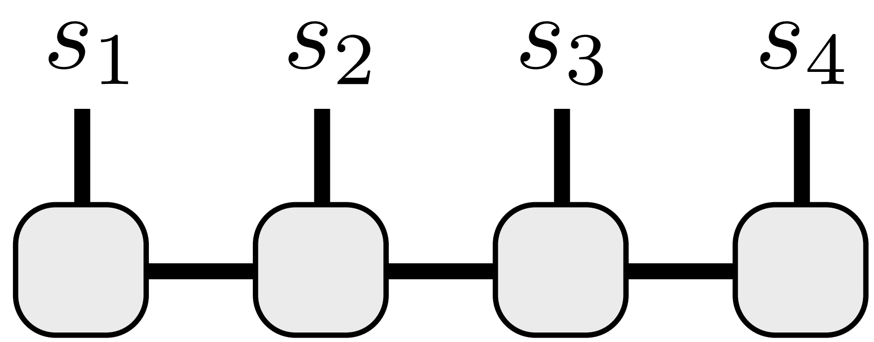
Say we have a 4-site MPS.
What can we do with it?



Depends on the gauge!

$$|\Psi\rangle = \sum_{\{s\},\{\alpha\}} M^{s_1}_{\alpha_1} M^{s_2}_{\alpha_1\alpha_2} M^{s_3}_{\alpha_2\alpha_3} M^{s_4}_{\alpha_3} |s_1 s_2 s_3 s_4\rangle$$

Assume we know nothing about the MPS
Put it in a useful gauge:



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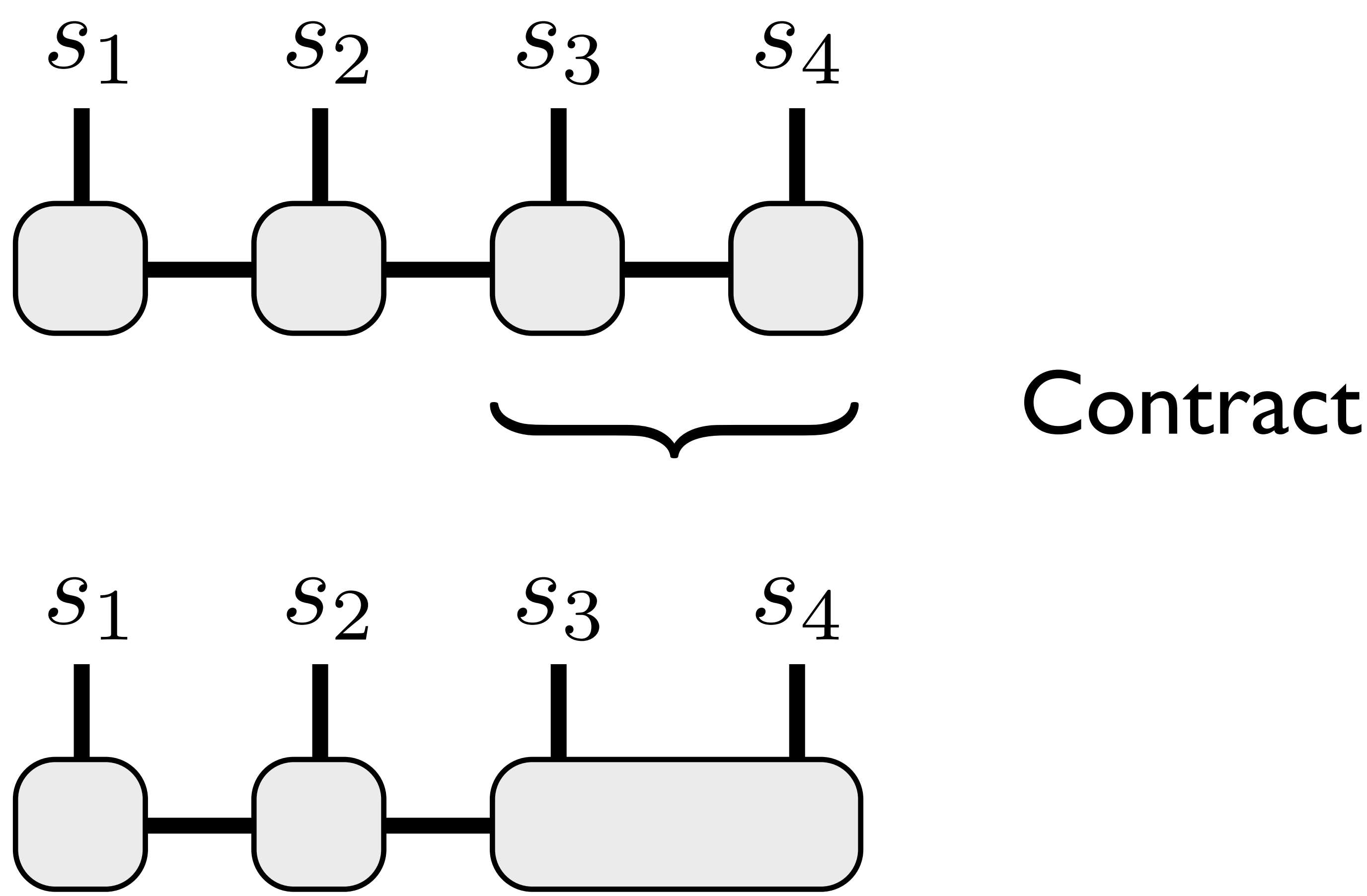

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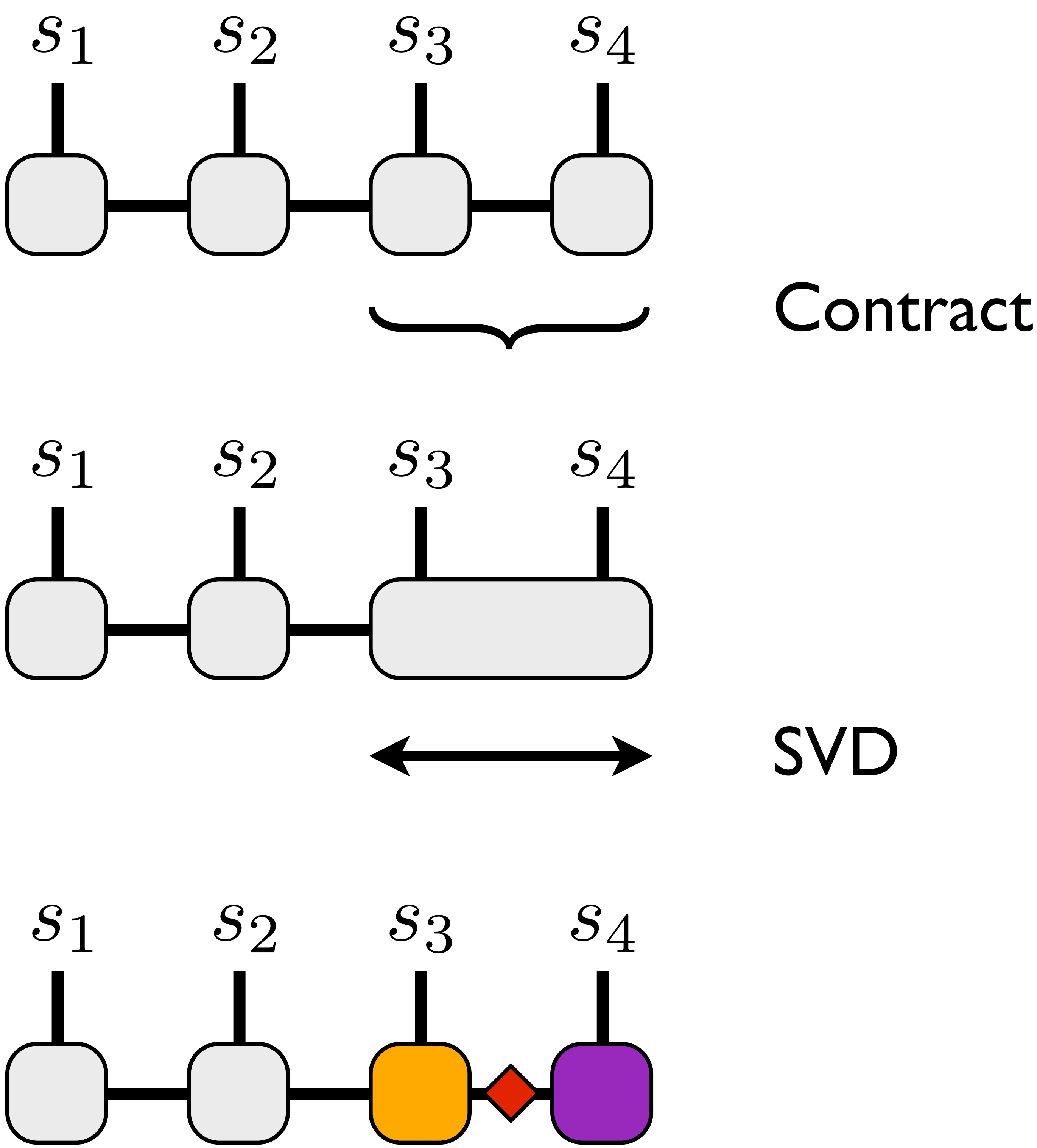

