

Analyzing Quantum Many-Body Systems with ITensor and PastaQ

Matthew Fishman

Center for Computational Quantum Physics (CCQ)

Flatiron Institute, NY

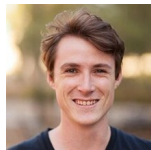
mtfishman.github.io

github.com/mtfishman/ITensorTutorials.jl

June 18, 2022

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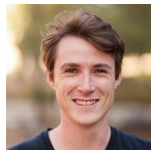
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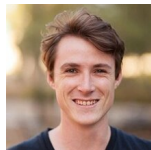
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- ▶ We are hiring postdocs, full-time scientists, part-time and full-time software developers, interns, etc.

What is the Center for Computation Quantum Physics (CCQ)?



SIMONS FOUNDATION

What is ITensor?

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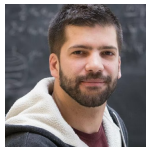


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- ▶ Find out more at: julialang.org.

What is PastaQ?

Pasta

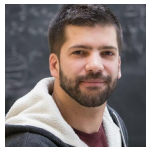
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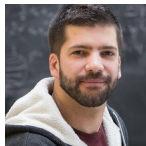


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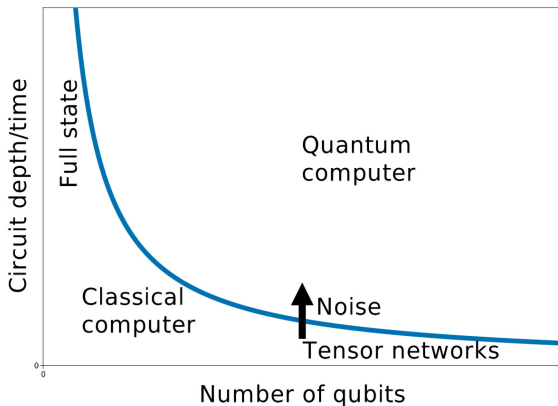
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- ▶ Find out more: github.com/GTorlai/PastaQ.jl

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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- ▶ Good for many sites or qubits but limited to shorter times/circuit depths (though better with noise).

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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

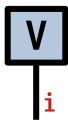


Tensor T_{ijk}
Order-3 tensor



What are tensor networks?

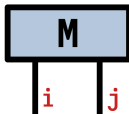
Vector V_i
Order-1 tensor



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



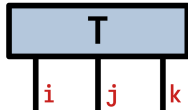
Matrix M_{ij}
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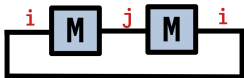
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$$\langle V|V \rangle = V_i V_i$$



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



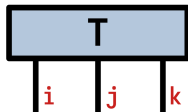
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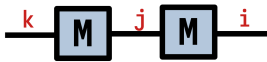
$$M|V \rangle = M_{ji} V_i$$



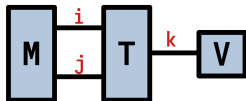
Tensor T_{ijk}
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$$MM = M_{kj} M_{ji}$$



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



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1 $ julia
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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)

Tutorial: One-site state basics

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3 i = Index(2)
4
5
```



Tutorial: One-site state basics

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

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

i

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

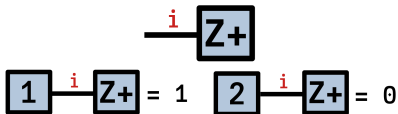
Construct from a Vector

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```

i



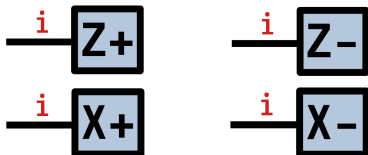
Tutorial: One-site state basics

