03 SVD

The density matrix renormalization group (DMRG) works with a variational wavefunction known as a **matrix product state** (MPS).

Matrix product states arise from compressing one-dimensional wavefunctions through the **singular-value decomposition** (SVD).

Let's see how this works...

Recall:
Singular-value decomposition

Given rectangular (4x3) matrix M

$$M = \begin{bmatrix} 0.435839 & 0.223707 & 0.10 \\ 0.435839 & 0.223707 & -0.10 \\ 0.223707 & 0.435839 & 0.10 \\ 0.223707 & 0.435839 & -0.10 \end{bmatrix}$$

Can decompose as

$$\begin{bmatrix} 1/2 & -1/2 & 1/2 \\ 1/2 & -1/2 & -1/2 \\ 1/2 & 1/2 & 1/2 \\ 1/2 & 1/2 & -1/2 \end{bmatrix} \begin{bmatrix} 0.933 & 0 & 0 \\ 0 & 0.300 & 0 \\ 0 & 0 & 0.200 \end{bmatrix} \begin{bmatrix} 0.707107 & 0.707107 & 0 \\ -0.707107 & 0.707107 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$
\begin{bmatrix} 1/2 & -1/2 & 1/2 \\ 1/2 & -1/2 & -1/2 \\ 1/2 & 1/2 & 1/2 \\ 1/2 & 1/2 & -1/2 \end{bmatrix}
\begin{bmatrix} 0.933 & 0 & 0 \\ 0 & 0.300 & 0 \\ 0 & 0 & 0.200 \end{bmatrix}
\begin{bmatrix} 0.707107 & 0.707107 & 0 \\ -0.707107 & 0.707107 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}
$$

A D B

Matrices A and B one-sided unitaries (isometries):

$$A^\dagger A = \mathbf{1}$$

$$BB^\dagger = \mathbf{1}$$

D diagonal

Elements of D can be chosen:

(I) Real

(II) Positive semi-definite

(III) Decreasing order

Keep fewer and fewer elements of D:

$$\begin{array}{ccc} A & D & B \\ \begin{bmatrix} 1/2 & -1/2 & 1/2 \\ 1/2 & -1/2 & -1/2 \\ 1/2 & 1/2 & 1/2 \\ 1/2 & 1/2 & -1/2 \end{bmatrix} & \begin{bmatrix} 0.933 & 0 & 0 \\ 0 & 0.300 & 0 \\ 0 & 0 & 0.200 \end{bmatrix} & \begin{bmatrix} 0.707107 & 0.707107 & 0 \\ -0.707107 & 0.707107 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \end{array}$$

$$= M = \begin{bmatrix} 0.435839 & 0.223707 & 0.10 \\ 0.435839 & 0.223707 & -0.10 \\ 0.223707 & 0.435839 & 0.10 \\ 0.223707 & 0.435839 & -0.10 \end{bmatrix}$$

$$||M - M||^2 = 0$$

Keep fewer and fewer elements of D:

$$
\begin{array}{ccc}
A & D & B \\
\begin{bmatrix} 1/2 & -1/2 & 1/2 \\ 1/2 & -1/2 & -1/2 \\ 1/2 & 1/2 & 1/2 \\ 1/2 & 1/2 & -1/2 \end{bmatrix} &
\begin{bmatrix} 0.933 & 0 & 0 \\ 0 & 0.300 & 0 \\ 0 & 0 & 0.200 \end{bmatrix} &
\begin{bmatrix} 0.707107 & 0.707107 & 0 \\ -0.707107 & 0.707107 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}
\end{array}
$$

$$
= M_2 = \begin{bmatrix} 0.435839 & 0.223707 & 0 \\ 0.435839 & 0.223707 & 0 \\ 0.223707 & 0.435839 & 0 \\ 0.223707 & 0.435839 & 0 \end{bmatrix}
$$

$$
||M - M||^2 = 0
$$

Keep fewer and fewer elements of D:

$$\overset{A}{\begin{bmatrix} 1/2 & -1/2 & 1/2 \\ 1/2 & -1/2 & -1/2 \\ 1/2 & 1/2 & 1/2 \\ 1/2 & 1/2 & -1/2 \end{bmatrix}} \overset{D}{\begin{bmatrix} 0.933 & 0 & 0 \\ 0 & 0.300 & 0 \\ 0 & 0 & 0 \end{bmatrix}} \overset{B}{\begin{bmatrix} 0.707107 & 0.707107 & 0 \\ -0.707107 & 0.707107 & 0 \\ 0 \quad 0 & 0 & 1 \end{bmatrix}}$$