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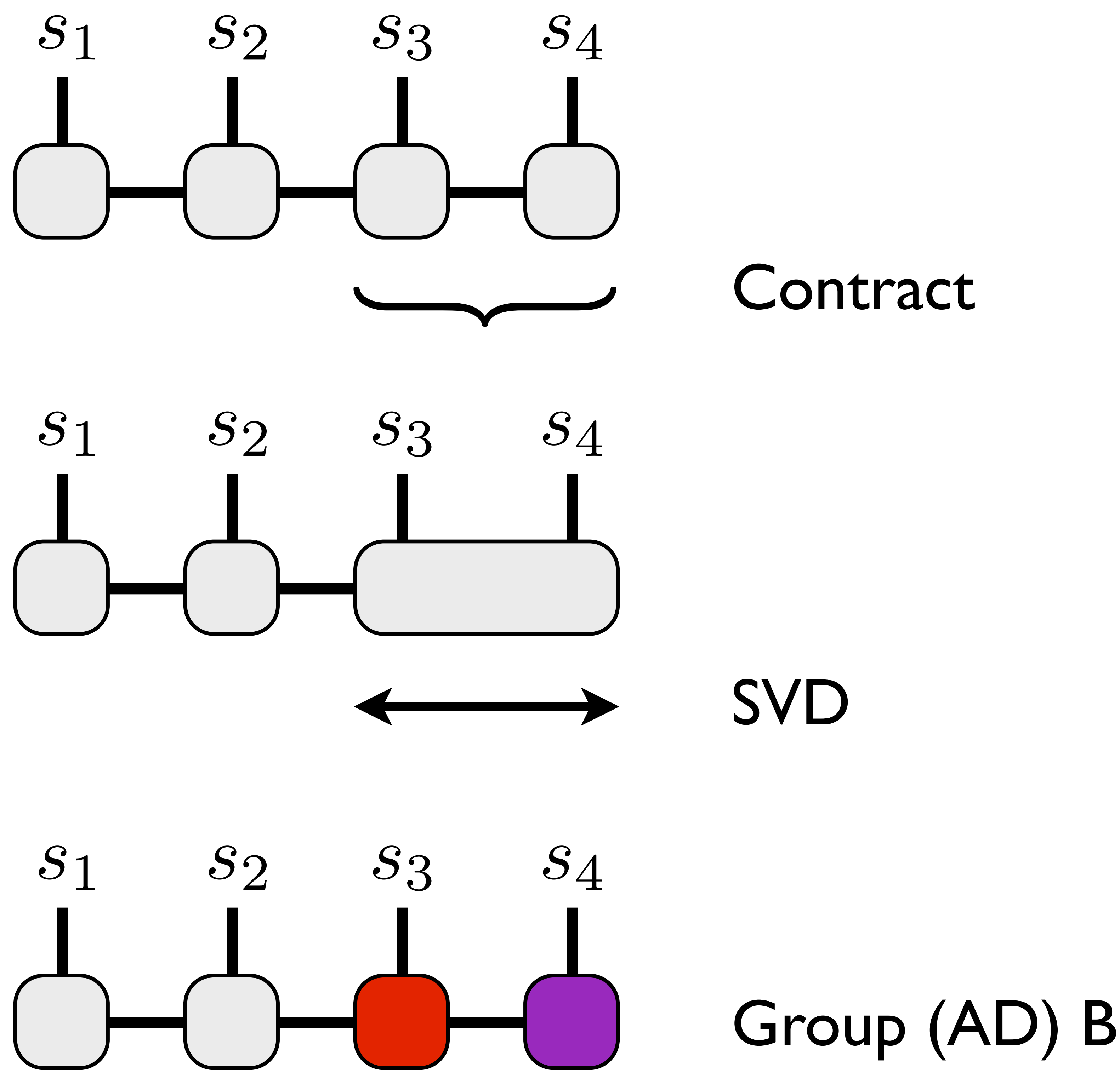
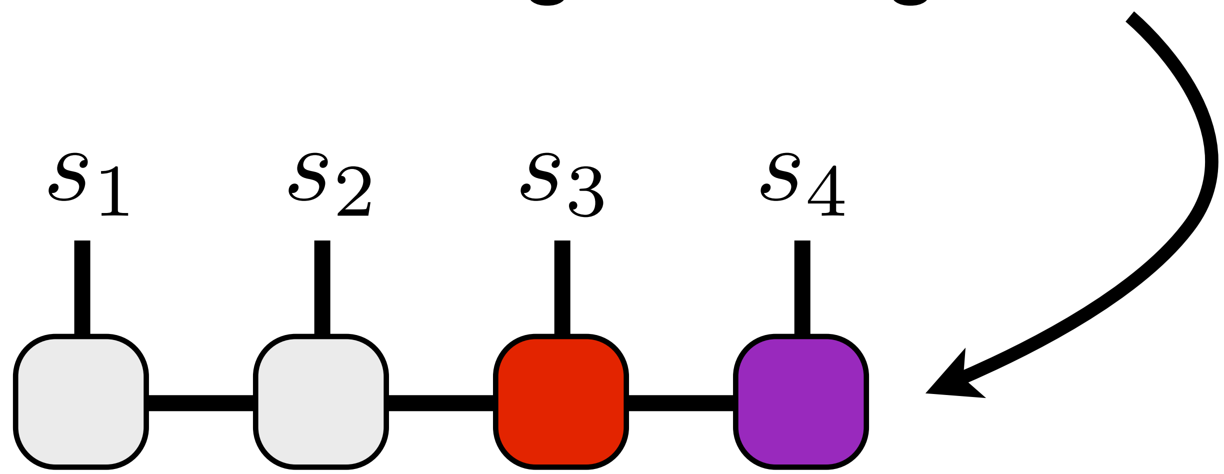