```
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)
```

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

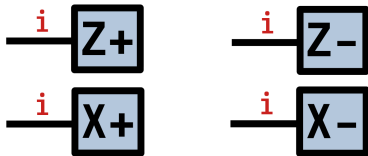
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```



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

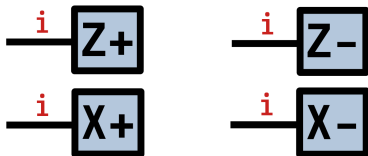
$$|X+\rangle = (|Z+\rangle + |Z-\rangle)/\sqrt{2}$$

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

Tutorial: One-site state basics

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2 Zm=ITensor([0,1],i)
3 Xp=ITensor([1,1]/√2,i)
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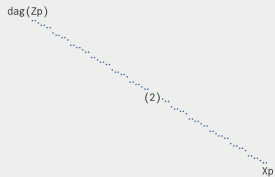
$$X_+ = \frac{Z_+ + Z_-}{\sqrt{2}}$$

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

Tutorial: One-site state basics

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

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



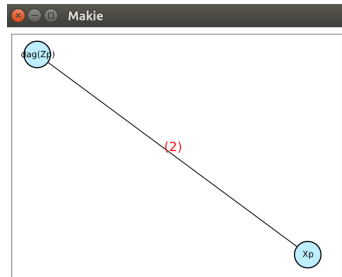
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```
1 using ITensorGLMakie
2
3 @visualize dag(Zp) * Xp
```



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
```

i \neq 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
```

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

$$\begin{array}{c} \underline{i} \\ \text{prime}(\underline{i}) = \underline{i'} \\ \underline{i} \neq \underline{i'} \end{array}$$

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

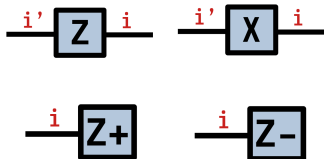
X

$|Z+\rangle$

$|Z-\rangle$

Tutorial: One-site operators

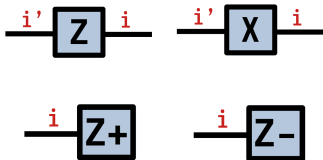
```
1  Z = op("Z", i)
2  X = op("X", i)
3
4  Zp = state("Zp", i)
5  Zm = state("Zm", i)
```



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
```

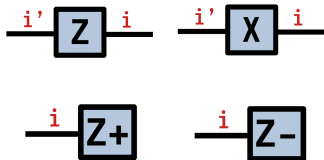


$$X|Z+\rangle = |Z-\rangle$$

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
```



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

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
```

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

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
```

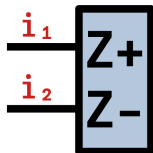
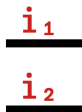
(dim=2|id=505|“S=1/2”)

(dim=2|id=576|“S=1/2”)

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

Tutorial: Two-site states

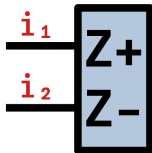
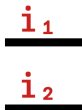
```
1 i1 = Index(2, "S=1/2,i1")
2 i2 = Index(2, "S=1/2,i2")
3
4 i1 != i2
5
6 ZpZm = ITensor(i1, i2)
7 ZpZm[i1=>1, i2=>2] = 1
```



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
```



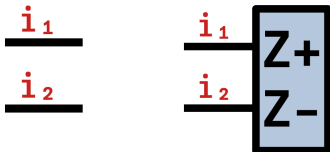
$$|Z+\rangle_1$$
$$|Z+\rangle_2$$

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

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

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

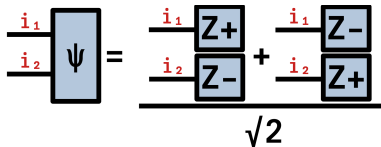
```
1   $\psi$  = ITensor(i1, i2)
2   $\psi[i1=>1, i2=>2]$  = 1/ $\sqrt{2}$ 
3   $\psi[i1=>2, i2=>1]$  = 1/ $\sqrt{2}$ 
4
5   $\psi$  = (Zp1 * Zm2 +
6        Zm1 * Zp2)/ $\sqrt{2}$ 
```

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

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

$$\psi = \frac{Z+ + Z-}{\sqrt{2}}$$

$$\text{svd}(Z+Z-) = U S V$$
$$S = \begin{bmatrix} 1 & 0 \end{bmatrix}$$

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

$$\psi = \frac{\psi_{i1 i2}^{\text{Z+}} + \psi_{i1 i2}^{\text{Z-}}}{\sqrt{2}}$$

$$\text{svd}(\text{ZpZm}) = \text{U} \text{S} \text{V}$$
$$\text{S} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

$$\text{svd}(\psi) = \text{U} \text{S} \text{V}$$
$$\text{S} = \begin{bmatrix} 1/\sqrt{2} & 0 \\ 0 & 1/\sqrt{2} \end{bmatrix}$$

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

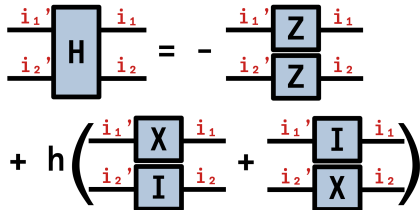
```
1 H = ITensor(i1', i2',  
2             i1, i2)  
3 H[i1'=>2, i2'=>1,  
4   i1=>2, i2=>1] = -1  
5 # ...
```