$$= M_2 = \begin{bmatrix} 0.435839 & 0.223707 & 0 \\ 0.435839 & 0.223707 & 0 \\ 0.223707 & 0.435839 & 0 \\ 0.223707 & 0.435839 & 0 \end{bmatrix}$$

$$||M_2 - M||^2 = 0.04 = (0.2)^2$$

Keep fewer and fewer elements of D:

$$
\begin{array}{ccc}
A & D & B \\
\begin{bmatrix} 1/2 & -1/2 & 1/2 \\ 1/2 & -1/2 & -1/2 \\ 1/2 & 1/2 & 1/2 \\ 1/2 & 1/2 & -1/2 \end{bmatrix} &
\begin{bmatrix} 0.933 & 0 & 0 \\ 0 & 0.300 & 0 \\ 0 & 0 & 0 \end{bmatrix} &
\begin{bmatrix} 0.707107 & 0.707107 & & 0 \\ -0.707107 & 0.707107 & & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}
\end{array}
$$

$$
= M_3 = \begin{bmatrix} 0.329773 & 0.329773 & 0 \\ 0.329773 & 0.329773 & 0 \\ 0.329773 & 0.329773 & 0 \\ 0.329773 & 0.329773 & 0 \end{bmatrix}
$$

$$
||M_2 - M||^2 = 0.04 = (0.2)^2
$$

Keep fewer and fewer elements of D:

$$
\begin{array}{ccc}
A & D & B \\
\begin{bmatrix} 1/2 & -1/2 & 1/2 \\ 1/2 & -1/2 & -1/2 \\ 1/2 & 1/2 & 1/2 \\ 1/2 & 1/2 & -1/2 \end{bmatrix}
&
\begin{bmatrix} 0.933 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}
&
\begin{bmatrix} 0.707107 & 0.707107 & 0 & \\ -0.707107 & 0.707107 & 0 & \\ 0 & 0 & 0 & 1 \end{bmatrix}
\end{array}
$$

$$
= M_3 = \begin{bmatrix} 0.329773 & 0.329773 & 0 \\ 0.329773 & 0.329773 & 0 \\ 0.329773 & 0.329773 & 0 \\ 0.329773 & 0.329773 & 0 \end{bmatrix}
$$

$$
||M_3 - M||^2 = 0.13 = (0.3)^2 + (0.2)^2
$$

Keep fewer and fewer elements of D:

$$\overset{A}{\begin{bmatrix} 1/2 & -1/2 & 1/2 \\ 1/2 & -1/2 & -1/2 \\ 1/2 & 1/2 & 1/2 \\ 1/2 & 1/2 & -1/2 \end{bmatrix}} \overset{D}{\begin{bmatrix} 0.933 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}} \overset{B}{\begin{bmatrix} 0.707107 & 0.707107 & 0 \\ -0.707107 & 0.707107 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}}$$

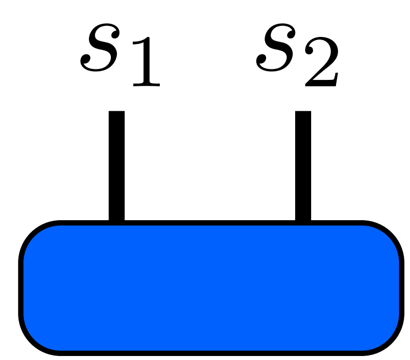
$$= M_3 = \boxed{\begin{array}{l} \text{Truncating SVD =} \\ \text{Controlled approximation} \\ \text{for M} \end{array}}$$

$$||M_3 - M||^2 = 0.13 = (0.3)^2 + (0.2)^2$$

Recall:

Most general two-spin wavefunction

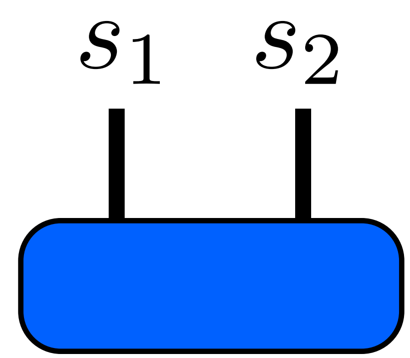
$$\psi_{s_1 s_2} =$$



Recall:

Most general two-spin wavefunction

$$\psi_{s_1 s_2} =$$

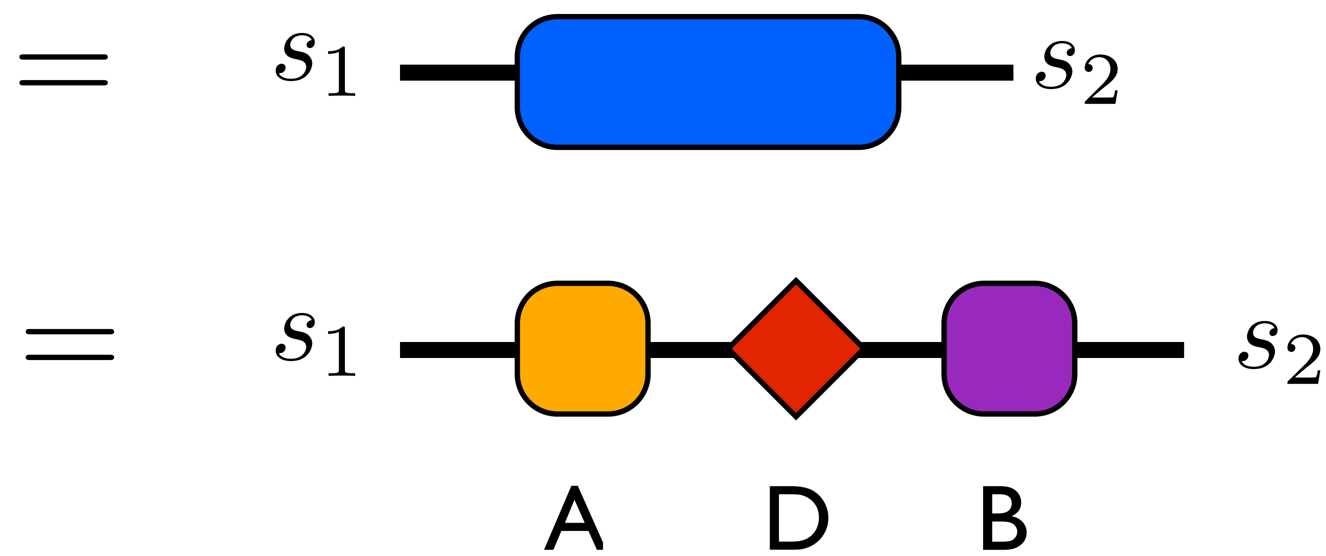


Can treat as a matrix:

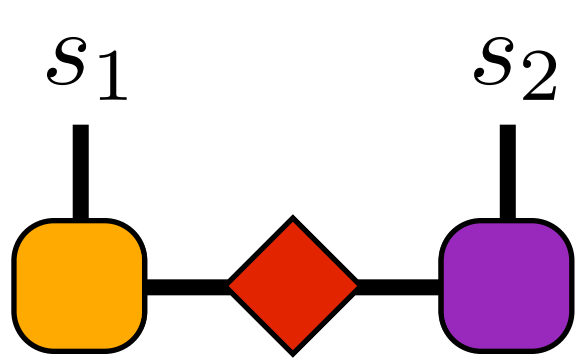
$$\psi_{s_1 s_2} =$$

SVD this matrix:

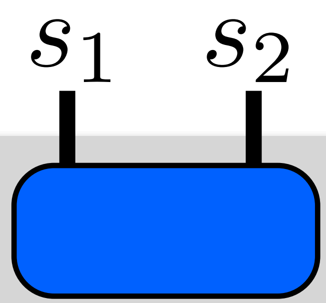
$$\psi_{s_1 s_2} = $$



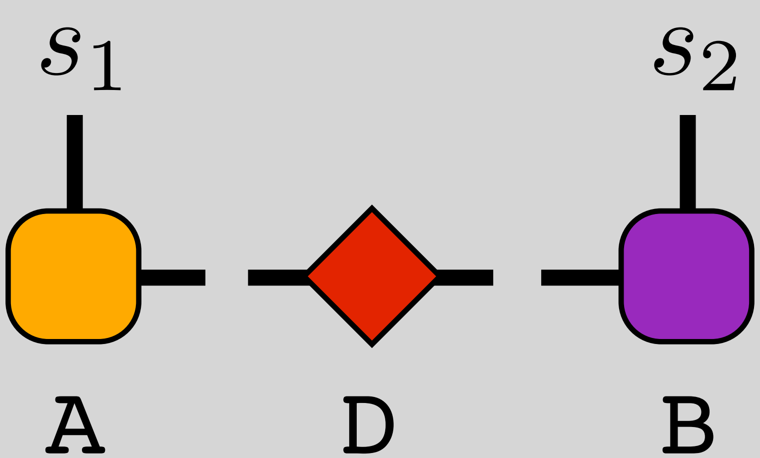
Bend lines back to look like wavefunction:



Using ITensor:

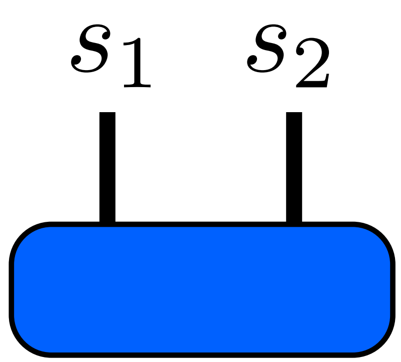



```
//Say we have a two-site ITensor psi

//Declare ITensors holding results:

ITensor A(s1),D,B;    //Indices of psi on A remain,
                      //rest go onto B

//Call svd function:
svd(psi,A,D,B);
```



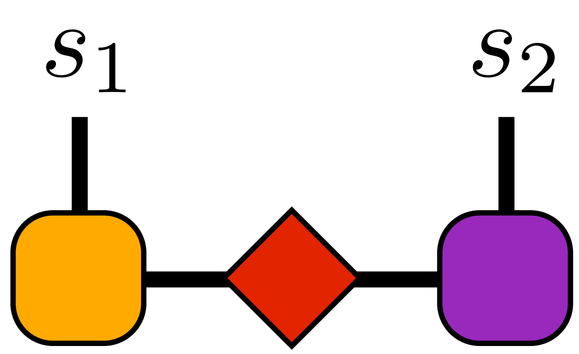
What have we gained from SVD?

Generic two-spin wavefunction (say spin S):



$(2S+1)^2$ parameters
Not clear which parameters important, unimportant

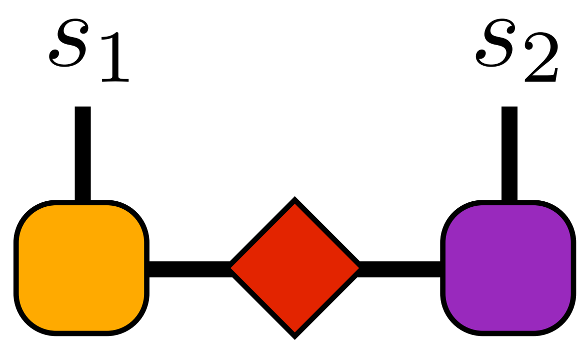
Compressed wavefunction:



SVD tells us which parameters are important, might be very few!

Later see that # parameters also scales much better

This form of wavefunction known as
matrix product state (MPS)



Why? Amplitude a product of matrices:

$$|\Psi\rangle = \sum_{s_1,\alpha,\alpha',s_2} A_{s_1\alpha} D_{\alpha\alpha'} B_{\alpha' s_2} |s_1\rangle |s_2\rangle$$

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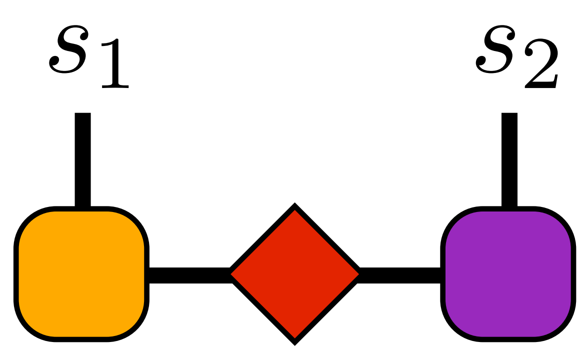
MPS have different equivalent forms, or "gauges"