Note that site 4 tensor now right orthogonal



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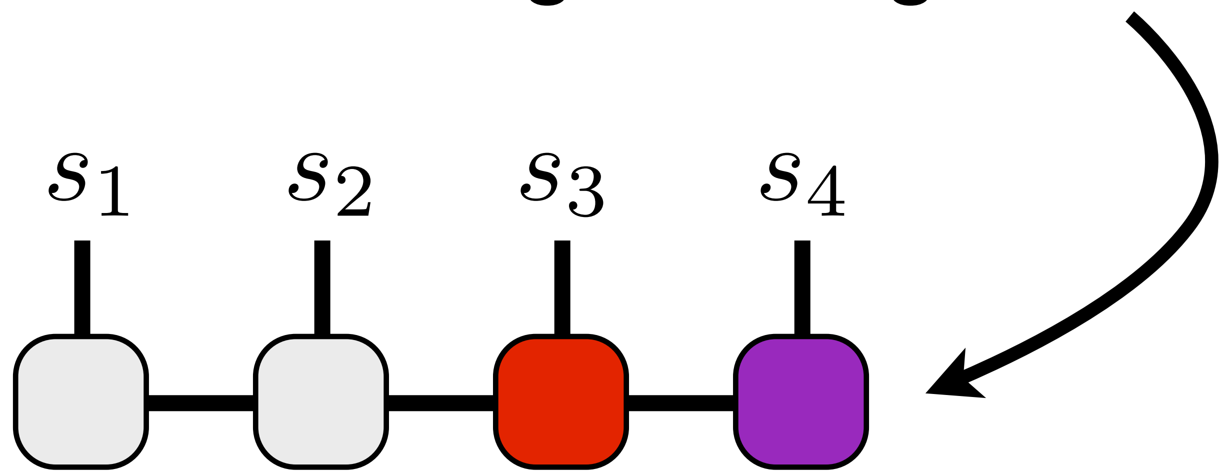
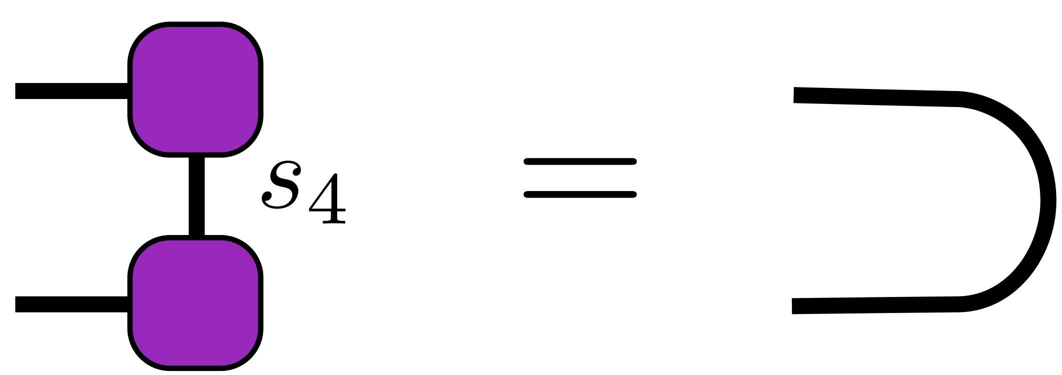
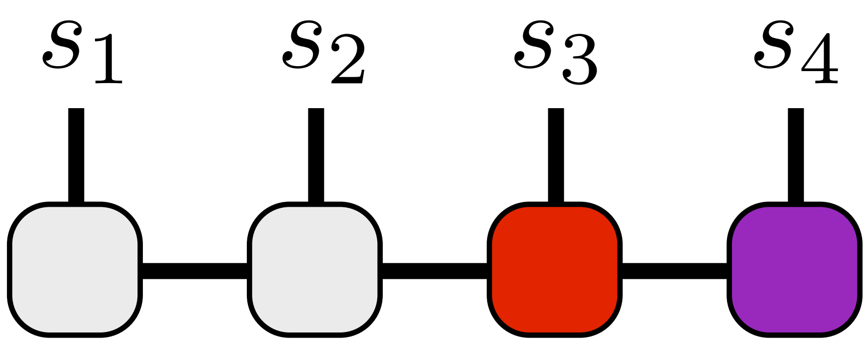


Recall this means



Can repeat gauge transformation (repeated SVD)



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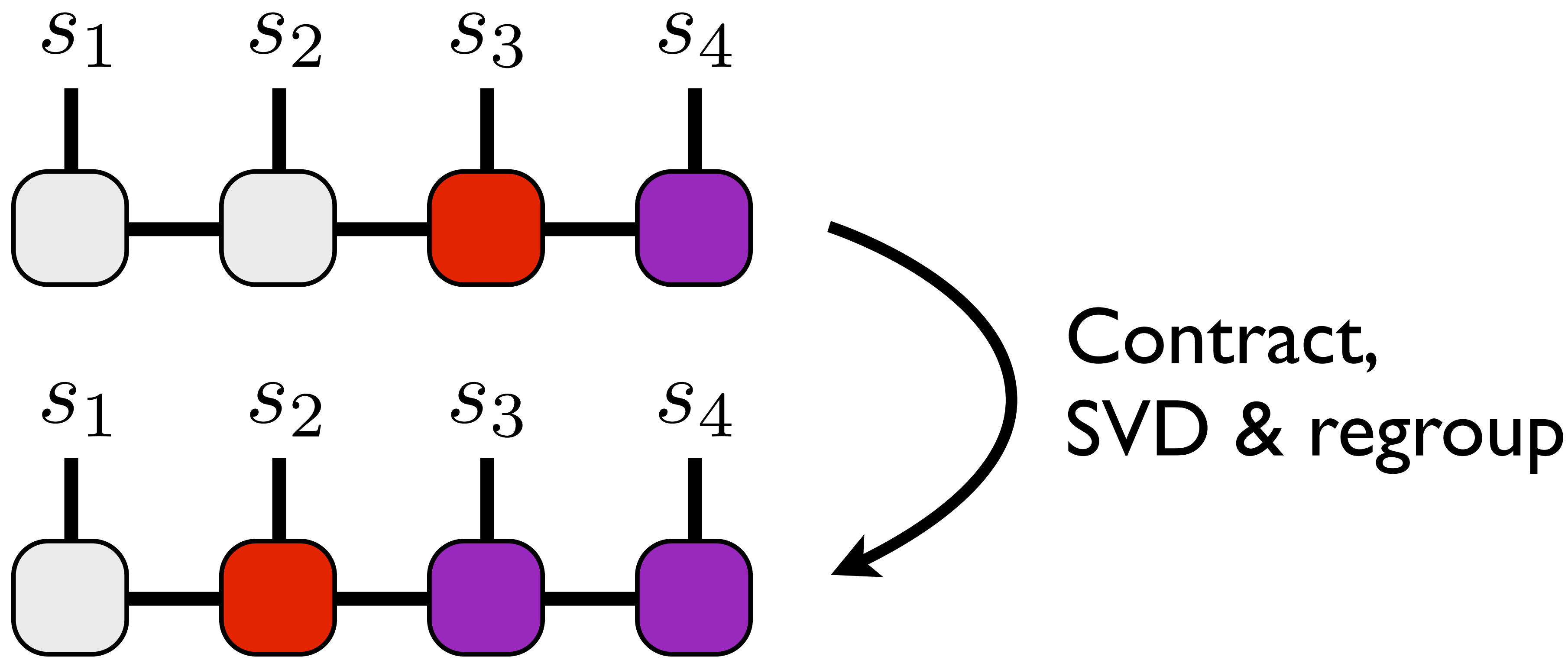

