

# Analyzing Quantum Many-Body Systems with ITensor and PastaQ

Matthew Fishman

Center for Computational Quantum Physics (CCQ)

Flatiron Institute, NY

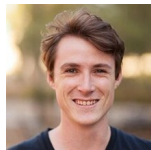
[mtfishman.github.io](https://mtfishman.github.io)

[github.com/mtfishman/ITensorTutorials.jl](https://github.com/mtfishman/ITensorTutorials.jl)

June 18, 2022

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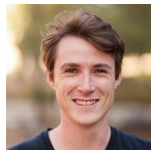
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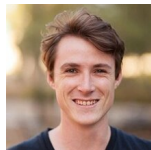
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- ▶ We are hiring postdocs, full-time scientists, part-time and full-time software developers, interns, etc.

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SIMONS FOUNDATION

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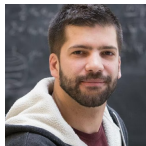


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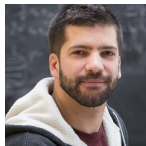
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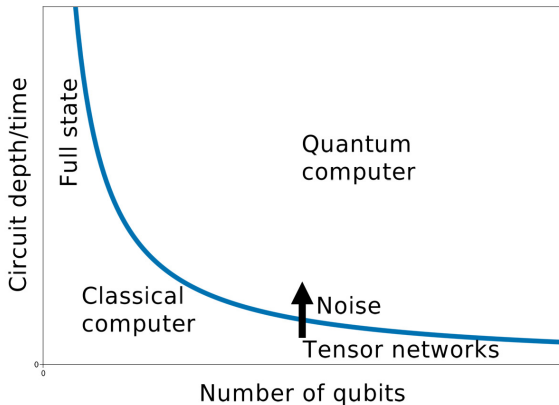
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- ▶ Find out more: [github.com/GTorlai/PastaQ.jl](https://github.com/GTorlai/PastaQ.jl)

## *When should I use tensor networks?*

- In my opinion, tensor networks are the best general purpose tool we have right now for simulating and analyzing quantum computers.



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  - ▶ ITensor and PastaQ handle this seamlessly.
  - ▶ This is not the focus of ITensor and PastaQ at the moment, specialized libraries like [Yao.jl](#) may be faster.
- ▶ Tensor networks are a common, general language for reasoning about quantum many-body systems (for example, quantum circuits).

# *What are tensor networks?*

Vector  $V_i$   
Order-1 tensor



Matrix  $M_{ij}$   
Order-2 tensor

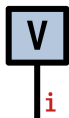


Tensor  $T_{ijk}$   
Order-3 tensor



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$$\langle V|V \rangle = V_i V_i$$



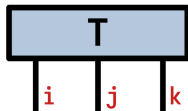
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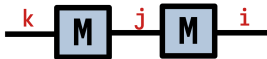
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$$MM = M_{kj} M_{ji}$$



# What are tensor networks?

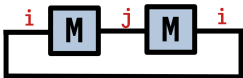
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$$\text{tr}(MM) = M_{ij} M_{ji}$$



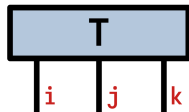
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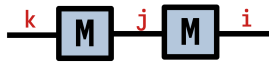
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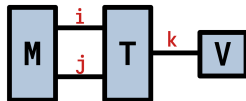
Tensor  $T_{ijk}$   
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$$MM = M_{kj} M_{ji}$$



$$M_{ij} T_{ijk} V_k$$



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2. Launch Julia:

```
1 $ julia
```

3. Type the following commands:

```
1 julia> using Pkg
2
3 julia> Pkg.add("ITensors")
4 [...]
5
6 julia> Pkg.add("PastaQ")
7 [...]
```

## *How do I install ITensor/PastaQ?*

Now you can use ITensors and PastaQ:

```
1 julia> using ITensors
2
3 julia> i = Index(2);
4
5 julia> A = ITensor(i);
```



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```
1 julia> using PastaQ
2
3 julia> gates = [("X", 1), ("CX", (1, 3))];
4
5 julia>  $\psi$  = runcircuit(gates);
```

## *Tutorial: One-site state basics*

```
1 using ITensors
2
3 i = Index(2)
4
5
```

Load ITensor

2-dimensional labeled  
Hilbert space  
(dim=2|id=510)

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## *Tutorial: One-site state basics*

```
1 using ITensors
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3 i = Index(2)
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```

```
1 Zp = ITensor(i)
2 Zp[i==1] = 1
3
4 Zp = ITensor([1, 0], i)
```

i

$$|Z+\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

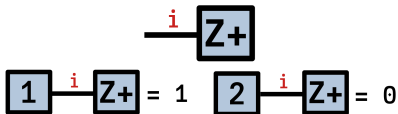
Construct from a Vector

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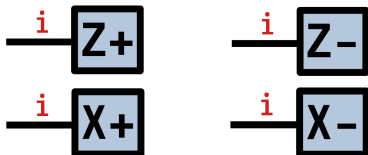
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```
1 Zp=ITensor([1,0],i)
2 Zm=ITensor([0,1],i)
3 Xp=ITensor([1,1]/sqrt(2),i)
4 Xm=ITensor([1,-1]/sqrt(2),i)
```

$$\begin{aligned} |Z+\rangle &= \begin{bmatrix} 1 \\ 0 \end{bmatrix}, & |Z-\rangle &= \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ |X+\rangle &= \begin{bmatrix} 1 \\ 1 \end{bmatrix} / \sqrt{2}, & |X-\rangle &= \begin{bmatrix} 1 \\ -1 \end{bmatrix} / \sqrt{2} \end{aligned}$$

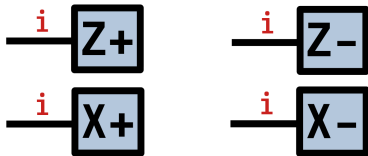
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```



```
1 Xp = (Zp + Zm)/sqrt(2)
2
3
4
5 (dag(Zp) * Xp)[]
6 inner(Zp, Xp)
```

$$|X+\rangle = (|Z+\rangle + |Z-\rangle)/\sqrt{2}$$

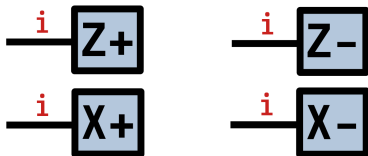
$$\langle Z+ | X+\rangle \approx 1/\sqrt{2}$$



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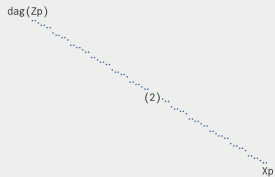
$$X_+ = \frac{Z_+ + Z_-}{\sqrt{2}}$$

$$Z_+ X_+ = 1/\sqrt{2}$$

## *Tutorial: One-site state basics*

```
1 using ITensorUnicodePlots
2
3 @visualize dag(Zp) * Xp
```

```
julia> @visualize dag(Zp) * Xp
```



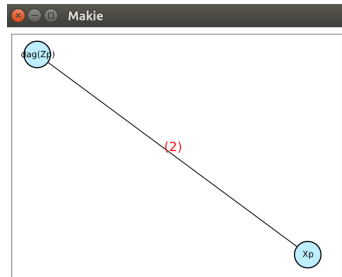
# Tutorial: One-site state basics

```
1 using ITensorUnicodePlots
2
3 @visualize dag(Zp) * Xp
```

```
julia> @visualize dag(Zp) * Xp
```



```
1 using ITensorGLMakie
2
3 @visualize dag(Zp) * Xp
```



## *Tutorial: One-site states*

```
1 i = Index(2, "S=1/2")
```

(dim=2|id=25|"S=1/2")

"S=1/2" defines an operator basis

Additionally:  
"Qubit", "Qudit",  
"Electron", ...

## Tutorial: One-site states

```
1 i = Index(2, "S=1/2")
```

(dim=2|id=25|"S=1/2")

"S=1/2" defines an operator basis

Additionally:

"Qubit", "Qudit",  
"Electron", ...

