

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

March 30, 2022

Who am I?

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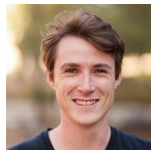
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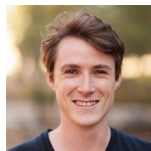
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- ▶ We are hiring postdocs, full-time scientists, part-time and full-time software developers, interns, etc.

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SIMONS FOUNDATION

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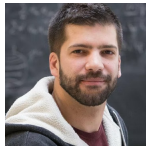


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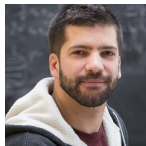
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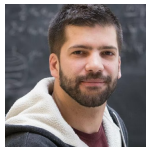


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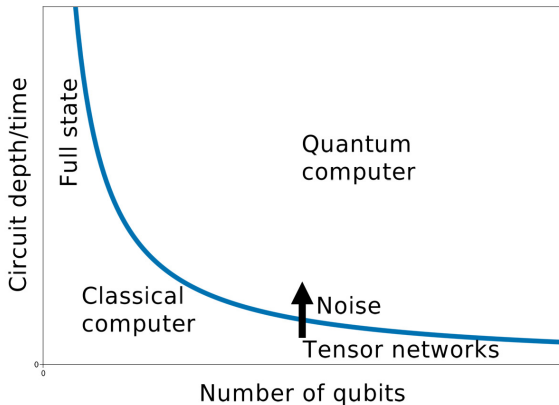


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- ▶ Find out more: github.com/GTorlai/PastaQ.jl



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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 - ▶ 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

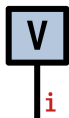


Tensor T_{ijk}
Order-3 tensor



What are tensor networks?

Vector V_i
Order-1 tensor



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



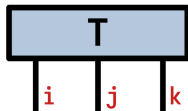
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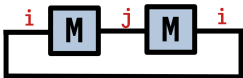
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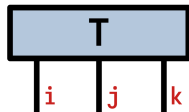
Matrix M_{ij}
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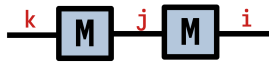
$$M|V \rangle = M_{ji} V_i$$



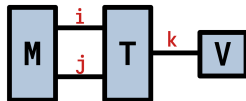
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$$MM = M_{kj} M_{ji}$$



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



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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

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

i

Tutorial: One-site state basics

```
1 using ITensors
2
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

Tutorial: One-site state basics

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```
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```

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```

i

$$\boxed{1} \overset{i}{-} \boxed{Z+} = 1 \quad \boxed{2} \overset{i}{-} \boxed{Z+} = 0$$

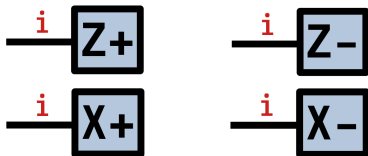
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```
1 Zp = ITensor([1, 0], i)
2 Zm = ITensor([0, 1], i)
3 Xp = ITensor([1, 1]/√2, i)
4 Xm = ITensor([1, -1]/√2, i)
```

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

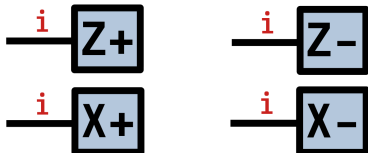
Tutorial: One-site state basics

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1 Zp = ITensor([1, 0], i)
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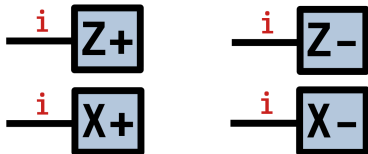
```
1 Xp = (Zp + Zm)/√2
2
3
4
5 dag(Zp) * Xp
6 inner(Zp, Xp)
```

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

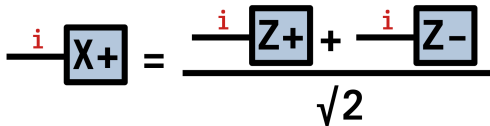
$$\langle Z+ | X+\rangle \approx 1/\sqrt{2}$$