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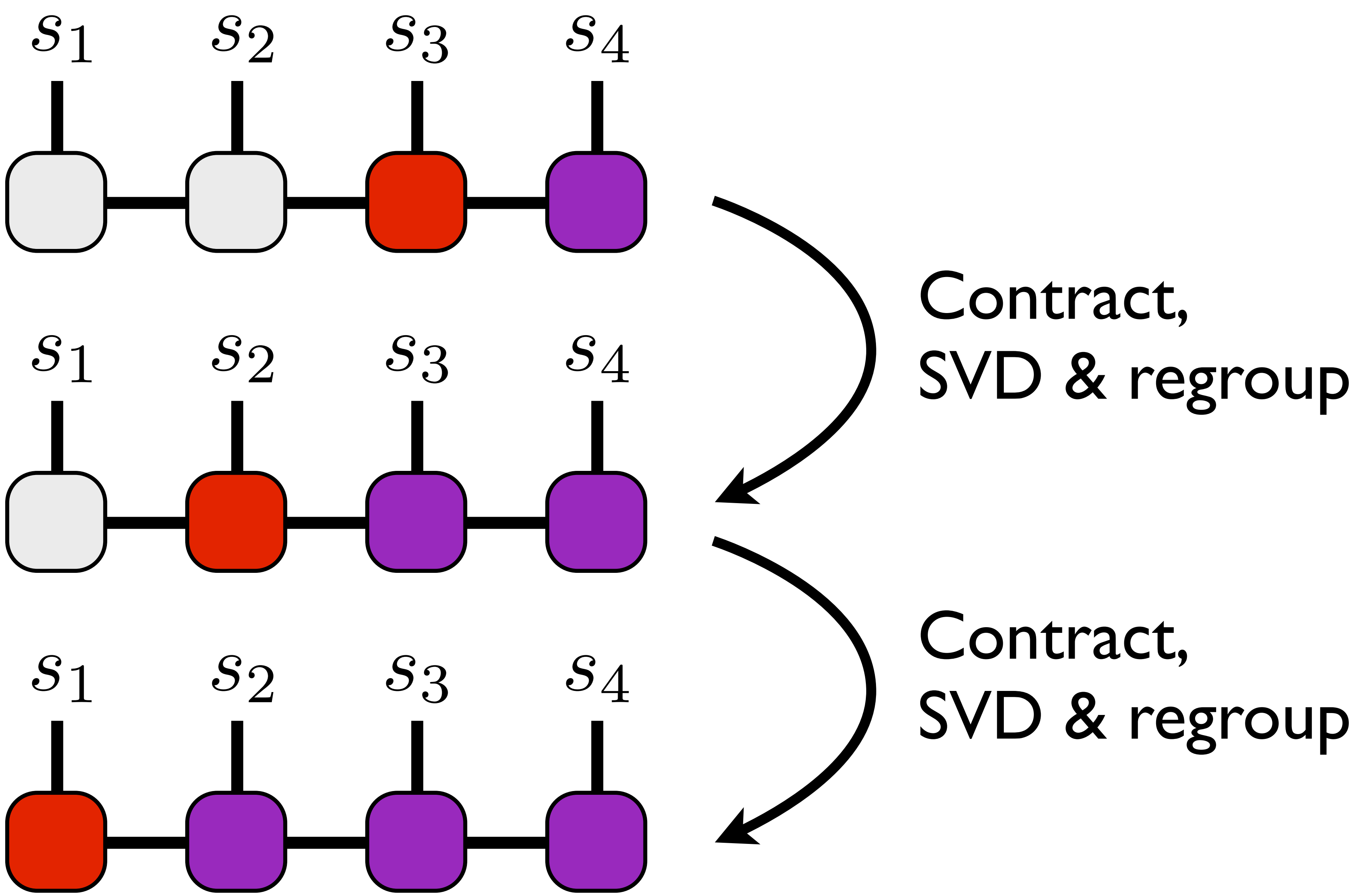
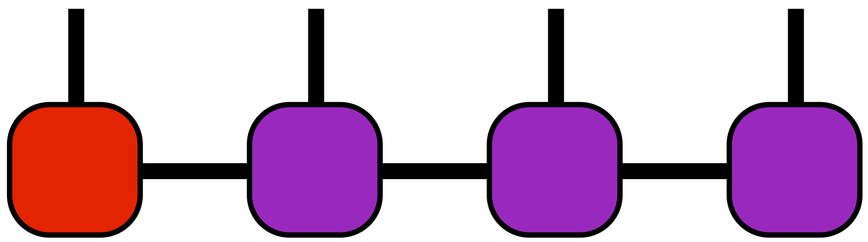


What have we gained?

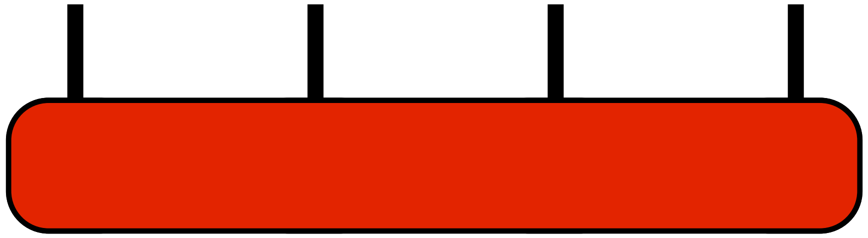
Consider measuring an operator on site 1



What have we gained?

Consider measuring an operator on site 1

First, general wavefunction:

$$|\Psi\rangle$$ 

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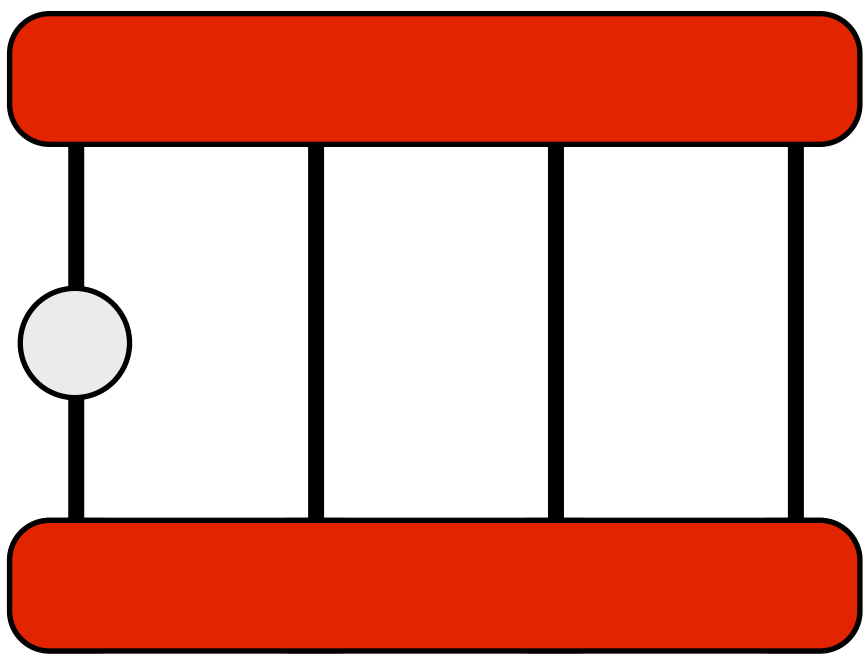
Consider measuring an operator on site 1

