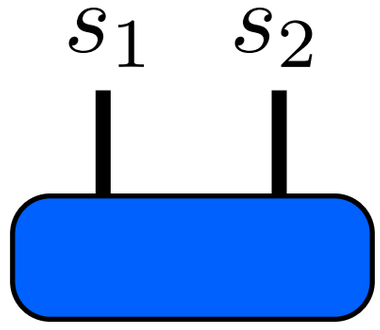
02 Two Sites

Most general two-spin wavefunction is

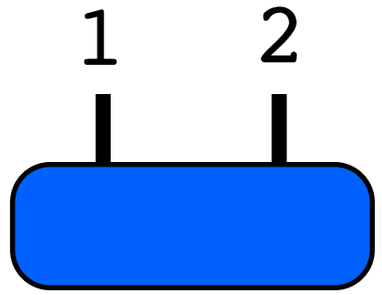
$$|\Psi\rangle = \sum_{s_1,s_2=1}^{2} \psi_{s_1 s_2} |s_1\rangle |s_2\rangle$$

Amplitudes a rank-2 tensor

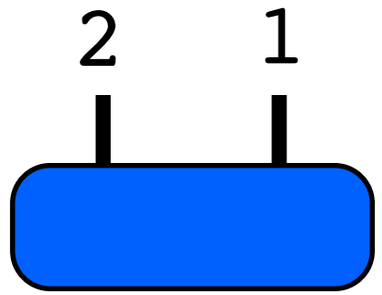
$$\psi_{s_1 s_2} =$$



Let's make a singlet



$= \ 1/\sqrt{2}$



$= -1/\sqrt{2}$

Using ITensor:

```
Index s1("s1",2,Site), s2("s2",2,Site);
ITensor psi(s1,s2); //default initialized to zero
psi(s1(1),s2(2)) =  1./sqrt(2);
psi(s1(2),s2(1)) = -1./sqrt(2);
```

Why **`Site`** tag in Index constructor?

```
Index s1("s1",2,Site),
      s2("s2",2,Site);
```

Two Index types: **`Link`** (default) and **`Site`**.

Useful for priming just one type of Index, for example.

Let's make the Heisenberg Hamiltonian $\hat{H} = \mathbf{S}_1 \cdot \mathbf{S}_2$

$$\hat{H} = S_1^z S_2^z + \frac{1}{2} S_1^+ S_2^- + \frac{1}{2} S_1^- S_2^+$$

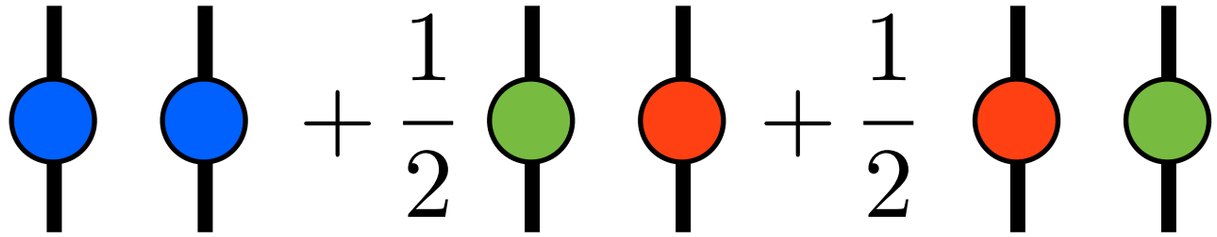
First create operators, for example S^+

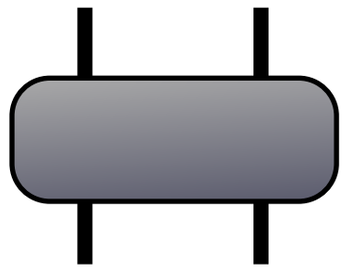
```
ITensor Sp1(s1,prime(s1));
commaInit(Sp1,s1,prime(s1)) = 0, 1,
                              0, 0;
```

Multiply and add operators to make H:

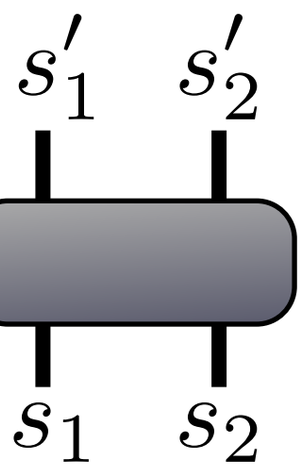
```
ITensor H = Sz1*Sz2 + 0.5*Sp1*Sm2 + 0.5*Sm1*Sp2;
```

Tensor form of H

$\hat{H} =$  $+ \frac{1}{2}$ $+ \frac{1}{2}$

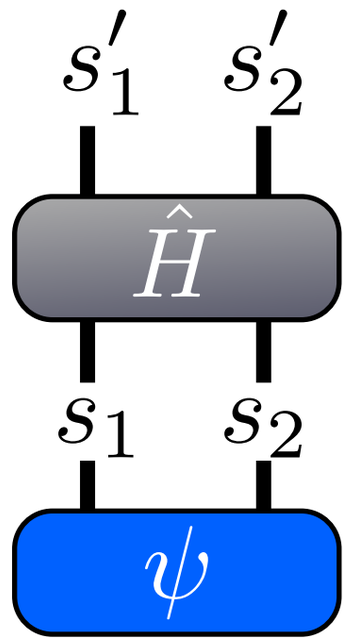
$=$ 

Showing Index labels

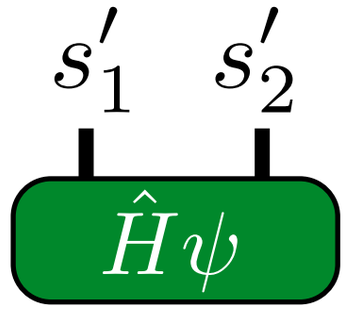
$\hat{H} =$ 

Compute singlet energy with this Hamiltonian:

$$\hat{H}|\psi\rangle =$$



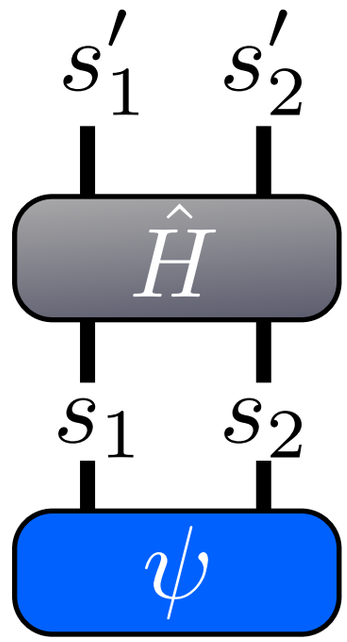
$=$



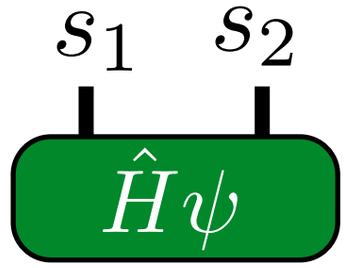

```
ITensor Hpsi = H * psi;
```

Compute singlet energy with this Hamiltonian:

$$\hat{H}|\psi\rangle =$$



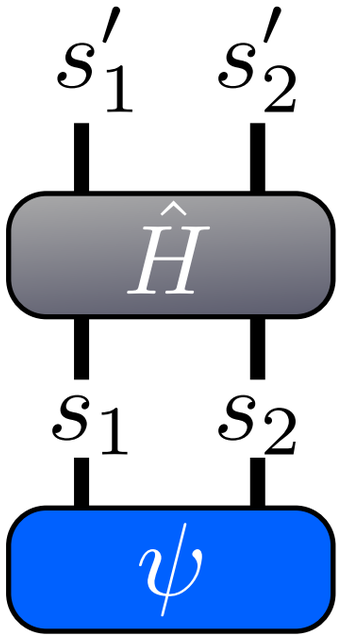
$=$



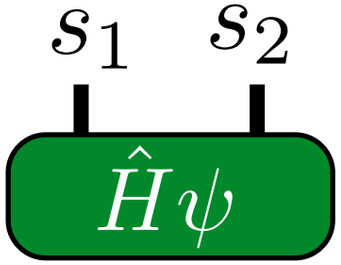

```
ITensor Hpsi = H * psi;

Hpsi.mapprime(1,0);
```

Compute singlet energy with this Hamiltonian:

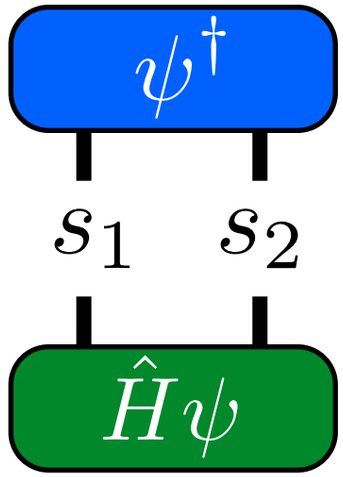
$$\hat{H}|\psi\rangle =$$



$=$



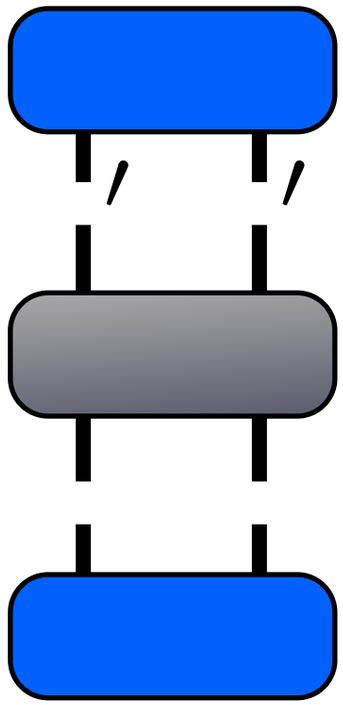
$;\ E =$




```
ITensor Hpsi = H * psi;

Hpsi.mapprime(1,0);

Real E = (dag(psi) * Hpsi).toReal();
Print(E);
//Prints:
//E = -0.75
```

Or compute energy in one shot:

$$E_{\text{sing}} =$$



dag(prime(psi))

```
Real E = (dag(prime(psi)) * H * psi).toReal();
Print(E);
//Prints:
//E = -0.75
```

We'll use imaginary time evolution to find this Hamiltonian's ground state

$$e^{-\beta H/2}|0\rangle \propto |\Psi_0\rangle$$

`<library folder>/tutorial/02_two_sites`

1. Read through **`two.cc`**, compile and run by typing "**`make two`**" then run by typing "**`./two`**"

2. Open **`imag_tevol.cc`** and implement the code to make $e^{-\beta H}$ using a Taylor series (summed using a recursive formula)

3. Try increasing β, compile, and re-run the code until it converges to the ground state

Solution for missing code (near line 120 of `imag_tevol.cc`):

```
for(int ord = max_order-1; ord >= 1; --ord)
    {
    expH = expH * (x/ord);
    expH.mapprime(2,1);
    expH += I;
    }
```