```
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 ($n = 2$)

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



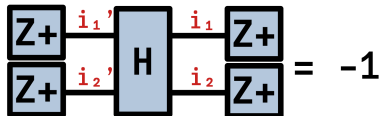
Tutorial: Two-site operators

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

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

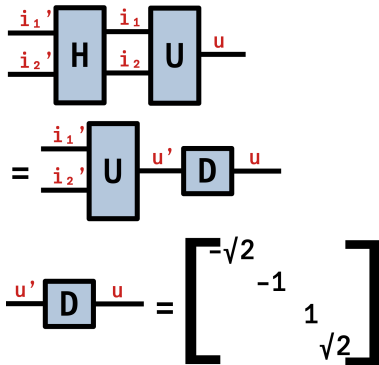
Tutorial: Two-site operators

```
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

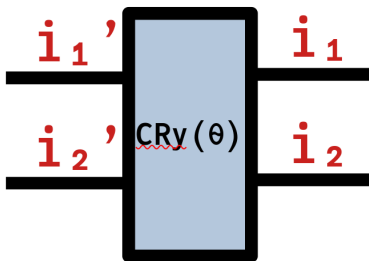
```
1 import ITensors: op
2
3 function op(
4     ::OpName"CRy",
5     ::SiteType"S=1/2";  $\theta$ )
6     c = cos( $\theta/2$ )
7     s = sin( $\theta/2$ )
8     return [
9         1 0 0 0
10        0 1 0 0
11        0 0 c -s
12        0 0 s  c]
13 end
```

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
```



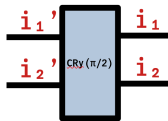
Tutorial: Custom two-site operators

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

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

Tutorial: Custom two-site operators

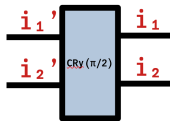
```
1 CRy = op("CRy", i1, i2;  $\theta=\pi/2$ )
```



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
```

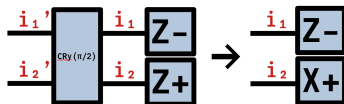
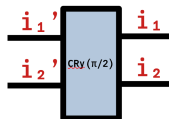


$$\text{CRy}(\pi/2)|Z-Z+\rangle = |Z-X+\rangle$$

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
```

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

Tutorial: Two-site state optimization

```
1 function E( $\psi$ )
2    $\psi H \psi$  = inner( $\psi'$ , H,  $\psi$ )
3    $\psi \psi$  = 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   end
6   return x
7 end
```

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

Gradient descent.

$f(x)$: function to minimize.

$\partial f(x)$: gradient of f .

γ : step size.

Tutorial: Two-site state optimization

```
1 function E( $\psi$ )
2    $\psi H \psi$  = inner( $\psi'$ , H,  $\psi$ )
3    $\psi \psi$  = 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   end
6   return x
7 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       $Z_{m1} * Z_{n2})/\sqrt{2}$   
3  
4   $E(\psi_0) == -1$   
5  
6  using Zygote # autodiff  
7  
8   $\partial E(\psi) = \text{gradient}(E, \psi)[1]$   
9   $\text{norm}(\partial E(\psi_0)) == 2$ 
```

$$E(\psi) = \frac{\text{Diagram 1}}{\text{Diagram 2}}$$

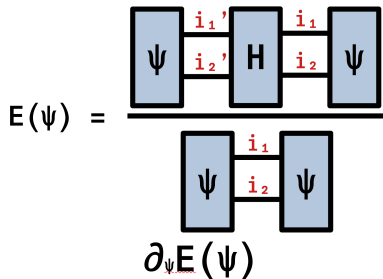
Diagram 1 (Numerator): A quantum circuit diagram representing the expectation value $E(\psi)$. It consists of three blue rectangular blocks labeled ψ , H , and ψ connected sequentially. The first ψ block has two red input lines labeled i_1' and i_2' . The H block has two red input lines labeled i_1 and i_2 . The second ψ block has two red output lines labeled i_1 and i_2 .