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2 Zm = ITensor([0, 1], i)
3 Xp = ITensor([1, 1]/√2, i)
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```
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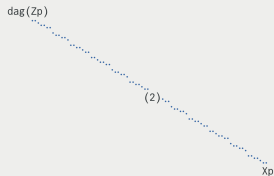
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6 inner(Zp, Xp)
```



Tutorial: One-site state basics

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

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



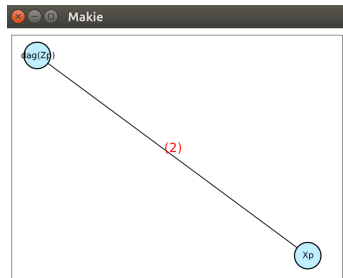
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```
1 using ITensorGLMakie
2
3 @visualize dag(Zp) * Xp
```



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")
```

```
2
```

```
3
```

```
4
```

```
5
```

```
6
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7
```

```
8
```

```
9
```

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

"S=1/2" defines an operator basis

Additionally:

"Qubit", "Qudit",

"Electron", ...

```
1 Zp = state("Z+", i)
```

```
2 Zm = state("Z-", i)
```

```
3 Xp = state("X+", i)
```

```
4 Xm = state("X-", 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 "iX-",
6     ::SiteType "S=1/2"
7 )
8     return [im -im]/√2
9 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 "iX-",
6     ::SiteType "S=1/2"
7 )
8     return [im -im]/√2
9 end
```

Overload ITensors.jl
behavior

Define a state with the
name “iX-”

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

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

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

Tutorial: Custom one-site states

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

Overload ITensors.jl
behavior

Define a state with the
name “iX-”

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

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

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 ≠ j

Tutorial: Priming

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

i ≠ j

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

(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 Z = ITensor(i', i)
2 Z[i'=>1, i=>1] = 1
3 Z[i'=>2, i=>2] = -1
```

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

Tutorial: One-site operators

```
1  Z = ITensor(i', i)
2  Z[i'=>1, i=>1] = 1
3  Z[i'=>2, i=>2] = -1
```



Tutorial: One-site operators

```
1 Z = ITensor(i', i)
2 Z[i'=>1, i=>1] = 1
3 Z[i'=>2, i=>2] = -1
```



```
1 z = [
2     1 0
3     0 -1
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("Z+", i)
```

```
5  Zm = state("Z-", i)
```

Z

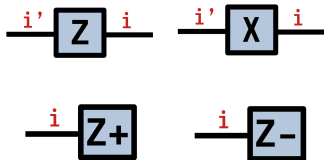
X

$|Z+\rangle$

$|Z-\rangle$

Tutorial: One-site operators

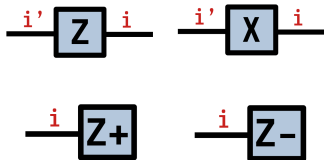
```
1 Z = op("Z", i)
2 X = op("X", i)
3
4 Zp = state("Z+", i)
5 Zm = state("Z-", i)
```



Tutorial: One-site operators

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

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

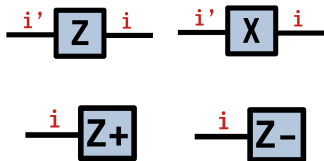


$$X|Z+\rangle = |Z-\rangle$$

Tutorial: One-site operators

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

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



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

```
1  import ITensors: op
2
3  function op(
4      ::OpName"iX",
5      ::SiteType"S=1/2"
6  )
7      return [
8          0 im
9          im 0
10     ]
11  end
```