```
1 Zp=state("Zp",i)
2 Zm=state("Zm",i)
3 Xp=state("Xp",i)
4 Xm=state("Xm",i)
```

```
1 ITensor([1,0],i)
2 ITensor([0,1],i)
3 ITensor([1,1]/√2,i)
4 ITensor([1,-1]/√2,i)
```

## *Tutorial: Custom one-site states*

```
1 import ITensors: state
2
3
4 function state(
5     ::StateName"iXm",
6     ::SiteType"S=1/2")
7     return [im,-im]/√2
8 end
```

Overload ITensors.jl  
behavior

Define a state with the  
name "iX-"

## Tutorial: Custom one-site states

```
1 import ITensors: state
2
3
4 function state(
5     ::StateName"iXm",
6     ::SiteType"S=1/2")
7     return [im,-im]/√2
8 end
```

```
1 iXm = state("iXm", i)
2
3
4 inner(Zm, iXm)
```

Overload ITensors.jl  
behavior

Define a state with the  
name “iX-”

$$|iX-\rangle = i|X-\rangle$$

$$\langle Z- | iX-\rangle = -i/\sqrt{2}$$

## Tutorial: Custom one-site states

```
1 import ITensors: state
2
3
4 function state(
5     ::StateName"iXm",
6     ::SiteType"S=1/2")
7     return [im, -im]/√2
8 end
```

```
1 iXm = state("iXm", i)
2
3
4 inner(Zm, iXm)
```

Overload ITensors.jl  
behavior

Define a state with the  
name “iX-”

$$\text{---} \boxed{\text{iX}^+} = \left( \text{---} \boxed{\text{X}^+} \right) * i$$



## *Tutorial: Priming*

```
1 i = Index(2)
2 j = Index(2)
3
4 i != j
```

(dim=2|id=837)

(dim=2|id=899)

## *Tutorial: Priming*

```
1 i = Index(2)
2 j = Index(2)
3
4 i != j
```

i  $\neq$  j

## Tutorial: Priming

```
1 i = Index(2)
2 j = Index(2)
3
4 i != j
```

```
1 i = Index(2)
2
3 prime(i) == i'
4
5 i != i'
6 noprime(i') == i
```

$$\underline{i} \neq \underline{j}$$

(dim=2|id=837)

(dim=2|id=837)'

## Tutorial: Priming

```
1 i = Index(2)
2 j = Index(2)
3
4 i != j
```

```
1 i = Index(2)
2
3 prime(i) == i'
4
5 i != i'
6 noprime(i') == i
```

$$\underline{i} \neq \underline{j}$$

$$\text{prime}\left(\frac{i}{\underline{\quad}}\right) = \underline{i'}$$
$$\underline{i} \neq \underline{i'}$$

## *Tutorial: One-site operators*

```
1 i = Index(2, "S=1/2")
2 Z = ITensor(i', i)
3 Z[i'=>1, i=>1] = 1
4 Z[i'=>2, i=>2] = -1
```

$$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

## Tutorial: One-site operators

```
1 i = Index(2, "S=1/2")
2 Z = ITensor(i', i)
3 Z[i'=>1, i=>1] = 1
4 Z[i'=>2, i=>2] = -1
```



## Tutorial: One-site operators

```
1 i = Index(2, "S=1/2")
2 Z = ITensor(i', i)
3 Z[i'=>1, i=>1] = 1
4 Z[i'=>2, i=>2] = -1
```

```
1 z = [1 0; 0 -1]
2
3
4
5 Z = ITensor(z, i', i)
6
7
8 Z = op("Z", i)
```



Matrix representation  $Z$

Convert to ITensor

Use predefined definition

## *Tutorial: One-site operators*

```
1 Z = op("Z", i)
2 X = op("X", i)
3
4 Zp = state("Zp", i)
5 Zm = state("Zm", i)
```

Z

X

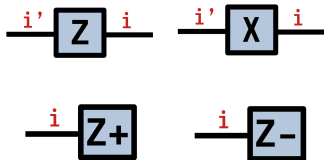
$|Z+\rangle$

$|Z-\rangle$



## Tutorial: One-site operators

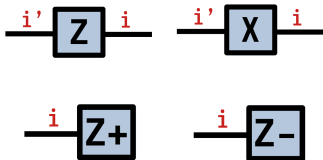
```
1 Z = op("Z", i)
2 X = op("X", i)
3
4 Zp = state("Zp", i)
5 Zm = state("Zm", i)
```



## Tutorial: One-site operators

```
1 Z = op("Z", i)
2 X = op("X", i)
3
4 Zp = state("Zp", i)
5 Zm = state("Zm", i)
```

```
1 X * Zp == Zm'
2 noprime(X * Zp) == Zm
```

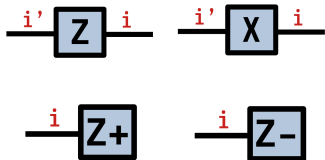


$$X|Z+\rangle = |Z-\rangle$$

## Tutorial: One-site operators

```
1 Z = op("Z", i)
2 X = op("X", i)
3
4 Zp = state("Zp", i)
5 Zm = state("Zm", i)
```

```
1 X * Zp == Zm'
2 noprime(X * Zp) == Zm
```



$$X \cdot Z_+ = Z_-$$

## *Tutorial: One-site operators*

```
1 (dag(Zm)' * X * Zp)[]  
2 inner(Zm', X, Zp)
```

$$\langle Z - |X|Z+ \rangle \approx 1$$

## *Tutorial: One-site operators*

```
1 (dag(Zm)' * X * Zp)[]  
2 inner(Zm', X, Zp)
```

$$\boxed{Z-} \overset{i'}{\text{---}} \boxed{X} \overset{i}{\text{---}} \boxed{Z+} = 1$$

## Tutorial: One-site operators

```
1 (dag(Zm)' * X * Zp)[]  
2 inner(Zm', X, Zp)
```

$$\boxed{Z-} \overset{i'}{\text{---}} \boxed{X} \overset{i}{\text{---}} \boxed{Z+} = 1$$

```
1 apply(X, Zp) ==  
2   noprime(X * Zp)  
3  
4  
5  
6 inner(Zm, apply(X, Zp))
```

$$X|Z+\rangle$$

$$\langle Z- | X | Z+ \rangle \approx 1$$

## Tutorial: One-site operators

```
1 (dag(Zm)' * X * Zp)[]  
2 inner(Zm', X, Zp)
```

$$\boxed{Z-} \overset{i'}{\text{---}} \boxed{X} \overset{i}{\text{---}} \boxed{Z+} = 1$$

```
1 apply(X, Zp) ==  
2   noprime(X * Zp)  
3  
4  
5  
6 inner(Zm, apply(X, Zp))
```

$$\begin{aligned} & \text{apply}\left(\overset{i'}{\text{---}} \boxed{X} \overset{i}{\text{---}}, \overset{i}{\text{---}} \boxed{Z+}\right) \\ &= \text{noprime}\left(\overset{i'}{\text{---}} \boxed{X} \overset{i}{\text{---}} \boxed{Z+}\right) \\ &= \overset{i}{\text{---}} \boxed{Z-} \end{aligned}$$

## *Tutorial: Custom one-site operators*

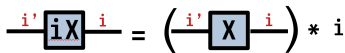
Overload ITensors.jl  
behavior