Diagram 2 (Denominator): A quantum circuit diagram representing the partial derivative $\partial_\psi E(\psi)$. It consists of two blue rectangular blocks labeled ψ connected sequentially. The first ψ block has two red input lines labeled i_1 and i_2 . The second ψ block has two red output lines labeled i_1 and i_2 .

Tutorial: Two-site state optimization

```
1   $\psi_0 = (\text{Zp1} * \text{Zp2} +$   
2       $\text{Zm1} * \text{Zn2})/\sqrt{2}$   
3  
4   $E(\psi_0) == -1$   
5  
6  using Zygote # autodiff  
7  
8   $\partial E(\psi) = \text{gradient}(E, \psi)[1]$   
9   $\text{norm}(\partial E(\psi_0)) == 2$ 
```

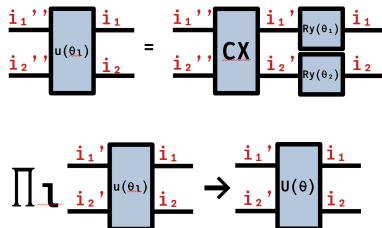
```
1   $\psi = \text{minimize}(E, \partial E, \psi_0;$   
2       $\text{nsteps}=10, \gamma=0.1)$   
3  
4   $E(\psi_0) == -1$   
5   $E(\psi) == -1.4142131 \approx -\sqrt{2}$   
6
```



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

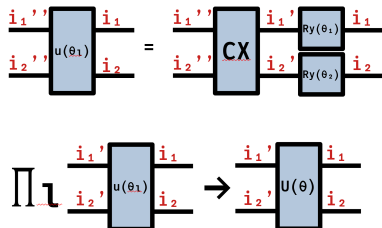
Tutorial: Two-site circuit optimization

```
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
11
```



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
10 U(θ, i1, i2) =
11     buildcircuit(u(θ), [i1, i2
12                     ])
```



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( $\psi_\theta$  ', H,  $\psi_\theta$ )
7  end
```

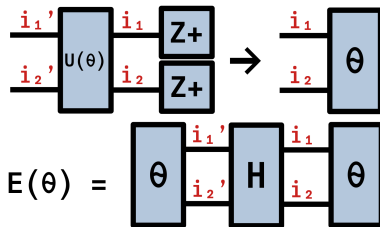
References state:

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

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

Tutorial: Two-site circuit optimization

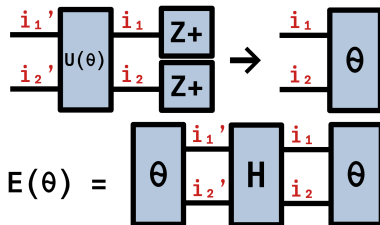
```
1  $\psi_0 = Z_{p1} * Z_{p2}$ 
2
3
4 function E( $\theta$ )
5      $\psi_\theta = \text{apply}(U(\theta, i_1, i_2), \psi_0)$ 
6     return inner( $\psi_\theta'$ , H,  $\psi_\theta$ )
7 end
```



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     nsteps=40,  $\gamma=0.5$ )
5
6  $E(\theta_0) == -1$ 
7  $E(\theta) == -1.4142077 \approx -\sqrt{2}$ 
```



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

Tutorial: Two-site fidelity optimization