Overload ITensors.jl
behavior

Tutorial: Custom one-site operators

```
1  import ITensors: op
2
3  function op(
4      ::OpName"iX",
5      ::SiteType"S=1/2"
6  )
7      return [
8          0 im
9          im 0
10     ]
11  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 )
7     return [
8         0 im
9         im 0
10    ]
11 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 )
7     return [
8         0 im
9         im 0
10    ]
11 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

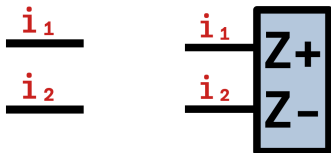
```
1 i1 = Index(2, "S=1/2")
2 i2 = Index(2, "S=1/2")
3
4 i1 ≠ i2
5
6 ZpZm = ITensor(i1, i2)
7 ZpZm[i1=>1, i2=>2] = 1
```

(dim=2|id=505|“S=1/2”)
(dim=2|id=576|“S=1/2”)

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

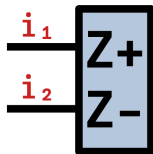
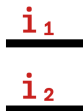
Tutorial: Two-site states

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



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

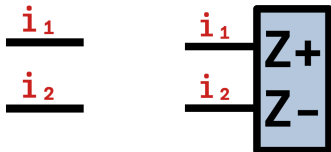
$$|Z+\rangle_1$$
$$|Z+\rangle_2$$

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

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

Tutorial: Two-site states

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



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



Tutorial: Two-site states

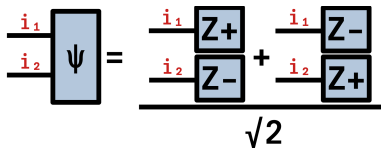
```
1   $\psi = \text{ITensor}(i1, i2)$ 
2   $\psi[i1=>1, i2=>2] = 1/\sqrt{2}$ 
3   $\psi[i1=>2, i2=>1] = 1/\sqrt{2}$ 
4
5   $\psi = (Z_{p1} * Z_{m2} +$ 
6       $Z_{m1} * Z_{p2})/\sqrt{2}$ 
```

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

From single-site states

Tutorial: Two-site states

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

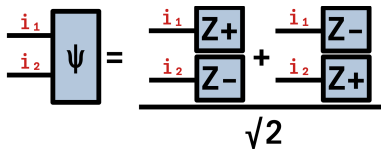


Tutorial: Two-site states

```

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

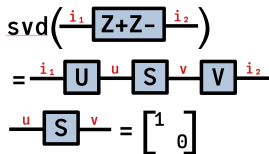
```



```

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

```



Tutorial: Two-site states

```

1   $\psi = \text{ITensor}(i1, i2)$ 
2   $\psi[i1=>1, i2=>2] = 1/\sqrt{2}$ 
3   $\psi[i1=>2, i2=>1] = 1/\sqrt{2}$ 
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   $\text{U}, \text{S}, \text{V} = \text{svd}(\text{ZmZp}, i1)$ 
5   $\text{diag}(\text{S}) == [1, 0]$ 
6
7   $\text{U}, \text{S}, \text{V} = \text{svd}(\psi, i1)$ 
8   $\text{diag}(\text{S}) == [1/\sqrt{2}, 1/\sqrt{2}]$ 

```

$$\psi = \frac{\begin{matrix} i_1 \\ i_2 \end{matrix} \left[\begin{matrix} \text{Z+} \\ \text{Z-} \end{matrix} \right] + \begin{matrix} i_1 \\ i_2 \end{matrix} \left[\begin{matrix} \text{Z-} \\ \text{Z+} \end{matrix} \right]}{\sqrt{2}}$$

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

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

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

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

Tutorial: Two-site operators

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

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

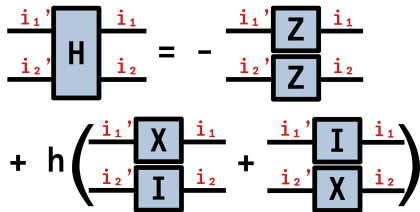
```
1 H = ITensor(i1', i2', i1, i2)
2 H[i1'=>2, i2'=>1,
3   i1=>2, i2=>1] = -1
4 # ...
```

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

Make a Hamiltonian:

Transverse field Ising ($n = 2$)

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



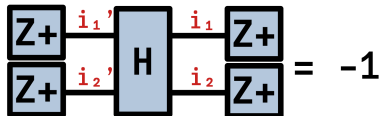
Tutorial: Two-site operators

$$1 \quad \text{inner}(\mathbf{Z}_p' * \mathbf{Z}_p', \mathbf{H}, \mathbf{Z}_p * \mathbf{Z}_p)$$

$$\langle \mathbf{Z} + \mathbf{Z} + | \mathbf{H} | \mathbf{Z} + \mathbf{Z} + \rangle$$

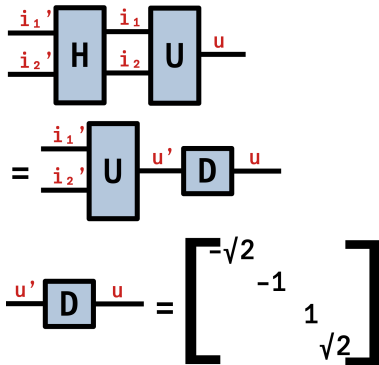
Tutorial: Two-site operators

$$1 \quad \text{inner}(Z_p' * Z_p', H, Z_p * Z_p)$$



Tutorial: Two-site operators

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



Tutorial: Custom two-site operators

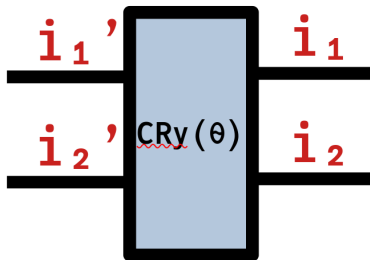
```
1 import ITensors: op
2
3 function op(
4     ::OpName"CRy",
5     ::SiteType"S=1/2";
6      $\theta$ 
7 )
8     c = cos( $\theta/2$ )
9     s = sin( $\theta/2$ )
10    return [
11        1 0 0 0
12        0 1 0 0
13        0 0 c -s
14        0 0 s  c
15    ]
16 end
```

Controlled-Ry (CRy)
rotation gate

CRy(θ)

Tutorial: Custom two-site operators