```
1 import ITensors: op
2
3 function op(
4     ::OpName"iX",
5     ::SiteType"S=1/2")
6     return [0 im; im 0]
7 end
```



## *Tutorial: Custom one-site operators*

```
1 import ITensors: op
2
3 function op(
4     ::OpName"iX",
5     ::SiteType"S=1/2")
6     return [0 im; im 0]
7 end
```



The diagram shows the definition of the  $iX$  operator in a tensor network notation. On the left, a horizontal line enters a blue square box labeled  $iX$  from the left, and another horizontal line exits the box to the right. Above the entry line is a red  $i'$  and above the exit line is a red  $i$ . This is set equal to the product of a term in parentheses and a scalar  $i$ . The term in parentheses consists of a horizontal line entering a blue square box labeled  $X$  from the left, and another horizontal line exiting the box to the right. Above the entry line is a red  $i'$  and above the exit line is a red  $i$ .

$$\text{---} \overset{i'}{\boxed{iX}} \text{---} \overset{i}{} = \left( \text{---} \overset{i'}{\boxed{X}} \text{---} \overset{i}{} \right) * i$$

## Tutorial: Custom one-site operators

```
1 import ITensors: op
2
3 function op(
4     ::OpName"iX",
5     ::SiteType"S=1/2")
6     return [0 im; im 0]
7 end
```

```
1 op("iX", i)
```

$$\text{---} \overset{i'}{\boxed{iX}} \text{---} = \left( \text{---} \overset{i'}{\boxed{X}} \text{---} \right) * i$$

## Tutorial: Custom one-site operators

```
1 import ITensors: op
2
3 function op(
4     ::OpName"iX",
5     ::SiteType"S=1/2")
6     return [0 im; im 0]
7 end
```

```
1 op("iX", i)
```

$$\text{---} \overset{i'}{\boxed{iX}} \text{---}^i = \left( \text{---} \overset{i'}{\boxed{X}} \text{---}^i \right) * i$$

```
1 X * im
```

## Tutorial: Two-site states

```
1 i1 = Index(2, "S=1/2,i1")
2 i2 = Index(2, "S=1/2,i2")
3
4 i1 != i2
5
6 ZpZm = ITensor(i1, i2)
7 ZpZm[i1=>1, i2=>2] = 1
```

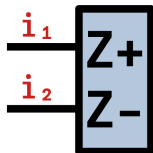
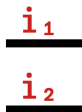
(dim=2|id=505|“S=1/2”)

(dim=2|id=576|“S=1/2”)

$$|Z+\rangle_1|Z-\rangle_2 = |Z+Z-\rangle$$

## Tutorial: Two-site states

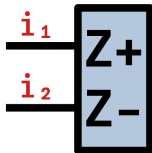
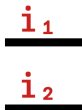
```
1 i1 = Index(2, "S=1/2,i1")
2 i2 = Index(2, "S=1/2,i2")
3
4 i1 != i2
5
6 ZpZm = ITensor(i1, i2)
7 ZpZm[i1=>1, i2=>2] = 1
```



## Tutorial: Two-site states

```
1 i1 = Index(2, "S=1/2,i1")
2 i2 = Index(2, "S=1/2,i2")
3
4 i1 != i2
5
6 ZpZm = ITensor(i1, i2)
7 ZpZm[i1=>1, i2=>2] = 1
```

```
1 Zp1=state("Zp",i1)
2 Zp2=state("Zp",i2)
3 Zm1=state("Zm",i1)
4 Zm2=state("Zm",i2)
5
6
7 ZpZm = Zp1 * Zm2
```



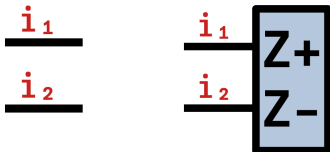
$$|Z+\rangle_1$$
$$|Z+\rangle_2$$

$$|Z-\rangle_1$$
$$|Z-\rangle_2$$

$$|Z+Z-\rangle = |Z+\rangle_1 |Z-\rangle_2$$

## Tutorial: Two-site states

```
1 i1 = Index(2, "S=1/2,i1")
2 i2 = Index(2, "S=1/2,i2")
3
4 i1 != i2
5
6 ZpZm = ITensor(i1, i2)
7 ZpZm[i1=>1, i2=>2] = 1
```



```
1 Zp1=state("Zp",i1)
2 Zp2=state("Zp",i2)
3 Zm1=state("Zm",i1)
4 Zm2=state("Zm",i2)
5
6
7 ZpZm = Zp1 * Zm2
```



## *Tutorial: Two-site states*

```
1   $\psi$  = ITensor(i1, i2)
2   $\psi[i1=>1, i2=>2]$  = 1/ $\sqrt{2}$ 
3   $\psi[i1=>2, i2=>1]$  = 1/ $\sqrt{2}$ 
4
5   $\psi$  = (Zp1 * Zm2 +
6         Zm1 * Zp2)/ $\sqrt{2}$ 
```

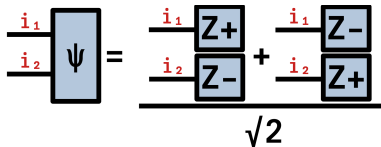
$$(|Z+\rangle|Z-\rangle + |Z-\rangle|Z+\rangle)/\sqrt{2}$$

From single-site states



## Tutorial: Two-site states

```
1   $\psi = \text{ITensor}(i1, i2)$ 
2   $\psi[i1 \Rightarrow 1, i2 \Rightarrow 2] = 1/\sqrt{2}$ 
3   $\psi[i1 \Rightarrow 2, i2 \Rightarrow 1] = 1/\sqrt{2}$ 
4
5   $\psi = (Z_{p1} * Z_{m2} +$ 
6          $Z_{m1} * Z_{p2})/\sqrt{2}$ 
```



## Tutorial: Two-site states

```
1   $\psi = \text{ITensor}(i1, i2)$ 
2   $\psi[i1 \Rightarrow 1, i2 \Rightarrow 2] = 1/\sqrt{2}$ 
3   $\psi[i1 \Rightarrow 2, i2 \Rightarrow 1] = 1/\sqrt{2}$ 
4
5   $\psi = (\text{Zp1} * \text{Zm2} +$ 
6          $\text{Zm1} * \text{Zp2})/\sqrt{2}$ 
```

```
1   $\text{inner}(\text{ZpZm}, \psi) == 1/\sqrt{2}$ 
2
3
4   $\_, S, \_ = \text{svd}(\text{ZpZm}, i1);$ 
5   $\text{diag}(S) == [1, 0]$ 
6
7   $\_, S, \_ = \text{svd}(\psi, i1);$ 
8   $\text{diag}(S) == [1/\sqrt{2}, 1/\sqrt{2}]$ 
```

$$\begin{array}{c} i_1 \\ i_2 \end{array} \psi = \frac{\begin{array}{c} i_1 \\ i_2 \end{array} \begin{array}{c} \boxed{Z+} \\ \boxed{Z-} \end{array} + \begin{array}{c} i_1 \\ i_2 \end{array} \begin{array}{c} \boxed{Z-} \\ \boxed{Z+} \end{array}}{\sqrt{2}}$$

$$\begin{array}{c} i_1 \\ i_2 \end{array} \boxed{Z+Z-} = \begin{array}{c} i_1 \\ u \end{array} \boxed{U} \begin{array}{c} u \\ v \end{array} \boxed{S} \begin{array}{c} v \\ i_2 \end{array} \boxed{V}$$
$$\begin{array}{c} u \\ v \end{array} \boxed{S} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

## Tutorial: Two-site states