```
1   $\psi_0 = Z_{p1} * Z_{p2}$ 
2   $\psi = (Z_p Z_p + Z_m Z_m) / \sqrt{2}$ 
3
4
5
6  function F( $\theta$ )
7       $\psi_\theta = \text{apply}(U(\theta, i1, i2), \psi$ 
8           $\theta)$ 
9      return  $-\text{abs}(\text{inner}(\psi, \psi_\theta))$ 
10         ^2
11 end
```

Reference state:

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

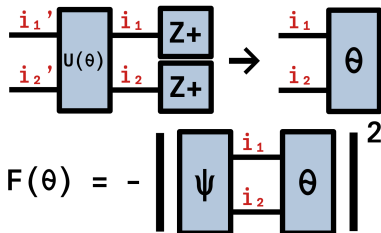
Target state:

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

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

Tutorial: Two-site fidelity optimization

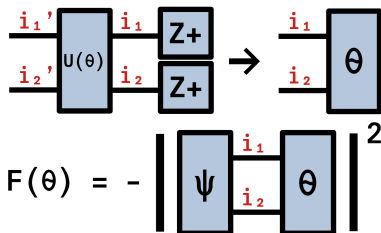
```
1  $\psi_0 = Z_{p1} * Z_{p2}$ 
2  $\psi = (Z_p Z_p + Z_m Z_m) / \sqrt{2}$ 
3
4
5
6 function F( $\theta$ )
7    $\psi_\theta = \text{apply}(U(\theta, i_1, i_2), \psi, \theta)$ 
8   return  $-\text{abs}(\text{inner}(\psi, \psi_\theta))^2$ 
9 end
```



Tutorial: Two-site fidelity optimization

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

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



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

Tutorial: n-site states with MPS

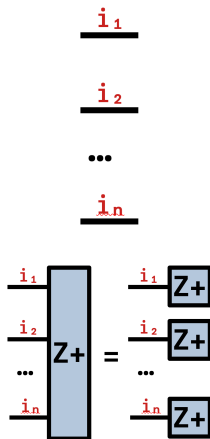
```
1  n = 30
2  i = [Index(2, "S=1/2")
3      for j
4        in 1:n]
5
6  Zp = MPS(i, "Zp")
7
8  maxlinkdim(Zp) == 1 #
   product state
```

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
4      in 1:n]
5
6  Zp = MPS(i, "Zp")
7
8  maxlinkdim(Zp) == 1 #
   product state
```



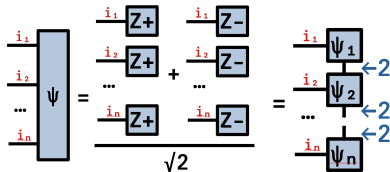
Tutorial: n-site states with MPS

```
1   $\psi = (Zp + Zm)/\sqrt{2}$ 
2
3
4  maxlinkdim( $\psi$ ) == 2 #
    entangled state
```

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

Tutorial: n -site states with MPS

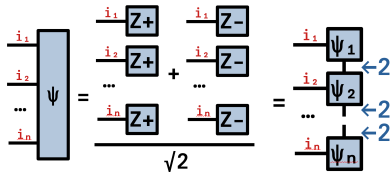
```
1  $\psi = (Z_p + Z_m)/\sqrt{2}$ 
2
3
4 maxlinkdim( $\psi$ ) == 2 #
   entangled state
```



Tutorial: n -site states with MPS

```

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



```

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

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

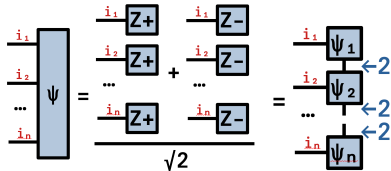
$$\langle Z_+ | \psi \rangle = 1/\sqrt{2}$$

Tutorial: n -site states with MPS

```

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

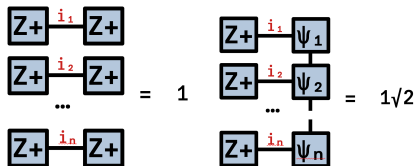
```



```

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

```



Tutorial: n-site states with MPS

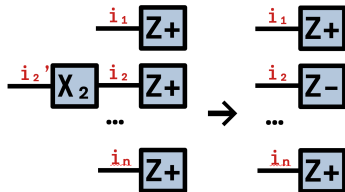
```
1  j = n ÷ 2
2  xj = op("X", i[j])
3
4  xjzp = apply(xj, zp)
5
6
7  state = [k == j ? "Zm" : "Zp"
8           for k
9           in 1:n]
9  xjzp = MPS(i, state)
```

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

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

Tutorial: n -site states with MPS

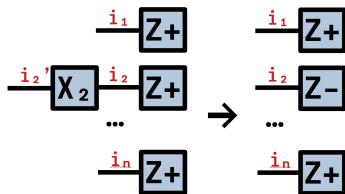
```
1  j = n ÷ 2
2  Xj = op("X", i[j])
3
4  XjZp = apply(Xj, Zp)
5
6
7  state = [k == j ? "Zm" : "Zp"
8           for k
9           in 1:n]
9  XjZp = MPS(i, state)
```