```
1  import ITensors: op
2
3  function op(
4      ::OpName"CRy",
5      ::SiteType"S=1/2";
6       $\theta$ 
7  )
8      c = cos( $\theta/2$ )
9      s = sin( $\theta/2$ )
10     return [
11         1 0 0 0
12         0 1 0 0
13         0 0 c -s
14         0 0 s  c
15     ]
16 end
```



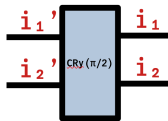
Tutorial: Custom two-site operators

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

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

Tutorial: Custom two-site operators

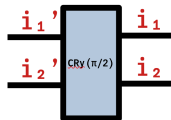
```
1 CRy = op("CRy", i1, i2;  $\theta=\pi/2$ )
```



Tutorial: Custom two-site operators

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

```
1 apply(CRy, Zm1 * Zp2) ==  
2     Zm1 * Xp2
```

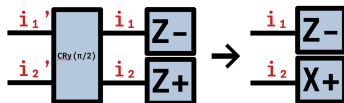
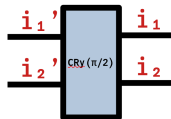


$$\text{CRy}(\pi/2)|Z-Z+\rangle = |Z-X+\rangle$$

Tutorial: Custom two-site operators

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

```
1 apply(CRy, Zm1 * Zp2) ==  
2      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    $\psi H \psi = \text{inner}(\psi', H, \psi)$ 
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   end
6   return x
7 end
```

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

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

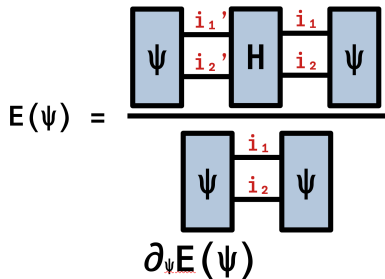
```
1 function minimize(f,  $\partial f$ , x;
2   nsteps,  $\gamma$ )
3   for n in 1:nsteps
4      $x = x - \gamma * \partial f(x)$ 
5   end
6   return x
7 end
```

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

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

Tutorial: Two-site state optimization

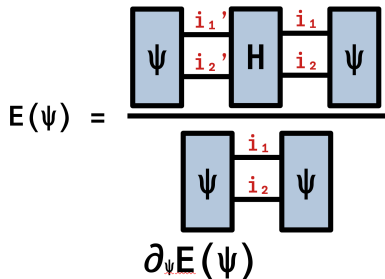
```
1  $\psi_0 = (Z_{p1} * Z_{m2} +$   
2  $Z_{m1} * Z_{p2})/\sqrt{2}$   
3  
4  $E(\psi_0) == -1$   
5  
6 using Zygote # autodiff  
7  
8  $\partial E(\psi) = \text{gradient}(E, \psi)[1]$   
9  $\text{norm}(\partial E(\psi_0)) == 2$ 
```



Tutorial: Two-site state optimization

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

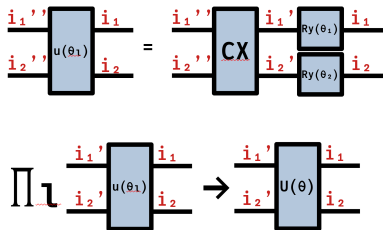
```
1  $\psi = \text{minimize}(E, \partial E, \psi_0;$   
2  $\text{nsteps}=10, \gamma=0.1)$   
3  
4  $E(\psi_0) == -1$   
5  $E(\psi) == -1.4142131 \approx -\sqrt{2}$   
6
```



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

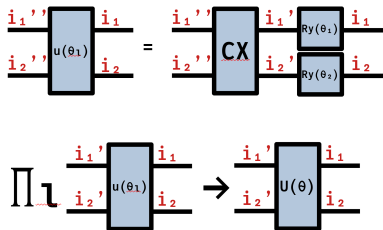
Tutorial: Two-site circuit optimization

