

Analyzing Quantum Many-Body Systems with ITensor and PastaQ

Matthew Fishman

Center for Computational Quantum Physics (CCQ)

Flatiron Institute, NY

<https://mtfishman.github.io/>

February 26, 2022



Who am I?

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mtfishman.github.io



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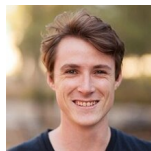
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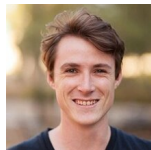
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- ▶ We are hiring postdocs, full-time scientists, part-time and full-time software developers, interns, etc.

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SIMONS FOUNDATION

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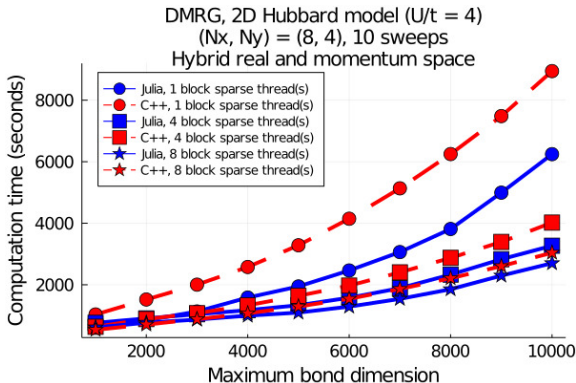
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- ▶ Great numerical libraries, code ended up faster.



What is PastaQ?

Pasta

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What is PastaQ?

Pasta

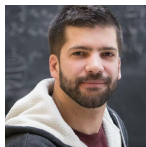
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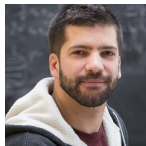
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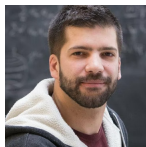
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- ▶ Find out more: github.com/GTorlai/PastaQ.jl



When should I use tensor networks?

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

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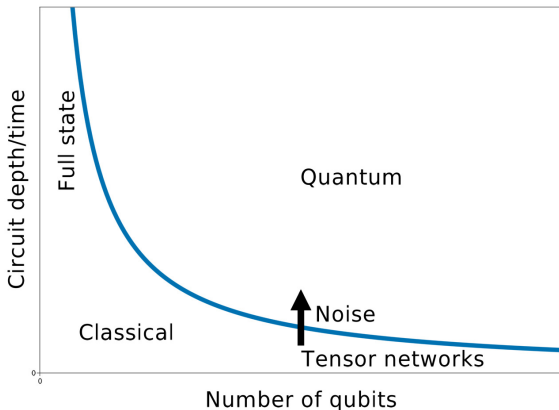
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- ▶ Tensor networks are a common, general language for reasoning about quantum many-body systems (for example, quantum circuits).

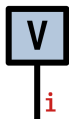
When should I use tensor networks?

- ▶ In my opinion, tensor networks are the best general purpose tool we have right now for studying quantum many-body systems (while we wait for a general purpose quantum computer).

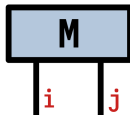


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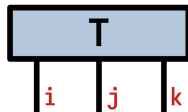
Vector V_i
Order-1 tensor



Matrix M_{ij}
Order-2 tensor

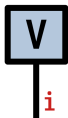


Tensor T_{ijk}
Order-3 tensor



What are tensor networks?

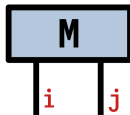
Vector V_i
Order-1 tensor



Vector inner
product



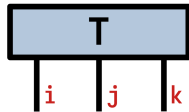
Matrix M_{ij}
Order-2 tensor



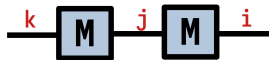
Matrix-vector
multiplication



Tensor T_{ijk}
Order-3 tensor



Matrix-matrix
multiplication

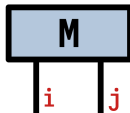


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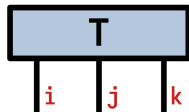
Vector V_i
Order-1 tensor



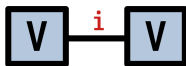
Matrix M_{ij}
Order-2 tensor



Tensor T_{ijk}
Order-3 tensor



Vector inner
product



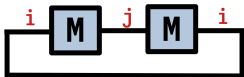
Matrix-vector
multiplication



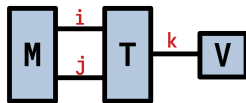
Matrix-matrix
multiplication



Trace of matrix-matrix
multiplication



General tensor
network



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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);
6
7 julia> using PastaQ
8
9 julia> gates = [("X", 1), ("CX", (1, 3))];
10
11 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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```

i

Tutorial: One-site state basics

```
1 using ITensors
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```

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

i

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

Construct from a Vector

Tutorial: One-site state basics

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```

```
2
```

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```

```
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```

```
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```
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```

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```

i

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

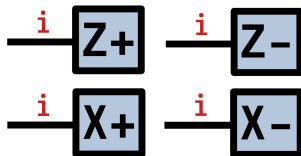
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2 Zm = ITensor([0, 1], i)
3 Xp = ITensor([1, 1]/√2, i)
4 Xm = ITensor([1, -1]/√2, i)
```