```

1   $\psi = \text{ITensor}(i1, i2)$ 
2   $\psi[i1 \Rightarrow 1, i2 \Rightarrow 2] = 1/\sqrt{2}$ 
3   $\psi[i1 \Rightarrow 2, i2 \Rightarrow 1] = 1/\sqrt{2}$ 
4
5   $\psi = (\text{Zp1} * \text{Zm2} +$ 
6       $\text{Zm1} * \text{Zp2})/\sqrt{2}$ 

```

```

1   $\text{inner}(\text{ZpZm}, \psi) == 1/\sqrt{2}$ 
2
3
4   $\_, S, \_ = \text{svd}(\text{ZpZm}, i1);$ 
5   $\text{diag}(S) == [1, 0]$ 
6
7   $\_, S, \_ = \text{svd}(\psi, i1);$ 
8   $\text{diag}(S) == [1/\sqrt{2}, 1/\sqrt{2}]$ 

```

$$\psi = \frac{\begin{matrix} i_1 \\ i_2 \end{matrix} \begin{matrix} \boxed{Z+} \\ \boxed{Z-} \end{matrix} + \begin{matrix} i_1 \\ i_2 \end{matrix} \begin{matrix} \boxed{Z-} \\ \boxed{Z+} \end{matrix}}{\sqrt{2}}$$

$$\text{svd}\left(\begin{matrix} i_1 & \boxed{Z+Z-} & i_2 \end{matrix}\right) = \begin{matrix} i_1 & \boxed{U} & u & \boxed{S} & v & \boxed{V} & i_2 \end{matrix}$$

$$\begin{matrix} u & \boxed{S} & v \end{matrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

$$\text{svd}\left(\begin{matrix} i_1 & \boxed{\psi} & i_2 \end{matrix}\right) = \begin{matrix} i_1 & \boxed{U} & u & \boxed{S} & v & \boxed{V} & i_2 \end{matrix}$$

$$\begin{matrix} u & \boxed{S} & v \end{matrix} = \begin{bmatrix} 1/\sqrt{2} & 0 \\ 0 & 1/\sqrt{2} \end{bmatrix}$$

## *Tutorial: Two-site operators*

```
1 H = ITensor(i1', i2',  
2           i1, i2)  
3 H[i1'=>2, i2'=>1,  
4   i1=>2, i2=>1] = -1  
5 # ...
```

Make a Hamiltonian:

Transverse field Ising ( $n = 2$ )

$$H = -\sum_j^{n-1} Z_j Z_{j+1} + h \sum_j^n X_j$$

## Tutorial: Two-site operators

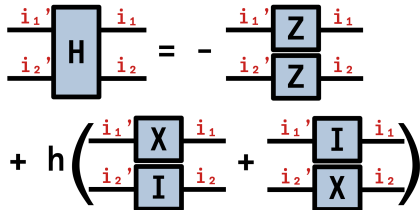
```
1 H = ITensor(i1', i2',  
2           i1, i2)  
3 H[i1'=>2, i2'=>1,  
4   i1=>2, i2=>1] = -1  
5 # ...
```

```
1 Id1 = op("Id", i1)  
2 Z1 = op("Z", i1)  
3 X1 = op("X", i1)  
4 Id2 = op("Id", i2)  
5 Z2 = op("Z", i2)  
6 X2 = op("X", i2)  
7  
8 ZZ = Z1 * Z2  
9 XI = X1 * Id2  
10 IX = Id1 * X2  
11  
12 h = 0.5  
13 H = -ZZ + h * (XI + IX)
```

Make a Hamiltonian:

Transverse field Ising ( $n = 2$ )

$$H = -\sum_j^{n-1} Z_j Z_{j+1} + h \sum_j^n X_j$$



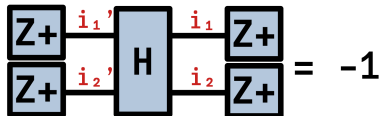
## *Tutorial: Two-site operators*

```
1 inner(Zp1' * Zp2', H,  
2       Zp1 * Zp2)
```

$$\langle Z+Z+ | H | Z+Z+ \rangle$$

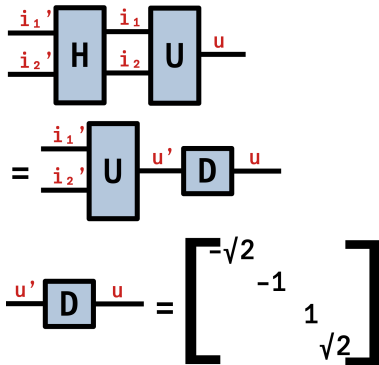
## *Tutorial: Two-site operators*

```
1 inner(Zp1' * Zp2', H,  
2       Zp1 * Zp2)
```



## Tutorial: Two-site operators

```
1 D, U = eigen(H);  
2 diag(D)  $\approx$   $[-\sqrt{2}, -1, 1, \sqrt{2}]$ 
```





## *Tutorial: Custom two-site operators*

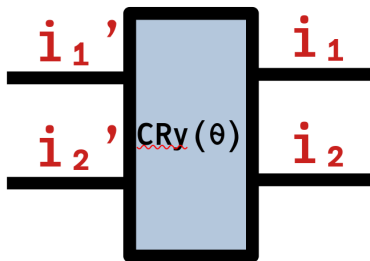
```
1 import ITensors: op
2
3 function op(
4     ::OpName"CRy",
5     ::SiteType"S=1/2";  $\theta$ )
6     c = cos( $\theta/2$ )
7     s = sin( $\theta/2$ )
8     return [
9         1 0 0 0
10        0 1 0 0
11        0 0 c -s
12        0 0 s  c]
13 end
```

Controlled-Ry (CRy)  
rotation gate

$\text{CRy}(\theta)$

## Tutorial: Custom two-site operators

```
1 import ITensors: op
2
3 function op(
4     ::OpName"CRy",
5     ::SiteType"S=1/2";  $\theta$ )
6     c = cos( $\theta/2$ )
7     s = sin( $\theta/2$ )
8     return [
9         1 0 0 0
10        0 1 0 0
11        0 0 c -s
12        0 0 s  c]
13 end
```



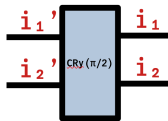
## *Tutorial: Custom two-site operators*

```
1 CRy = op("CRy", i1, i2;  $\theta=\pi/2$ )
```

Controlled-rotation gate  
 $\text{CRy}(\pi/2)$

## *Tutorial: Custom two-site operators*

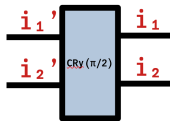
```
1 CRy = op("CRy", i1, i2;  $\theta=\pi/2$ )
```



## Tutorial: Custom two-site operators

```
1 CRy = op("CRy", i1, i2;  $\theta=\pi/2$ )
```

```
1 Xp1=state("Xp",i1)
2 Xm1=state("Xm",i1)
3 Xp2=state("Xp",i2)
4 Xm2=state("Xm",i2)
5
6 apply(CRy, Zm1 * Zp2)  $\approx$ 
7     Zm1 * Xp2
```

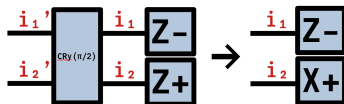
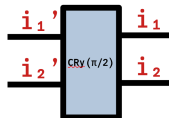


$$\text{CRy}(\pi/2)|Z-Z+\rangle = |Z-X+\rangle$$

## Tutorial: Custom two-site operators

```
1 CRy = op("CRy", i1, i2;  $\theta=\pi/2$ )
```

```
1 Xp1=state("Xp",i1)
2 Xm1=state("Xm",i1)
3 Xp2=state("Xp",i2)
4 Xm2=state("Xm",i2)
5
6 apply(CRy, Zm1 * Zp2)  $\approx$ 
7     Zm1 * Xp2
```



## *Tutorial: Two-site state optimization*