Canonical form

$$|\Psi\rangle = \sum_{s_1,\alpha,\alpha',s_2} A_{s_1\alpha} D_{\alpha\alpha'} B_{\alpha' s_2} |s_1\rangle |s_2\rangle$$

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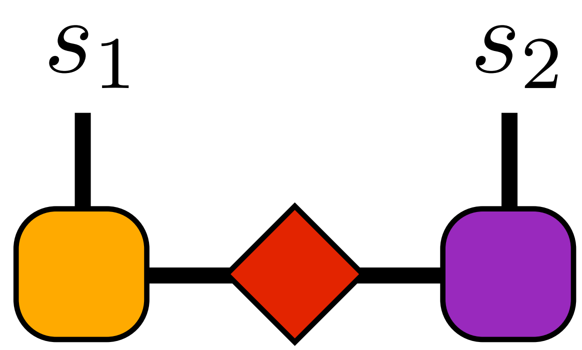

$$|\Psi\rangle = \sum_{s_1,\alpha,\alpha',s_2} A_{s_1\alpha} D_{\alpha\alpha'} B_{\alpha' s_2} |s_1\rangle |s_2\rangle$$

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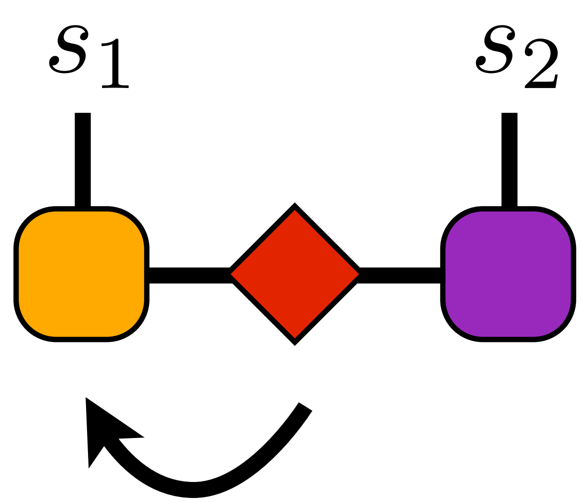

Left-canonical

$$|\Psi\rangle = \sum_{s_1,\alpha,\alpha',s_2} A_{s_1\alpha} D_{\alpha\alpha'} B_{\alpha' s_2} |s_1\rangle |s_2\rangle$$

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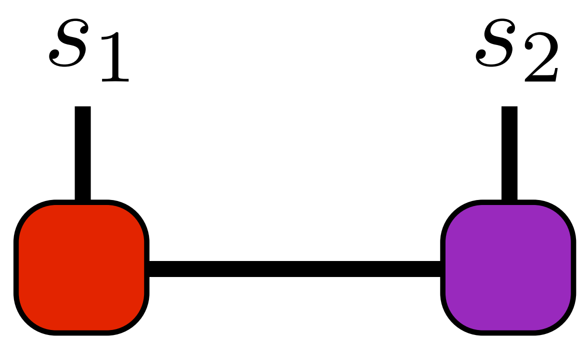

Left-canonical

$$|\Psi\rangle = \sum_{s_1,\alpha',s_2} \psi_{s_1\alpha'} B_{\alpha' s_2} |s_1\rangle |s_2\rangle$$