Tutorial: n -site states with MPS

```
1  j = n ÷ 2
2   $x_j = \text{op}(\text{"X"}, i[j])$ 
3
4   $x_j Z_p = \text{apply}(x_j, Z_p)$ 
5
6
7  state = [k == j ? "Zm" : "Zp"
8           for k
9           in 1:n]
10  $x_j Z_p = \text{MPS}(i, \text{state})$ 
```

```
1  maxlinkdim( $x_j Z_p$ ) == 1
2  inner( $Z_p, x_j Z_p$ ) == 0
```



Tutorial: n -site operators with MPO

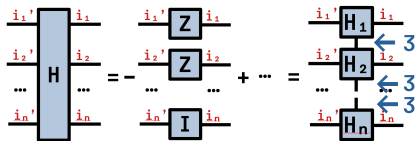
```
1 function ising(n; h)
2   H = OpSum()
3   for j in 1:(n - 1)
4     H -= "Z", j, "Z", j + 1
5   end
6   for j in 1:n
7     H += h, "X", j
8   end
9   return H
10 end
11
12 h = 0.5 # field
13 H = MPO(ising(n; h), i)
14 maxlinkdim(H) == 3
```

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

```

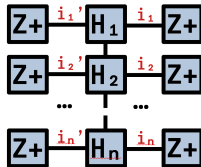
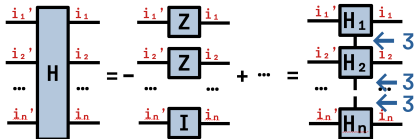
1  function ising(n; h)
2      H = OpSum()
3      for j in 1:(n - 1)
4          H -= "Z", j, "Z", j + 1
5      end
6      for j in 1:n
7          H += h, "X", j
8      end
9      return H
10 end
11
12 h = 0.5 # field
13 H = MPO(ising(n; h), i)
14 maxlinkdim(H) == 3

```

```

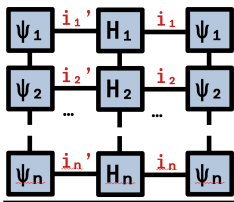
1  Zp = MPS(i, "Zp")
2  inner(Zp', H, Zp) == -(n-1)
3

```



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
```

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


Tutorial: n -site state optimization

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

```
1  $\psi_0$  = MPS(i, "Zp")
2
3  $\psi$  = minimize(E,  $\partial E$ ,  $\psi_0$ ;
4           nsteps=50,  $\gamma$ =0.1,
5           maxdim=10, cutoff=1e-
6           5)
7
8  $E_{dmrg}$ ,  $\psi_{dmrg}$  = dmrg(H,  $\psi_0$ ;
9           nsweeps=10,
10          maxdim=10, cutoff=1e-
11          5)
```

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

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

Tutorial: n -site state optimization

```

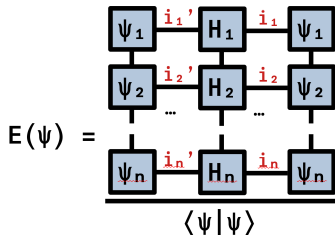
1 function E( $\psi$ )
2    $\psi H \psi = \text{inner}(\psi', H, \psi)$ 
3    $\psi \psi = \text{inner}(\psi, \psi)$ 
4   return  $\psi H \psi / \psi \psi$ 
5 end

```

```

1  $\psi_0 = \text{MPS}(i, \text{"Zp"})$ 
2
3  $\psi = \text{minimize}(E, \partial E, \psi_0;$ 
4    $\text{nsteps}=50, \gamma=0.1,$ 
5    $\text{maxdim}=10, \text{cutoff}=1e-$ 
6    $5)$ 
7  $E_{\text{dmrg}}, \psi_{\text{dmrg}} = \text{dmrg}(H, \psi_0;$ 
8    $\text{nsweeps}=10,$ 
9    $\text{maxdim}=10, \text{cutoff}=1e-$ 
10   $5)$ 

```



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