```
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])
```



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
```

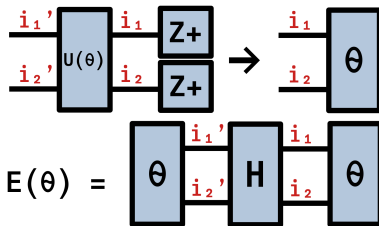
References state:

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

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

Tutorial: Two-site circuit optimization

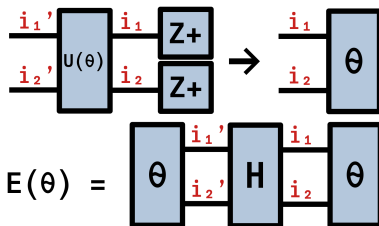
```
1  $\psi_0 = Z_{p1} * Z_{p2}$ 
2
3
4 function E( $\theta$ )
5    $\psi_\theta = \text{apply}(U(\theta, i_1, i_2), \psi_0)$ 
6   return inner( $\psi_\theta'$ , H,  $\psi_\theta$ )
7 end
```



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( $\psi_\theta$ , 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  $E(\theta) == -1.4142077 \approx -\sqrt{2}$ 
```



$$E(\theta) = \text{Tr}(\theta^\dagger H \theta)$$

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

Tutorial: Two-site fidelity optimization

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

Reference state:

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

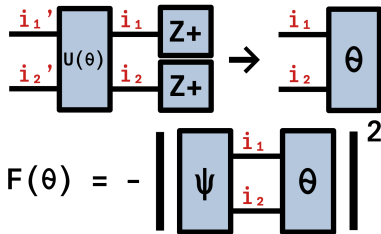
Target state:

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

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

Tutorial: Two-site fidelity optimization

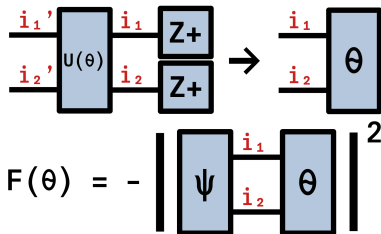
```
1  $\psi_0 = Z_{p1} * Z_{p2}$ 
2  $\psi = (Z_p Z_p + Z_m Z_m) / \sqrt{2}$ 
3
4
5
6 function F( $\theta$ )
7    $\psi_\theta = \text{apply}(U(\theta, i_1, i_2), \psi_0)$ 
8   return  $-\text{abs}(\text{inner}(\psi, \psi_\theta))^2$ 
9 end
```



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    $\psi_\theta = \text{apply}(U(\theta, i_1, i_2), \psi_0)$ 
8   return -abs(inner( $\psi, \psi_\theta$ ))^2
9 end
```

```
1  $\theta_0 = [0, 0, 0, 0]$ 
2  $\partial F(\theta) = \text{gradient}(F, \theta)[1]$ 
3  $\theta = \text{minimize}(F, \partial F, \theta_0;$ 
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

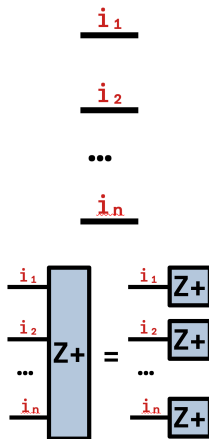
```
1  n = 30
2  i = [Index(2, "S=1/2")
3       for j in 1:n]
4
5
6  Zp = MPS(i, "Z+")
7
8  maxlinkdim(Zp) == 1 #
   product state
```

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



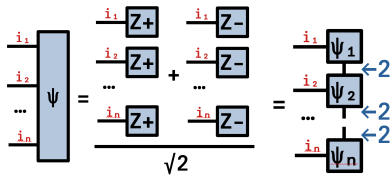
Tutorial: n-site states with MPS

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