First, general wavefunction:

$$\langle \Psi | \quad \hat{A}_1 \quad | \Psi \rangle$$



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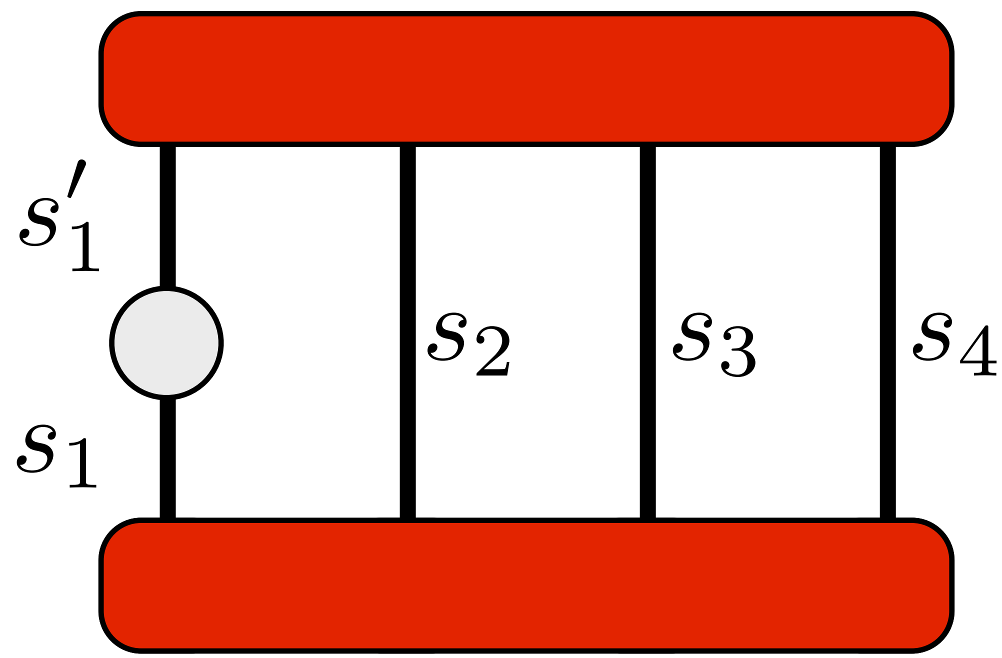


Cost scales exponentially!

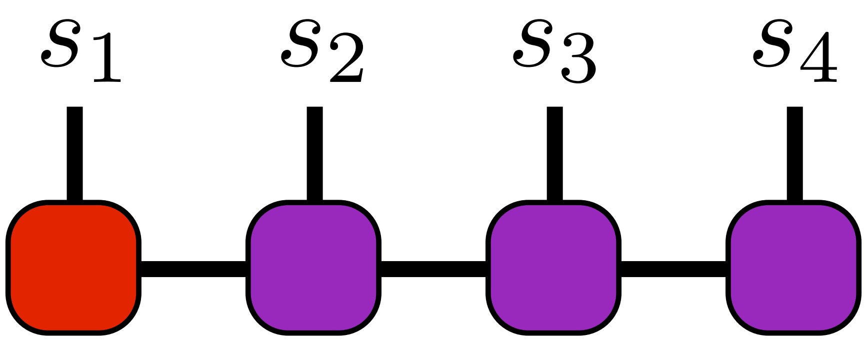
2^4 in this case

$$\langle \hat{A}_1 \rangle = \sum_{\{s\}} \bar{\psi}_{s_1' s_2 s_3 s_4} A_{s_1' s_1} \psi_{s_1 s_2 s_3 s_4}$$

What have we gained?

Consider measuring an operator on site 1

Now gauged MPS:



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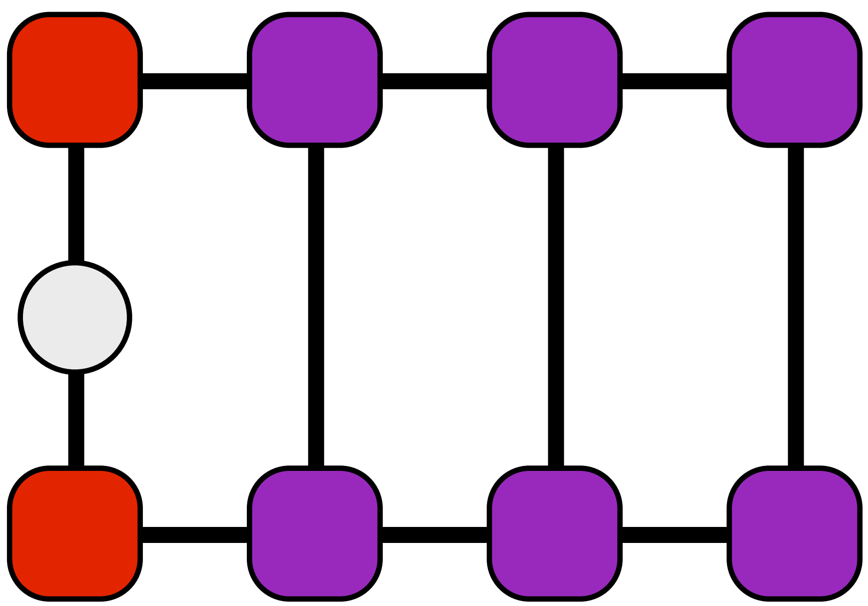

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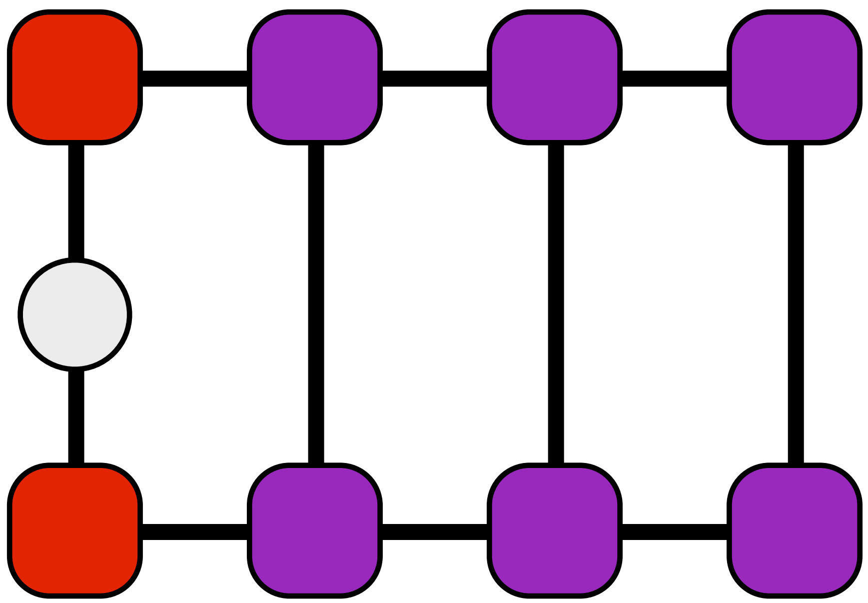
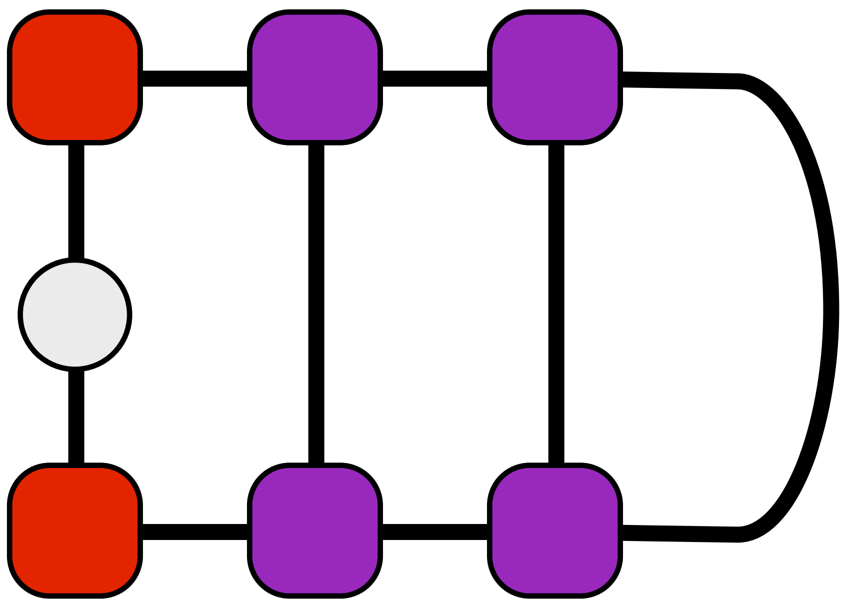


Use right orthogonality

What have we gained?