```
1 function E( $\psi$ )  
2    $\psi H \psi = \text{inner}(\psi', H, \psi)$   
3    $\psi \psi = \text{inner}(\psi, \psi)$   
4   return  $\psi H \psi / \psi \psi$   
5 end
```

$$E(\psi) = \langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle$$

## Tutorial: Two-site state optimization

```
1 function E( $\psi$ )  
2    $\psi H \psi = \text{inner}(\psi', H, \psi)$   
3    $\psi \psi = \text{inner}(\psi, \psi)$   
4   return  $\psi H \psi / \psi \psi$   
5 end
```

$$E(\psi) = \frac{\begin{array}{c} \boxed{\psi} \begin{array}{c} i_1' \\ i_2' \end{array} \boxed{H} \begin{array}{c} i_1 \\ i_2 \end{array} \boxed{\psi} \end{array}}{\begin{array}{c} \boxed{\psi} \begin{array}{c} i_1 \\ i_2 \end{array} \boxed{\psi} \end{array}}$$



### *Tutorial: Two-site state optimization*

```

1 function E( $\psi$ )
2      $\psi H \psi = \text{inner}(\psi', H, \psi)$ 
3      $\psi \psi = \text{inner}(\psi, \psi)$ 
4     return  $\psi H \psi / \psi \psi$ 
5 end

```

```

1 function minimize(f, ∂f, x;
2                   nsteps, γ)
3     for n in 1:nsteps
4         x = x - γ * ∂f(x)
5         println("Step = $(n),
6                 f(x) = $(f(x))")
7     end
8     return x
9 end

```

Diagram illustrating the decomposition of a quantum circuit  $E(\psi)$  into two parts. The top part shows a sequence of three blue boxes:  $\Psi$ ,  $H$ , and  $\Psi$ . The first  $\Psi$  box has two red inputs labeled  $i_1'$  and  $i_2'$ . The  $H$  box has two red inputs labeled  $i_1$  and  $i_2$ . The second  $\Psi$  box has two red inputs labeled  $i_1$  and  $i_2$ . The bottom part shows a single blue box  $\Psi$  with two red inputs labeled  $i_1$  and  $i_2$ .

Gradient descent.

$f(x)$ : function to minimize.

$\partial f(\mathbf{x})$ : gradient of  $f$ .

$\gamma$ : step size.

# Tutorial: Two-site state optimization

```
1 function E( $\psi$ )
2    $\psi H \psi = \text{inner}(\psi', H, \psi)$ 
3    $\psi \psi = \text{inner}(\psi, \psi)$ 
4   return  $\psi H \psi / \psi \psi$ 
5 end
```

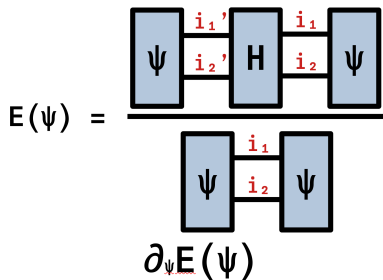
```
1 function minimize(f,  $\partial f$ , x;
2   nsteps,  $\gamma$ )
3   for n in 1:nsteps
4      $x = x - \gamma * \partial f(x)$ 
5     println("Step = $(n),
6        $f(x) = $(f(x))"$ )
7   end
8   return x
9 end
```

$$E(\psi) = \frac{\begin{array}{|c|} \hline \psi \\ \hline \end{array} \begin{array}{|c|} \hline i_1' \\ \hline \end{array} \begin{array}{|c|} \hline H \\ \hline \end{array} \begin{array}{|c|} \hline i_1 \\ \hline \end{array} \begin{array}{|c|} \hline \psi \\ \hline \end{array}}{\begin{array}{|c|} \hline \psi \\ \hline \end{array} \begin{array}{|c|} \hline i_2' \\ \hline \end{array} \begin{array}{|c|} \hline i_2 \\ \hline \end{array} \begin{array}{|c|} \hline \psi \\ \hline \end{array}}$$

$$\min_{\psi} E(\psi) \quad \partial_{\psi} E(\psi)$$

## Tutorial: Two-site state optimization

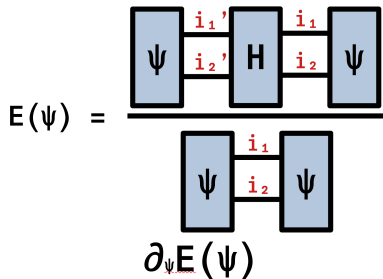
```
1   $\psi_0 = (Z_{p1} * Z_{p2} +$   
2       $Z_{m1} * Z_{m2})/\sqrt{2}$   
3  
4   $E(\psi_0) == -1$   
5  
6  using Zygote # autodiff  
7  
8   $\partial E(\psi) = \text{gradient}(E, \psi)[1]$   
9   $\text{norm}(\partial E(\psi_0)) == 2$ 
```



## Tutorial: Two-site state optimization

```
1   $\psi_0 = (\text{Zp1} * \text{Zp2} +$   
2       $\text{Zm1} * \text{Zm2})/\sqrt{2}$   
3  
4   $E(\psi_0) == -1$   
5  
6  using Zygote # autodiff  
7  
8   $\partial E(\psi) = \text{gradient}(E, \psi)[1]$   
9   $\text{norm}(\partial E(\psi_0)) == 2$ 
```

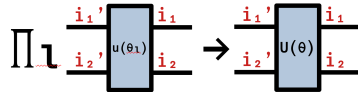
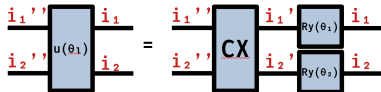
```
1   $\psi = \text{minimize}(E, \partial E, \psi_0;$   
2       $\text{nsteps}=10, \gamma=0.1)$   
3  
4   $E(\psi_0) == -1$   
5   $E(\psi) \# \approx -1.4142131 \approx -\sqrt{2}$   
6
```



$$\min_{\psi} E(\psi) = \min_{\psi} \langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle$$

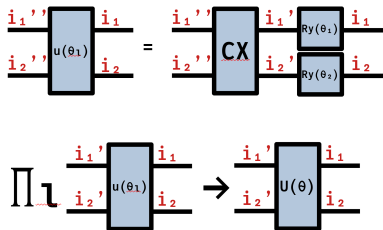
# Tutorial: Two-site circuit optimization

```
1 # Circuit as a vector of
   gates:
2 U( $\theta$ , i1, i2) = [
3   op("Ry", i1;  $\theta$ = $\theta$ [1]),
4   op("Ry", i2;  $\theta$ = $\theta$ [2]),
5   op("CX", i1, i2),
6   op("Ry", i1;  $\theta$ = $\theta$ [3]),
7   op("Ry", i2;  $\theta$ = $\theta$ [4])]
8
9
10
```



## Tutorial: Two-site circuit optimization

```
1 # PastaQ notation:
2 u(θ) = [
3     ("Ry",1,(;θ=θ[1])),
4     ("Ry",2,(;θ=θ[2])),
5     ("CNOT",1,2),
6     ("Ry",1,(;θ=θ[3])),
7     ("Ry",2,(;θ=θ[4]))]
8
9 U(θ,i1,i2) =
10     buildcircuit([i1,i2],u(θ))
```



## *Tutorial: Two-site circuit optimization*