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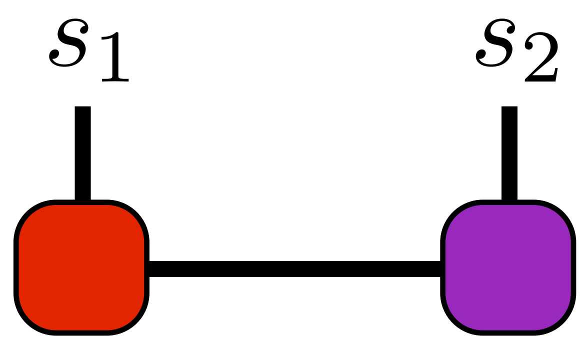
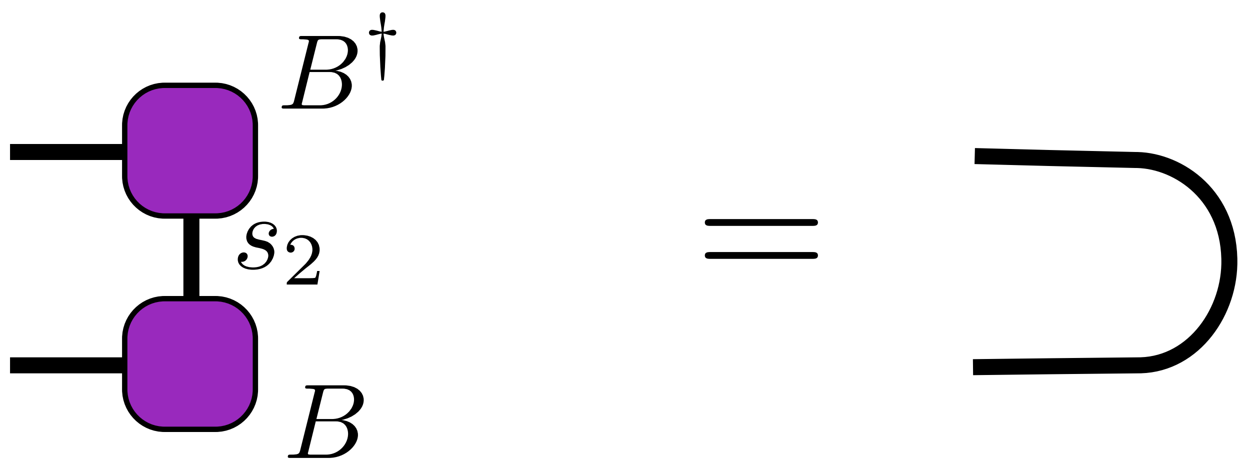


Matrix B is "right orthogonal" (from SVD)



$$BB^\dagger = I$$

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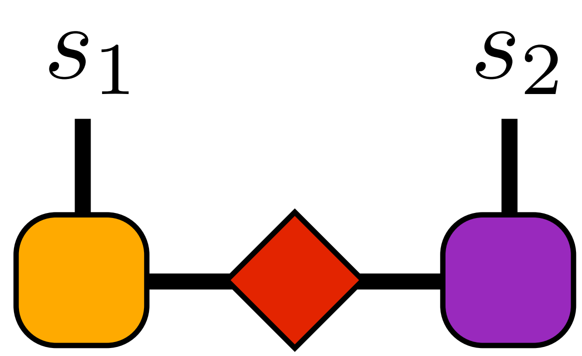

Canonical form

$$|\Psi\rangle = \sum_{s_1,\alpha,\alpha',s_2} A_{s_1\alpha} D_{\alpha\alpha'} B_{\alpha' s_2} |s_1\rangle|s_2\rangle$$

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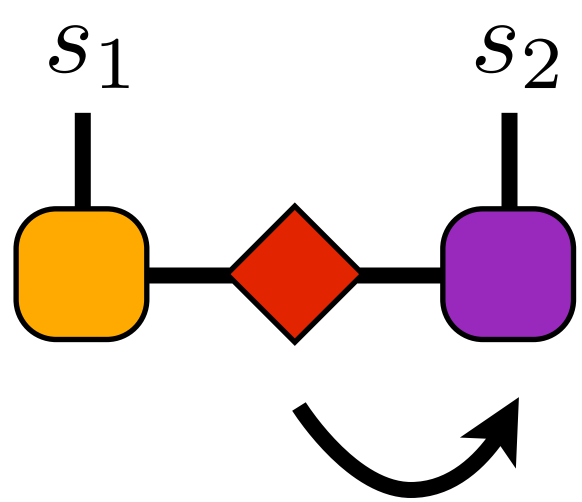
MPS have different equivalent forms, or "gauges"



Right-canonical

$$|\Psi\rangle = \sum_{s_1,\alpha,\alpha',s_2} A_{s_1\alpha} D_{\alpha\alpha'} B_{\alpha' s_2} |s_1\rangle |s_2\rangle$$