Consider measuring an operator on site 1

Now gauged MPS:



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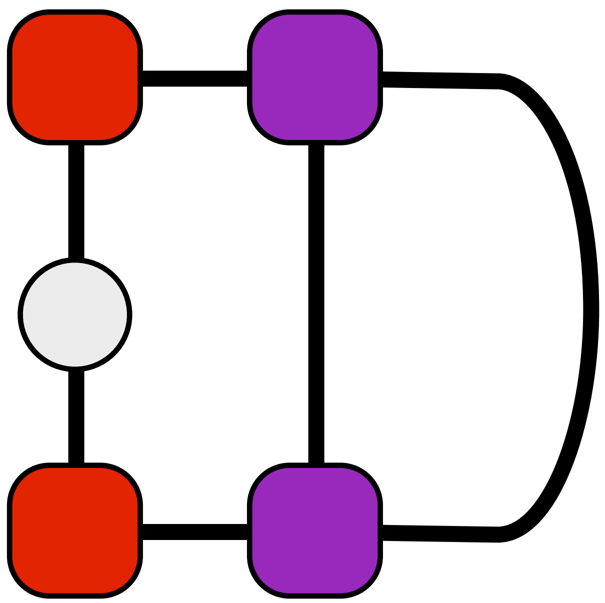

Use right orthogonality

What have we gained?

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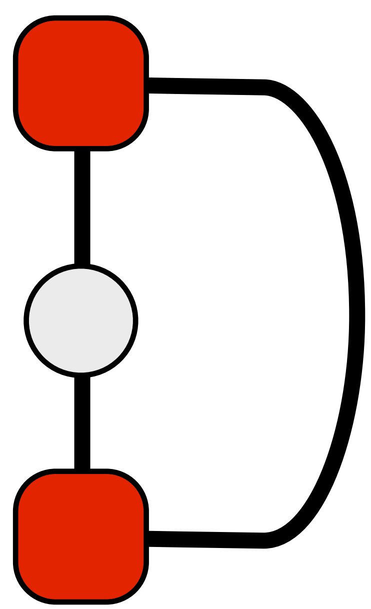


Use right orthogonality

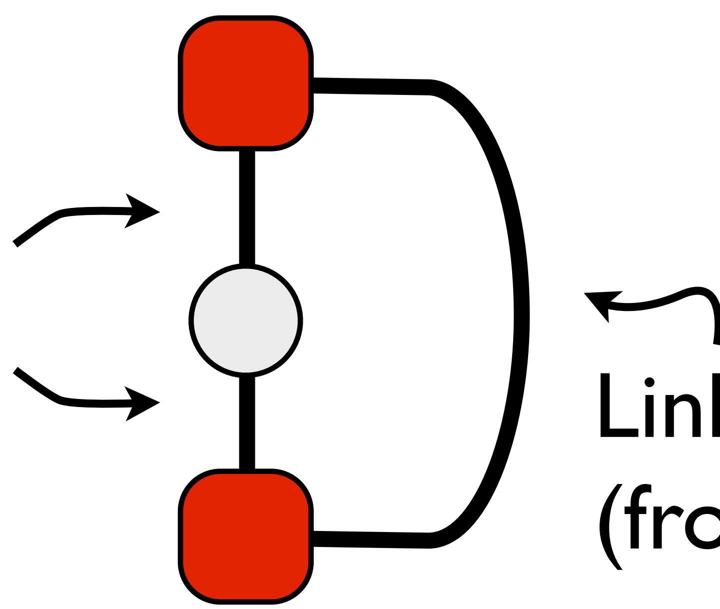
Much simpler computation!

What have we gained?

How much simpler a computation?

Choose always $\leq m$ singular values in each SVD

Site indices run from 1...d



Link index runs from 1...m (from SVD)

Computational cost ~ d^2 m (compared to d^4)

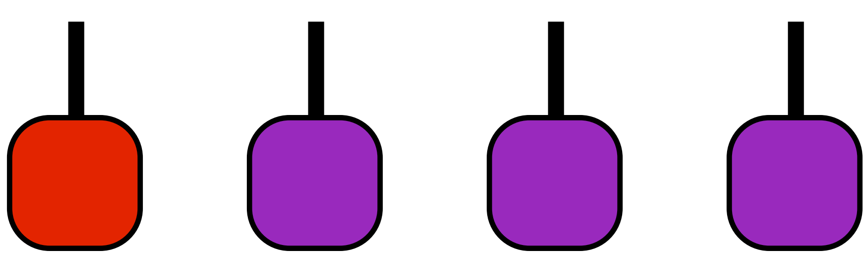
Gauging an MPS Using ITensor:

```
//Define lattice sites

SpinHalf sites(N);
```

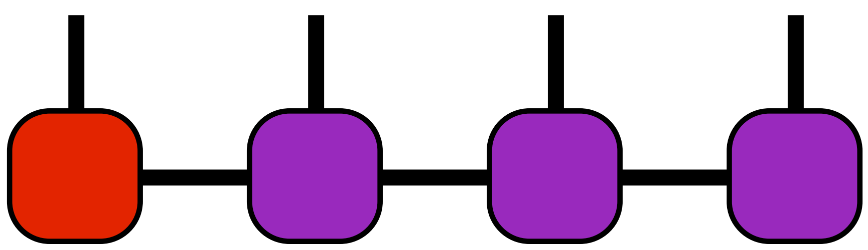
Gauging an MPS Using ITensor:

```
//Define lattice sites
SpinHalf sites(N);
MPS psi(sites);
```



Gauging an MPS Using ITensor:

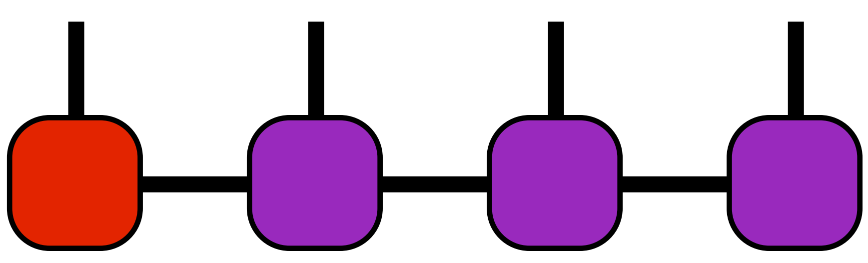
```
//Define lattice sites
SpinHalf sites(N);
MPS psi(sites);
computeGroundState(H,psi); //optimize psi
```



Gauging an MPS Using ITensor:

```
//Define lattice sites
SpinHalf sites(N);
MPS psi(sites);
computeGroundState(H,psi); //optimize psi


//Gauge MPS to second site
psi.position(2);
```