```
1   $\psi_0 = Z_{p1} * Z_{p2}$ 
2
3
4  function E( $\theta$ )
5       $\psi_\theta = \text{apply}(U(\theta, i1, i2), \psi_0)$ 
6      return inner( $\psi_\theta^\dagger, H, \psi_\theta$ )
7  end
```

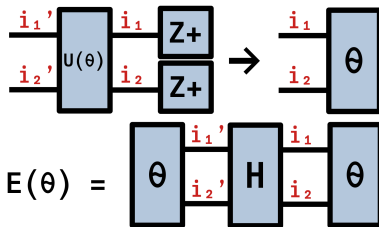
References state:

$$|0\rangle = |Z+Z+\rangle$$

$$\begin{aligned} \min_{\theta} E(\theta) \\ &= \min_{\theta} \langle 0 | U(\theta)^\dagger H U(\theta) | 0 \rangle \\ &= \min_{\theta} \langle \theta | H | \theta \rangle \end{aligned}$$

## Tutorial: Two-site circuit optimization

```
1  $\psi_0 = Z_{p1} * Z_{p2}$ 
2
3
4 function E( $\theta$ )
5      $\psi_\theta = \text{apply}(U(\theta, i_1, i_2), \psi_0)$ 
6     return inner( $\psi_{\theta'}, H, \psi_\theta$ )
7 end
```

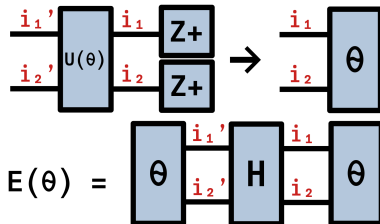




## Tutorial: Two-site circuit optimization

```
1  $\psi_0 = Z_{p1} * Z_{p2}$ 
2
3
4 function E( $\theta$ )
5      $\psi_\theta = \text{apply}(U(\theta, i_1, i_2), \psi_0)$ 
6     return inner( $\psi_\theta^\dagger, H, \psi_\theta$ )
7 end
```

```
1  $\theta_0 = [0, 0, 0, 0]$ 
2  $\partial E(\theta) = \text{gradient}(E, \theta)[1]$ 
3  $\theta = \text{minimize}(E, \partial E, \theta_0;$ 
4                $\text{nsteps}=40, \gamma=0.5)$ 
5
6  $E(\theta_0) == -1$ 
7  $E(\theta) \# \approx -1.4142077 \approx -\sqrt{2}$ 
```



$E(\theta) =$

$$\min_{\theta} E(\theta) \quad \partial_{\theta} E(\theta)$$

## *Tutorial: Two-site fidelity optimization*

```
1   $\psi_0 = Z_{p1} * Z_{p2}$ 
2   $\psi = (Z_{p1} * Z_{p2} + Z_{m1} * Z_{m2})$ 
    $/ \sqrt{2}$ 
3
4
5
6  function F( $\theta$ )
7       $\psi_\theta = \text{apply}(U(\theta, i1, i2), \psi_0)$ 
8      return -abs2(inner( $\psi, \psi_\theta$ ))
9  end
```

Reference state:

$$|0\rangle = |Z+Z+\rangle$$

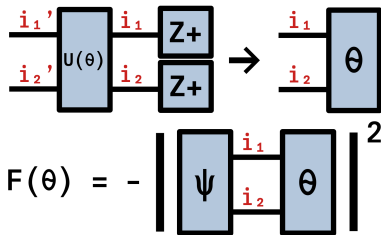
Target state:

$$|\psi\rangle = (|Z+Z+\rangle + |Z-Z-\rangle)/\sqrt{2}$$

$$\min_{\theta} F(\theta) = \min_{\theta} -|\langle\psi|U(\theta)|0\rangle|^2$$

## Tutorial: Two-site fidelity optimization

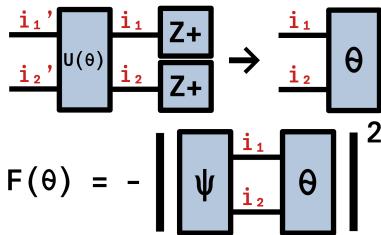
```
1   $\psi_0 = Z_{p1} * Z_{p2}$ 
2   $\psi = (Z_{p1} * Z_{p2} + Z_{m1} * Z_{m2})$ 
   /  $\sqrt{2}$ 
3
4
5
6  function F( $\theta$ )
7     $\psi_\theta = \text{apply}(U(\theta, i_1, i_2), \psi_0)$ 
8    return -abs2(inner( $\psi, \psi_\theta$ ))
9  end
```



## Tutorial: Two-site fidelity optimization

```
1   $\psi_0 = Z_{p1} * Z_{p2}$ 
2   $\psi = (Z_{p1} * Z_{p2} + Z_{m1} * Z_{m2})$ 
   /  $\sqrt{2}$ 
3
4
5
6  function F( $\theta$ )
7     $\psi_\theta = \text{apply}(U(\theta, i_1, i_2), \psi_0)$ 
8    return -abs2(inner( $\psi, \psi_\theta$ ))
9  end
```

```
1   $\theta_0 = [0, 0, 0, 0]$ 
2   $\partial F(\theta) = \text{gradient}(F, \theta)[1]$ 
3   $\theta = \text{minimize}(F, \partial F, \theta_0;$ 
   nsteps=50,  $\gamma=0.1)$ 
4
5
6   $F(\theta_0) == -0.5$ 
7   $F(\theta) \# \approx -0.9938992 \approx -1$ 
```



$$\min_{\theta} F(\theta) \quad \partial_{\theta} F(\theta)$$

## Tutorial: $n$ -site states with MPS

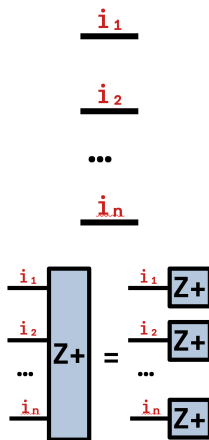
```
1  n = 30
2  i = [Index(2, "S=1/2")
3       for j in 1:n];
4
5
6  Zp = MPS(i, "Zp");
7  Zm = MPS(i, "Zm");
8
9  maxlinkdim(Zp) == 1
10     # product state
```

$n$ -site state

$|Z + Z + \dots Z+\rangle$

# Tutorial: $n$ -site states with MPS

```
1  n = 30
2  i = [Index(2, "S=1/2")
3       for j in 1:n];
4
5
6  Zp = MPS(i, "Zp");
7  Zm = MPS(i, "Zm");
8
9  maxlinkdim(Zp) == 1
10     # product state
```



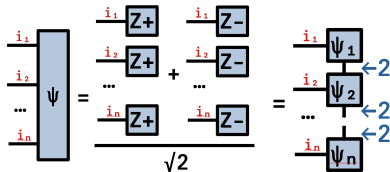
## *Tutorial: n-site states with MPS*

```
1   $\psi = (Z_p + Z_m)/\sqrt{2};$   
2  
3  
4  maxlinkdim( $\psi$ ) == 2  
5      # entangled state
```

$$\frac{(|Z + Z + \dots Z + \rangle + |Z - Z - \dots Z - \rangle)}{\sqrt{2}}$$

# Tutorial: $n$ -site states with MPS

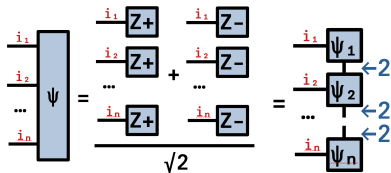
```
1  $\psi = (Z_p + Z_m)/\sqrt{2};$   
2  
3  
4 maxlinkdim( $\psi$ ) == 2  
5   # entangled state
```





## Tutorial: $n$ -site states with MPS

```
1  $\psi = (Z_p + Z_m)/\sqrt{2};$ 
2
3
4 maxlinkdim( $\psi$ ) == 2
5 # entangled state
```