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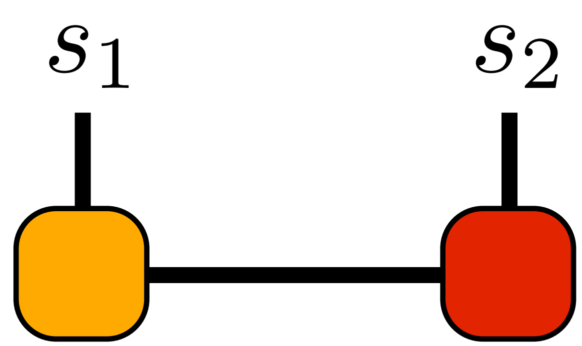
MPS have different equivalent forms, or “gauges”



Right-canonical

$$|\Psi\rangle = \sum_{s_1,\alpha,s_2} A_{s_1\alpha}\psi_{\alpha s_2}|s_1\rangle|s_2\rangle$$

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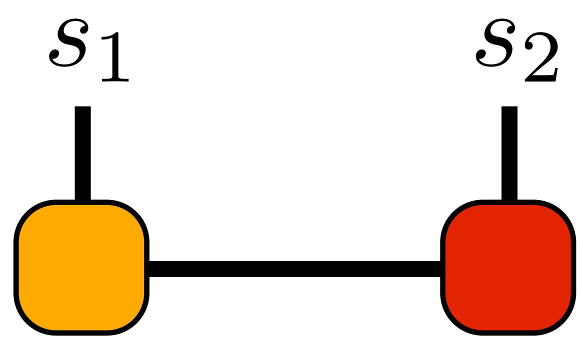
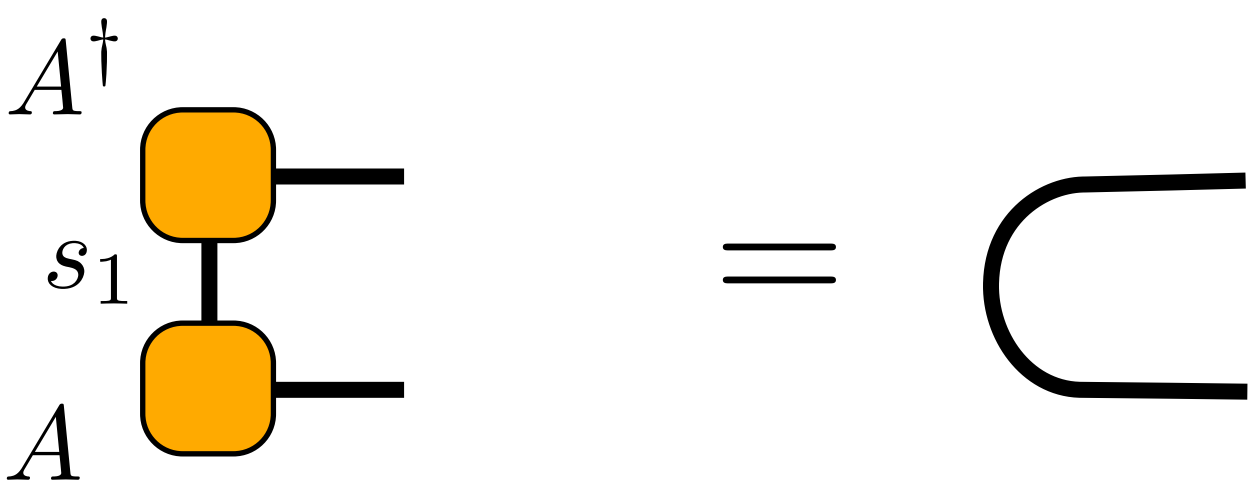
MPS have different equivalent forms, or "gauges"



Matrix A is "left orthogonal" (from SVD)



$$A^\dagger A = I$$

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We'll use the SVD to study the entanglement of a two-site wavefunction

```
<library folder>/tutorial/03_svd
```

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

2. Make a *normalized* wavefunction that is the sum

```
ITensor psi = (1-mix)*prod + mix*sing;
psi *= 1./psi.norm();
```

3. SVD this wavefunction

```
ITensor A(s1),D,B;

Spectrum spec = svd(psi,A,D,B);
```

3. Compute the entanglement entropy using the density-matrix eigenvalue spectrum "spec" returned by svd.

n^{th} eigenvalue: `spec.eig(n);` 1−indexed!

number of eigenvalues: `spec.numEigsKept();`