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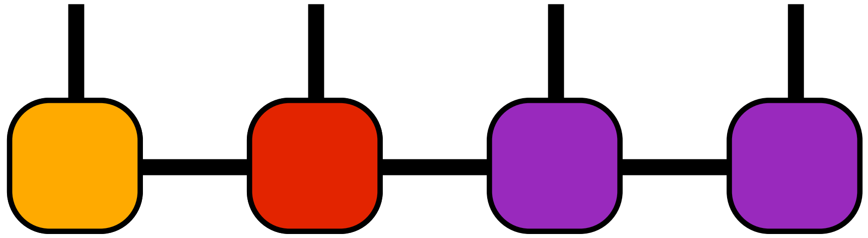
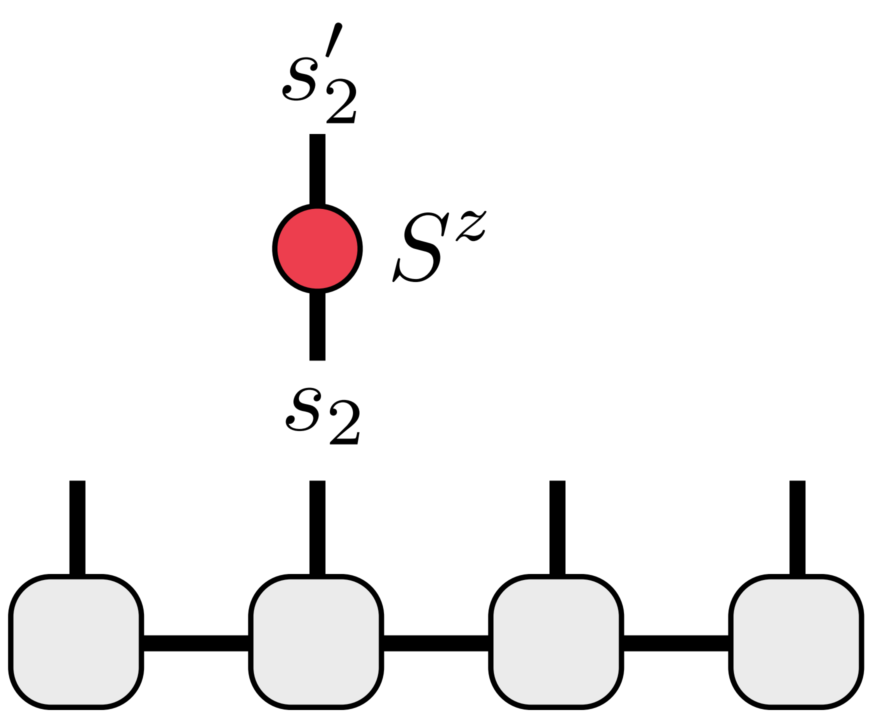


Measuring an MPS Using ITensor:

Can obtain single-site operators from “SiteSet” object:

```
//Obtain single-site operators
ITensor Sz = sites.op("Sz",2);
```

```
sites.op("Sz",2) ==
```

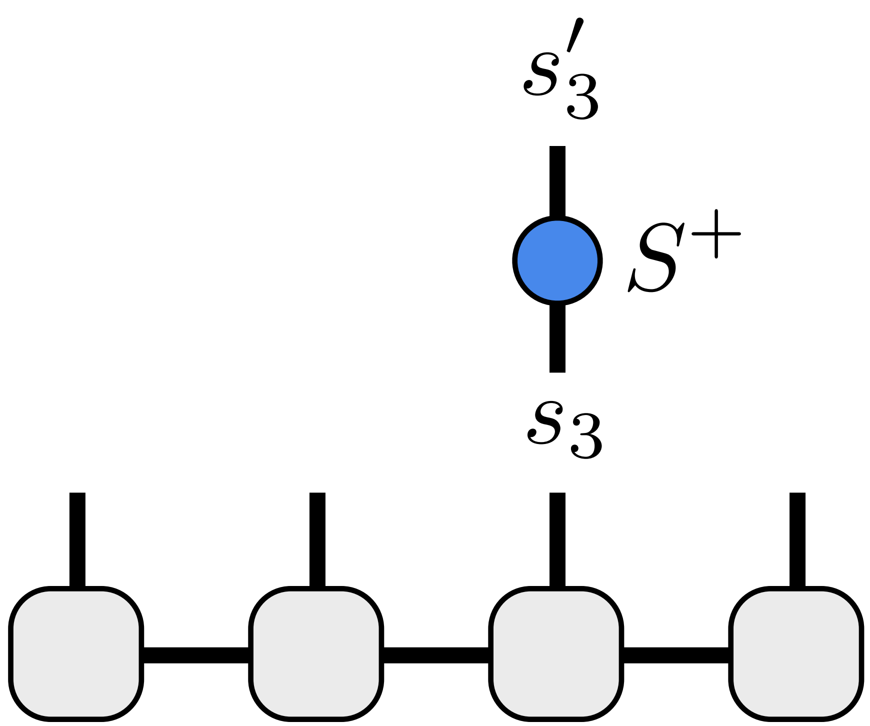


Measuring an MPS Using ITensor:

Can obtain single-site operators from “SiteSet” object:

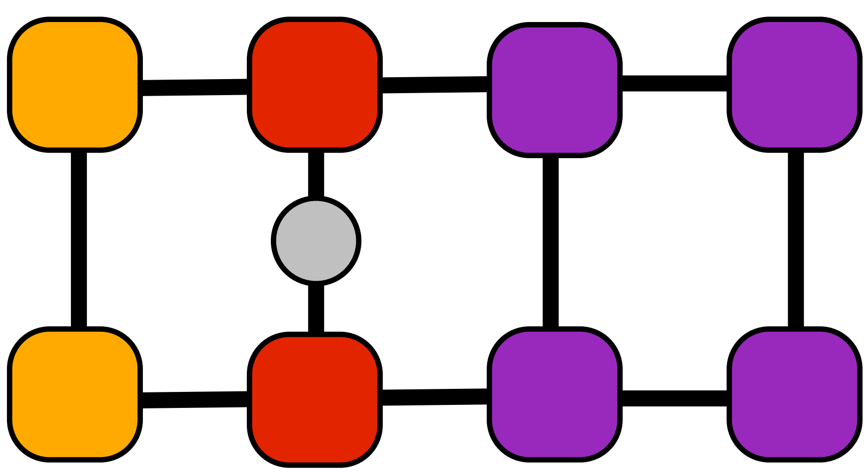
```
//Obtain single-site operators
ITensor Sz = sites.op("Sz",2);
ITensor Sp = sites.op("S+",3);
```

```
sites.op("S+",3) ==
```

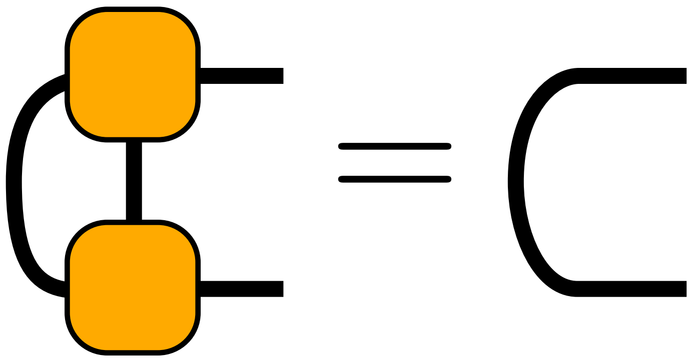


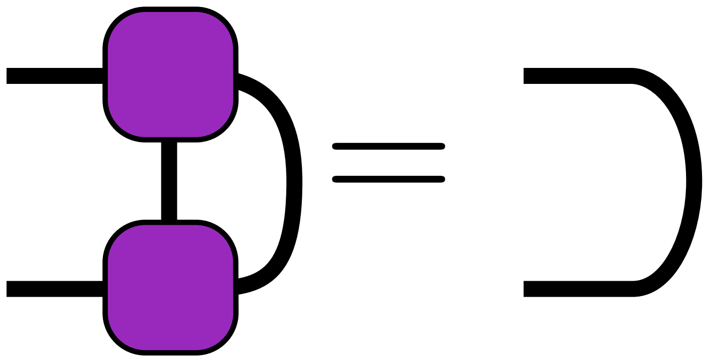
Measuring an MPS Using ITensor:

```
//Measure Sz on second site
```