```
1 inner( $Z_p, Z_p$ )  $\approx 1$ 
2
3
4 inner( $Z_p, \psi$ )  $\approx 1/\sqrt{2}$ 
```

$$\langle Z_+ | Z_+ \rangle = 1$$

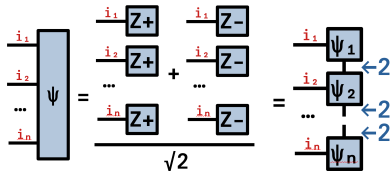
$$\langle Z_+ | \psi \rangle = 1/\sqrt{2}$$

# Tutorial: $n$ -site states with MPS

```

1   $\psi = (Z_p + Z_m)/\sqrt{2}$ ;
2
3
4  maxlinkdim( $\psi$ ) == 2
5  # entangled state

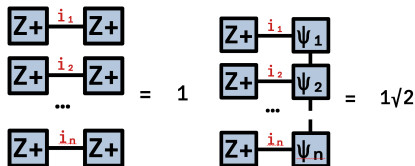
```



```

1  inner( $Z_p, Z_p$ )  $\approx 1$ 
2
3
4  inner( $Z_p, \psi$ )  $\approx 1/\sqrt{2}$ 

```



## Tutorial: $n$ -site states with MPS

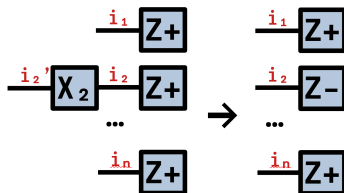
```
1  j = n ÷ 2
2  Xj = op("X", i[j])
3
4  XjZp = apply(Xj, Zp);
5
6
7  st = [k == j ? "Zm" : "Zp"
8        for k in 1:n];
9  XjZp = MPS(i, st);
```

$$X_j |Z + Z + \dots Z + \rangle = \\ |Z + Z + \dots Z - \dots Z + \rangle$$

$$|Z + Z + \dots Z - \dots Z + \rangle$$

## Tutorial: $n$ -site states with MPS

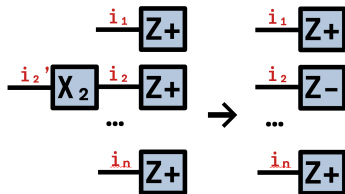
```
1  j = n ÷ 2
2  Xj = op("X", i[j])
3
4  XjZp = apply(Xj, Zp);
5
6
7  st = [k == j ? "Zm" : "Zp"
8        for k in 1:n];
9  XjZp = MPS(i, st);
```



## Tutorial: $n$ -site states with MPS

```
1  j = n ÷ 2
2  Xj = op("X", i[j])
3
4  XjZp = apply(Xj, Zp);
5
6
7  st = [k == j ? "Zm" : "Zp"
8        for k in 1:n];
9  XjZp = MPS(i, st);
```

```
1  maxlinkdim(XjZp) == 1
2  inner(Zp, XjZp) == 0
```



## Tutorial: $n$ -site operators with MPO

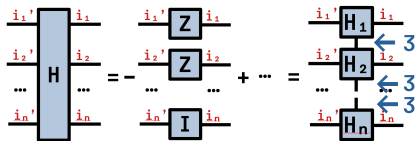
```
1 function ising(n; h)
2   H = OpSum()
3   for j in 1:(n - 1)
4     H -= "Z", j, "Z", j + 1
5   end
6   for j in 1:n
7     H += h, "X", j
8   end
9   return H
10 end
11
12 h = 0.5 # field
13 H = MPO(ising(n; h), i);
14 maxlinkdim(H) == 3
```

$n$  sites

$$H = -\sum_j^{n-1} Z_j Z_{j+1} + h \sum_j^n X_j$$

## Tutorial: $n$ -site operators with MPO

```
1 function ising(n; h)
2   H = OpSum()
3   for j in 1:(n - 1)
4     H -= "Z", j, "Z", j + 1
5   end
6   for j in 1:n
7     H += h, "X", j
8   end
9   return H
10 end
11
12 h = 0.5 # field
13 H = MPO(ising(n; h), i);
14 maxlinkdim(H) == 3
```



# Tutorial: $n$ -site operators with MPO

```

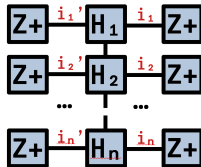
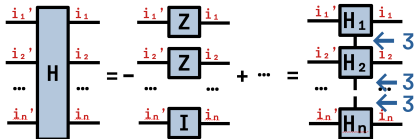
1  function ising(n; h)
2      H = OpSum()
3      for j in 1:(n - 1)
4          H -= "Z", j, "Z", j + 1
5      end
6      for j in 1:n
7          H += h, "X", j
8      end
9      return H
10 end
11
12 h = 0.5 # field
13 H = MPO(ising(n; h), i);
14 maxlinkdim(H) == 3

```

```

1  Zp = MPS(i, "Zp");
2  inner(Zp', H, Zp) ≈ -(n-1)
3

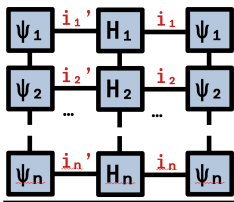
```





## Tutorial: $n$ -site state optimization

```
1 function E( $\psi$ )  
2    $\psi H \psi = \text{inner}(\psi', H, \psi)$   
3    $\psi \psi = \text{inner}(\psi, \psi)$   
4   return  $\psi H \psi / \psi \psi$   
5 end
```

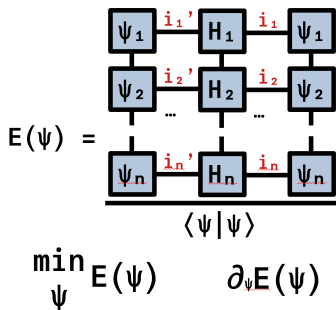
$$E(\psi) = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}$$


$\min_{\psi} E(\psi) \quad \partial_{\psi} E(\psi)$

## Tutorial: $n$ -site state optimization

```
1 function minimize(f, ∂f, x;  
2                   nsteps, γ,  
3                   cutoff)  
4     for n in 1:nsteps  
5       x = -(x, γ * ∂f(x); cutoff)  
6       println("Step = $(n),  
7               f(x) = $(f(x))")  
8     end  
9     return x  
10 end
```

```
1 ψ0 = MPS(i, "Zp");  
2 ψ = minimize(E, ∂E, ψ0;  
3             nsteps=50, γ=0.1,  
4             cutoff=1e-5);  
5  
6 Edmrg, ψdmrg = dmrg(H, ψ0;  
7                    nsweeps=10, cutoff=1e-5);
```


$$E(\psi) = \langle \psi | \psi \rangle$$
$$\min_{\psi} E(\psi) \quad \partial_{\psi} E(\psi)$$

# Tutorial: $n$ -site state optimization

```

1  function minimize(f, ∂f, x;
2                      nsteps, γ,
3                      cutoff)
4      for n in 1:nsteps
5          x = -(x, γ * ∂f(x); cutoff)
6          println("Step = $(n),
7                  f(x) = $(f(x))")
8      end
9      return x
10 end

```

$$E(\psi) = \frac{\langle \psi | \psi \rangle}{\langle \psi | \psi \rangle}$$

```

1  ψ0 = MPS(i, "Zp");
2  ψ = minimize(E, ∂E, ψ0;
3              nsteps=50, γ=0.1,
4              cutoff=1e-5);
5
6  Edmrg, ψdmrg = dmrg(H, ψ0;
7                      nsweeps=10, cutoff=1e-5);

```