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

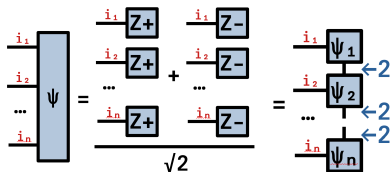
Tutorial: n -site states with MPS

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



Tutorial: n -site states with MPS

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



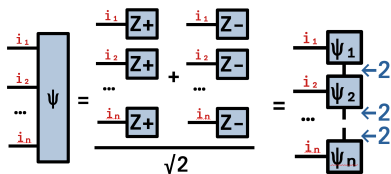
- 1 $\text{inner}(Z_p, Z_p) == 1$
- 2
- 3
- 4 $\text{inner}(Z_p, \psi) == 1/\sqrt{2}$

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

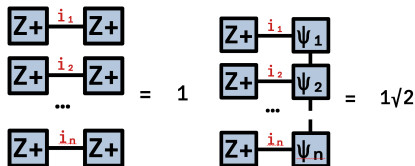
$$\langle Z_+ | \psi \rangle = 1/\sqrt{2}$$

Tutorial: n -site states with MPS

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



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



Tutorial: n -site states with MPS

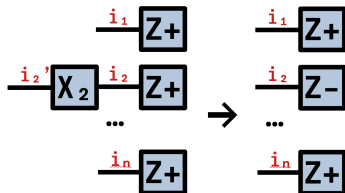
```
1  j = n ÷ 2
2  Xj = op("X", i[j])
3
4  XjZp = apply(Xj, Zp)
5
6
7  state = [k == j ? "Z-" : "Z+"
8           for k in 1:n]
9  XjZp = MPS(i, state)
```

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

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

Tutorial: n -site states with MPS

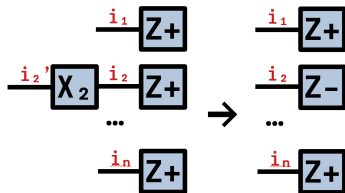
```
1  j = n ÷ 2
2  Xj = op("X", i[j])
3
4  XjZp = apply(Xj, Zp)
5
6
7  state = [k == j ? "Z-" : "Z+"
8           for k in 1:n]
9  XjZp = MPS(i, state)
```



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 ? "Z-" : "Z+"
8           for k in 1:n]
9  XjZp = MPS(i, state)
```

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



Tutorial: n-site operators with MPO

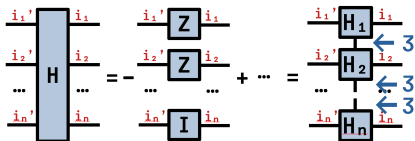
```
1 function ising(n; h)
2   H = OpSum()
3   for j in 1:(n - 1)
4     H -= "Z", j, "Z", j + 1
5   end
6   for j in 1:n
7     H += h, "X", j
8   end
9   return H
10 end
11
12 h = 0.5
13 H = MPO(ising(n; h=h), i)
14 maxlinkdim(H) == 3
```

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
13 H = MPO(ising(n; h=h), i)
14 maxlinkdim(H) == 3
```



Tutorial: n -site operators with MPO

```

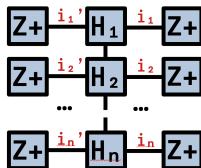
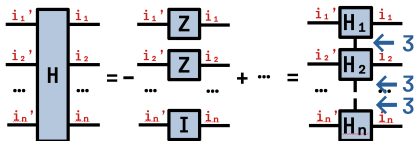
1  function ising(n; h)
2    H = OpSum()
3    for j in 1:(n - 1)
4      H -= "Z", j, "Z", j + 1
5    end
6    for j in 1:n
7      H += h, "X", j
8    end
9    return H
10 end
11
12 h = 0.5
13 H = MPO(ising(n; h=h), i)
14 maxlinkdim(H) == 3

```