```

1 maxlinkdim( $\psi_0$ ) == 1
2 maxlinkdim( $\psi$ ) == 3
3 maxlinkdim( $\psi_{\text{dmrg}}$ ) == 3
4  $E(\psi_0) == -29$ 
5  $E(\psi) == -31.0317917$ 
6  $E(\psi_{\text{dmrg}}) == -31.0356110$ 

```

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)]
```

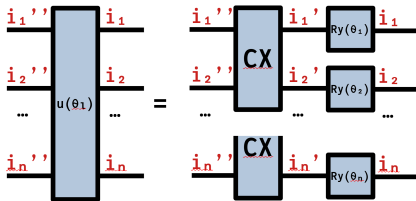
```
1 function U( $\theta$ , i; nlayers)
2     n = length(i)
3     for l in 1:(nlayers - 1)
4          $\theta_l$  =  $\theta[(1:n) .+ l * n]$ 
5          $U_\theta$  = [ $U_\theta$ ; Ry_layer( $\theta_l$ , i)
6             ]
7          $U_\theta$  = [ $U_\theta$ ; CX_layer(i)]
8     end
9     return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

$$U(\theta) = \text{Ry}_1(\theta_1) \dots \text{Ry}_n(\theta_n) \\ * \text{CX}_{1,2} \dots \text{CX}_{n-1,n} \\ * \text{Ry}_1(\theta_{n+1}) \dots \text{Ry}_n(\theta_{2n}) \\ *$$

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   for l in 1:(nlayers - 1)
4      $\theta_l$  =  $\theta[(1:n) .+ l * n]$ 
5      $U_\theta$  = [ $U_\theta$ ; Ry_layer( $\theta_l$ , i)
6           ]
7      $U_\theta$  = [ $U_\theta$ ; CX_layer(i)]
8   end
9   return  $U_\theta$ 
end
```



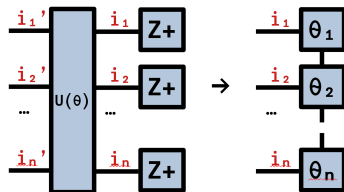
$$\prod_l U(\theta_l) \rightarrow U(\theta)$$

Tutorial: n -site states with MPS

```

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

```



$$E(\theta) =$$

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

Tutorial: n -site states with MPS

```

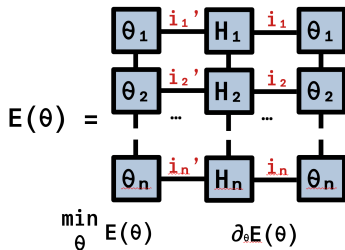
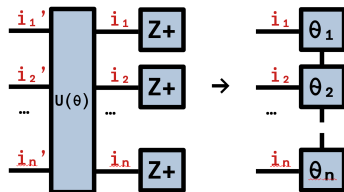
1   $\psi_0$  = MPS(i, "Zp")
2  nlayers = 6
3  function E( $\theta$ )
4       $\psi_\theta$  = apply(U( $\theta$ , i; nlayers),
                     $\psi_0$ )
5      return inner( $\psi_\theta$ ', H,  $\psi_\theta$ )
6  end
7
8   $\theta_0$  = zeros(nlayers * n)
9   $\theta$  = minimize(E,  $\partial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

```

```

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

```

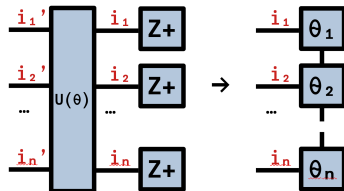


Tutorial: n -site states with MPS

```

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 -abs(inner( $\psi'$ ,  $\psi_\theta$ ))^2
6  end
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8   $\theta_0$  = zeros(nlayers * n)
9   $\theta$  = minimize(F,  $\partial F$ ,  $\theta_0$ ;
10               nsteps=20,  $\gamma=0.1$ )

```



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

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

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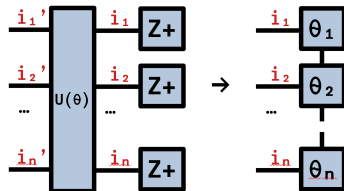
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```

```

1  maxlinkdim( $\psi_0$ ) == 1
2  maxlinkdim( $\psi_\theta$ ) == 2
3  F( $\theta_0$ ) == -0.556066
4  F( $\theta$ ) == -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.

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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!