```

1  maxlinkdim(ψ0) == 1
2  maxlinkdim(ψ) == 3
3  maxlinkdim(ψdmrg) == 3
4  E(ψ0) # ≈ -29
5  E(ψ) # ≈ -31.0317917
6  E(ψdmrg) # ≈ -31.0356110

```

## *Tutorial: n-site circuit optimization*

```
1 Ry_layer( $\theta$ , i) = [op("Ry", i[j];  $\theta=\theta[j]$ ) for j in 1:n]
2 CX_layer(i) = [op("CX", i[j], i[j+1]) for j in 1:2:(n-1)]
```

## *Tutorial: n-site circuit optimization*

```
1 Ry_layer( $\theta$ , i) = [op("Ry", i[j];  $\theta=\theta[j]$ ) for j in 1:n]
2 CX_layer(i) = [op("CX", i[j], i[j+1]) for j in 1:2:(n-1)]
```

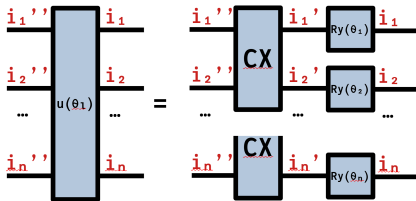
```
1 function U( $\theta$ , i; nlayers)
2     n = length(i)
3     U $\theta$  = ITensor[]
4     for l in 1:(nlayers-1)
5          $\theta l = \theta[(1:n) .+ l*n]$ 
6         U $\theta = [U\theta; Ry\_layer(\theta l, i)]$ 
7         U $\theta = [U\theta; CX\_layer(i)]$ 
8     end
9     return U $\theta$ 
10 end
```

$$U(\theta) = Ry_1(\theta_1) \dots Ry_n(\theta_n) \\ * CX_{1,2} \dots CX_{n-1,n} \\ * Ry_1(\theta_{n+1}) \dots Ry_n(\theta_{2n}) \\ * \dots$$

## Tutorial: $n$ -site circuit optimization

```
1 Ry_layer( $\theta$ , i) = [op("Ry", i[j];  $\theta$ = $\theta$ [j]) for j in 1:n]
2 CX_layer(i) = [op("CX", i[j], i[j+1]) for j in 1:2:(n-1)]
```

```
1 function U( $\theta$ , i; nlayers)
2     n = length(i)
3     U $\theta$  = ITensor[]
4     for l in 1:(nlayers-1)
5          $\theta$ l= $\theta$ [(1:n) .+ l*n]
6         U $\theta$ =[U $\theta$ ;Ry_layer( $\theta$ l,i)]
7         U $\theta$ =[U $\theta$ ;CX_layer(i)]
8     end
9     return U $\theta$ 
10 end
```



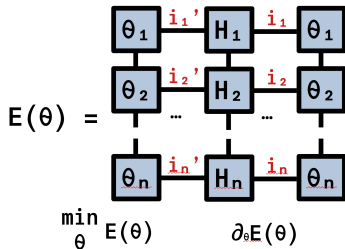
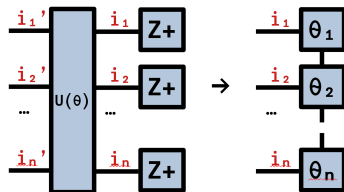
$$\prod_l U(\theta_l) \rightarrow U(\theta)$$

# Tutorial: $n$ -site states with MPS

```

1   $\psi_0$  = MPS( $i$ , "Zp");
2  nlayers = 6
3  function E( $\theta$ )
4       $\psi_\theta$ =apply(U( $\theta$ , $i$ ;nlayers), $\psi_0$ )
5      return inner( $\psi_\theta'$ ,H, $\psi_\theta$ )
6  end
7
8   $\theta_0$  = zeros(nlayers*n);
9   $\theta$  = minimize(E,  $\partial E$ ,  $\theta_0$ ;
10              nsteps=20,  $\gamma$ =0.1);

```



# Tutorial: $n$ -site states with MPS

```

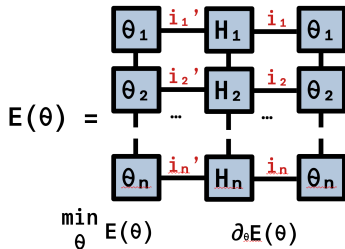
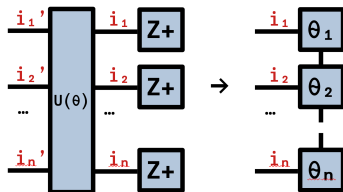
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```

```

1  maxlinkdim( $\psi_0$ ) = 1
2  maxlinkdim( $\psi_\theta$ ) = 3
3  E( $\theta_0$ ) #  $\approx -29$ 
4  E( $\theta$ ) #  $\approx -31.017062$ 

```



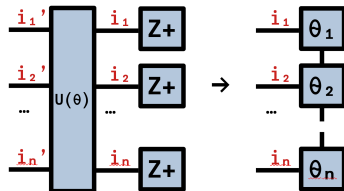


# Tutorial: $n$ -site states with MPS

```

1   $\psi_0$  = MPS(i, "Zp");
2  nlayers = 6
3  function F( $\theta$ )
4       $\psi_\theta$ =apply(U( $\theta$ ,i;nlayers), $\psi_0$ )
5      return -abs2(inner( $\psi'$ , $\psi_\theta$ ))
6  end
7
8   $\theta_0$  = zeros(nlayers*n);
9   $\theta$  = minimize(F,  $\partial F$ ,  $\theta_0$ ;
10              nsteps=20,  $\gamma$ =0.1);

```



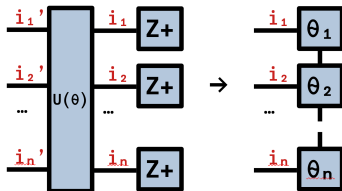
$$F(\theta) = - \left| \begin{array}{ccc} \psi_1 & i_1 & \theta_1 \\ \psi_2 & i_2 & \theta_2 \\ \vdots & \vdots & \vdots \\ \psi_n & i_n & \theta_n \end{array} \right|^2$$

$$\min_{\theta} F(\theta) \quad \partial_{\theta} F(\theta)$$

## Tutorial: $n$ -site states with MPS

```
1  $\psi_0 = \text{MPS}(i, \text{"Zp"})$ ;  
2  $\text{nlayers} = 6$   
3 function  $F(\theta)$   
4    $\psi_\theta = \text{apply}(U(\theta, i; \text{nlayers}), \psi_0)$   
5   return  $-\text{abs2}(\text{inner}(\psi', \psi_\theta))$   
6 end  
7  
8  $\theta_0 = \text{zeros}(\text{nlayers} * n)$ ;  
9  $\theta = \text{minimize}(F, \partial F, \theta_0$ ;  
10                $\text{nsteps}=20, \gamma=0.1)$ ;
```

```
1  $\text{maxlinkdim}(\psi_0) == 1$   
2  $\text{maxlinkdim}(\psi_\theta) == 2$   
3  $F(\theta_0) \# \approx -0.556066$   
4  $F(\theta) \# \approx -0.995230$ 
```



$$F(\theta) = - \left| \begin{array}{ccc} \psi_1 & i_1 & \theta_1 \\ \psi_2 & i_2 & \theta_2 \\ \vdots & \vdots & \vdots \\ \psi_n & i_n & \theta_n \end{array} \right|^2$$
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- ▶ More that I am probably forgetting... Ask Giacomo and me for more details.

## *Future directions/in progress*

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- ▶ Improved gradient optimization: higher order derivatives, preconditioners, isometrically constrained gradient optimization, etc.

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- ▶ I'm interested in building general tools and algorithms, and I'm looking for people with problems to solve. Also, we need help, code to contributions are welcome!