Recall:





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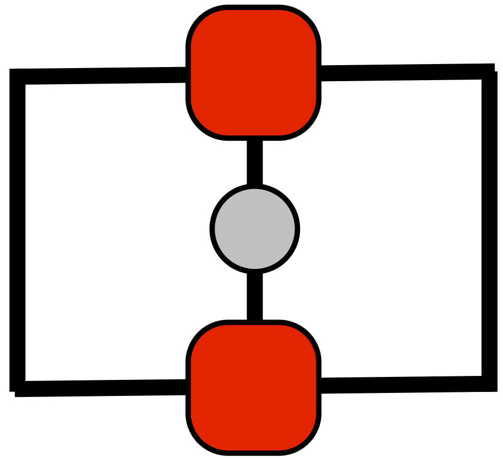

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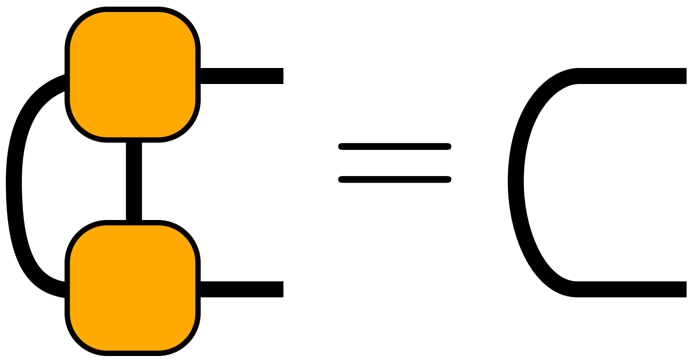
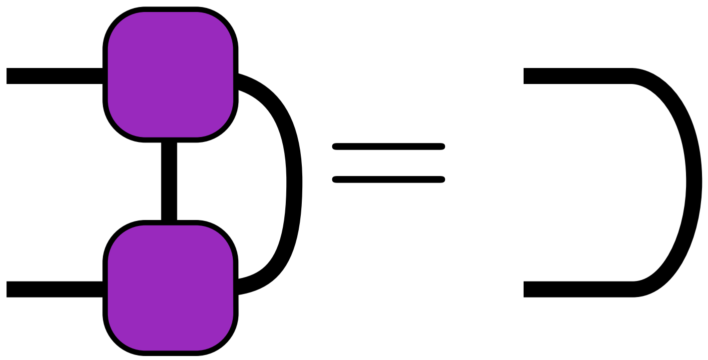
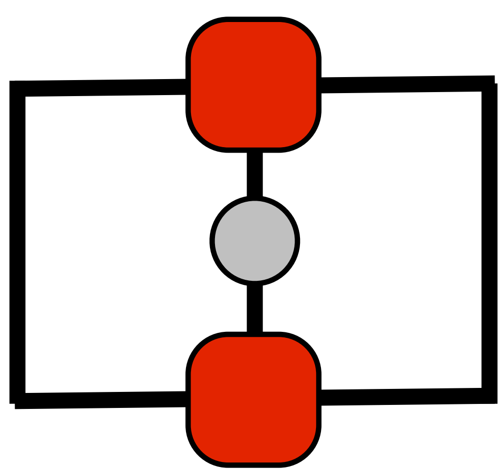




Measuring an MPS Using ITensor:

```
//Measure Sz on second site
Real sz_expect = (dag(prime(psi.A(2),Site))
                  * sites.op("Sz",2)
                  * psi.A(2)).toReal();
```



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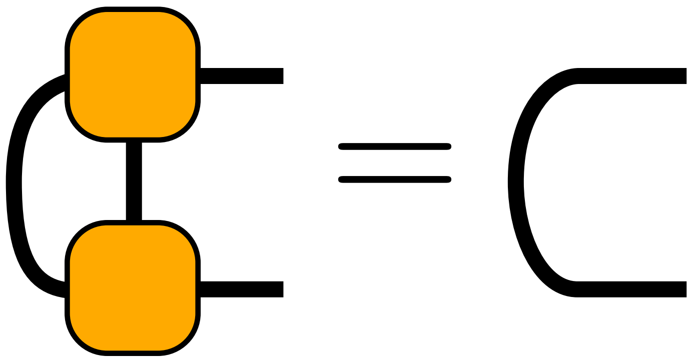

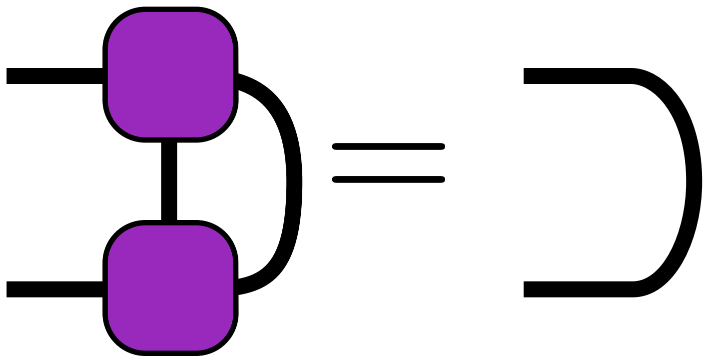

We'll measure the dimer order of the J_1-J_2 model

`<library folder>/tutorial/04_mps`

1. Read through **`j1j2.cc`**; compile; and run

2. Call `psi.position(N/2);` to gauge the MPS to site `N/2`

3. Measure $\hat{B}_{N/2} = \mathbf{S}_{N/2} \cdot \mathbf{S}_{N/2+1}$

```
ITensor wf = psi.A(N/2)*psi.A(N/2+1);
Real b = (dag(prime(wf,Site))*B(sites,N/2)*wf).toReal();
```

4. Repeat for bonds $(N/2\text{-}1)$ and $(N/2\text{+}1)$. (Don't forget to call `psi.position(b);` to include the "gauge center" `b` in each bond!!) Use to compute and save dimer order parameter:

$$D = \langle \hat{B}_{N/2} \rangle - \frac{1}{2}\langle \hat{B}_{N/2-1} \rangle - \frac{1}{2}\langle \hat{B}_{N/2+1} \rangle$$

Solution for missing code (near line 40 of `j1j2.cc`):

```
psi.position(N/2-1);
ITensor wf = psi.A(N/2-1)*psi.A(N/2);
val += -0.5*(dag(prime(wf,Site))*B(sites,N/2-1)*wf).toReal();

psi.position(N/2);
wf = psi.A(N/2)*psi.A(N/2+1);
val += (dag(prime(wf,Site))*B(sites,N/2)*wf).toReal();

psi.position(N/2+1);
wf = psi.A(N/2+1)*psi.A(N/2+2);
val += -0.5*(dag(prime(wf,Site))*B(sites,N/2+1)*wf).toReal();
```