```

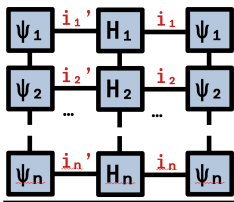
1  Zp = MPS(i, "Z+")
2  inner(Zp', H, Zp) == -(n-1)

```



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

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

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

```

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

```

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)]
```

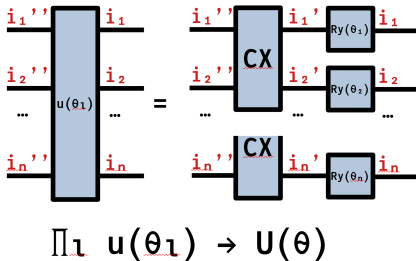
```
1 function U( $\theta$ , i; nlayers)
2   n = length(i)
3   for l in 1:(nlayers - 1)
4      $\theta_l = \theta[(1:n) .+ l * n]$ 
5      $U_\theta = [U_\theta; \text{Ry\_layer}(\theta_l, i)]$ 
6      $U_\theta = [U_\theta; \text{CX\_layer}(i)]$ 
7   end
8   return  $U_\theta$ 
9 end
```

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

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      $U_\theta = [U_\theta; \text{Ry\_layer}(\theta_l, i)]$ 
6      $U_\theta = [U_\theta; \text{CX\_layer}(i)]$ 
7   end
8   return  $U_\theta$ 
9 end
```

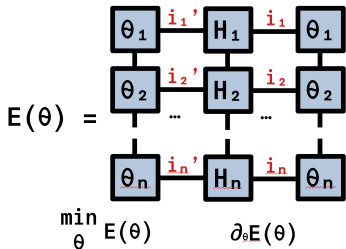
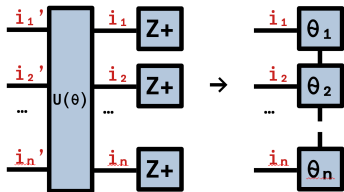


Tutorial: n -site states with MPS

```

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

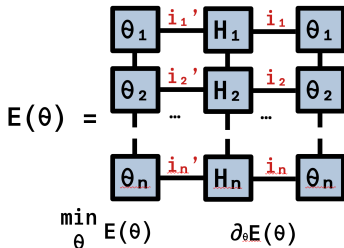
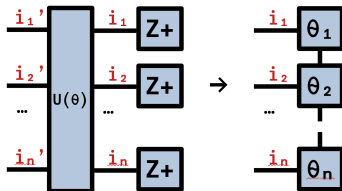
```



Tutorial: n -site states with MPS

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

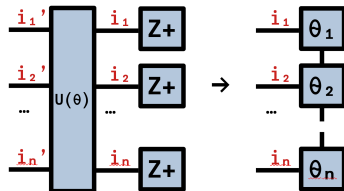
```
1 maxlinkdim( $\psi_0$ ) = 1
2 maxlinkdim( $\psi_\theta$ ) = 3
3  $E(\theta_0) == -29$ 
4  $E(\theta) == -31.017062$ 
```



Tutorial: n -site states with MPS

```

1   $\psi_0 = \text{MPS}(i, \text{"Z+"})$ 
2  nlayers = 6
3  function F( $\theta$ )
4     $\psi_\theta = \text{apply}(U(\theta, i; \text{nlayers}), \psi_0)$ 
5    return  $-\text{abs}(\text{inner}(\psi', \psi_\theta))^2$ 
6  end
7
8   $\theta_0 = \text{zeros}(\text{nlayers} * n)$ 
9   $\theta = \text{minimize}(F, \partial F, \theta_0;$ 
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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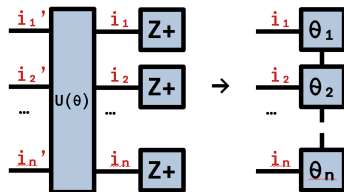
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3  function F( $\theta$ )
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5    return -abs(inner( $\psi'$ ,  $\psi_\theta$ ))2
6  end
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8   $\theta_0 = \text{zeros}(\text{nlayers} * n)$ 
9   $\theta = \text{minimize}(\text{F}, \partial \text{F}, \theta_0;$ 
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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

```



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

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Other features not mentioned

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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!