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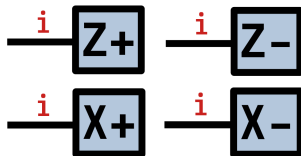
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```

```
1 (Zp + Zm)/√2
2 dag(Zp) * Xp
3 (dag(Zp) * Xp)[]
4 inner(Zp, Xp)
5 norm(Xp)
```

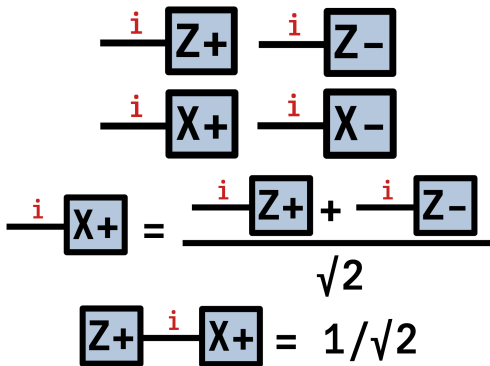


$\approx Xp$
 $\approx \text{ITensor}(1/\sqrt{2})$
 $\approx 1/\sqrt{2}$
 $\approx 1/\sqrt{2}$
 ≈ 1

Tutorial: One-site state basics

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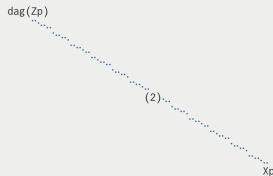
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Tutorial: One-site state basics

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

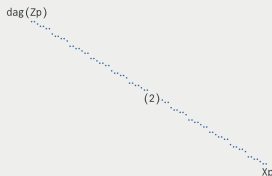
```
julia> @visualize dag(Zp) * Xp
```



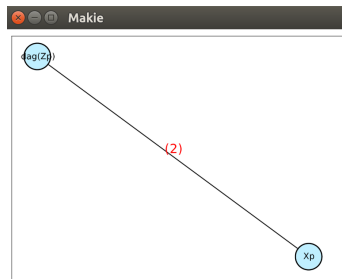
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```
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```



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



Tutorial: One-site states

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

```
2
```

```
3
```

```
4
```

```
5
```

```
6
```

“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
```

“ $S=1/2$ ” 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 (Zp + Zm)/sqrt(2)
4 (Zp - Zm)/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-”

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 inner(Zp, iXm)
4 inner(Zm, iXm)
```

$\approx \text{im} * X_m$

$\approx \text{im}/\sqrt{2}$

$\approx -\text{im}/\sqrt{2}$

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 inner(Zp, iXm)
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)

false

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)
4 i'
5 i ≠ i'
6 noprime(i') == i
```

i ≠ j

(dim=2|id=837)

(dim=2|id=837)'

(dim=2|id=837)'

true

true

Tutorial: Priming

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

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

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

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

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
6 Z = ITensor(z, i', dag(i))
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

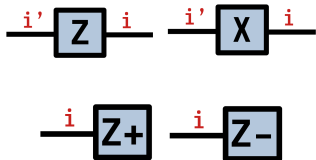
X

$|Z+\rangle$

$|Z-\rangle$

Tutorial: One-site operators

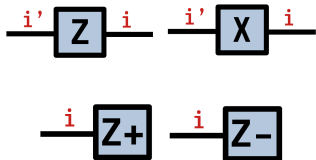
```
1 Z = op("Z", i)
2 X = op("X", i)
3
4 Zp = state("Z+", i)
5 Zm = state("Z-", i)
```



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 XZp = X * Zp
2 XZp == Zm
3 XZp == Zm'
4 noprime(XZp) == Zm
```



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

false

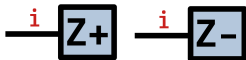
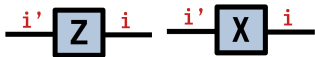
true

true

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 XZp = X * Zp
2 XZp == Zm
3 XZp == Zm'
4 noprime(XZp) == Zm
```



Tutorial: One-site operators

```
1 XZp = X * Zp
2
3 dag(Zm) * XZp
4
5 dag(Zm') * XZp
6 dag(Zp') * XZp
7
8 dag(Zm)' * X * Zp
9 inner(Zm', X, Zp)
```

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

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

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

$$\langle Z+|X|Z+\rangle \approx 0$$

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

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

Tutorial: One-site operators

- 1 $XZ_p = X * Z_p$
- 2
- 3 $\text{dag}(Z_m) * XZ_p$
- 4
- 5 $\text{dag}(Z_m') * XZ_p$
- 6 $\text{dag}(Z_p') * XZ_p$
- 7
- 8 $\text{dag}(Z_m)' * X * Z_p$
- 9 $\text{inner}(Z_m', X, Z_p)$

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

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

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

$$\boxed{Z_+} \overset{i'}{\text{---}} \boxed{X} \overset{i}{\text{---}} \boxed{Z_+} = 0$$

Tutorial: One-site operators

```

1  XZp = X * Zp
2
3  dag(Zm) * XZp
4
5  dag(Zm') * XZp
6  dag(Zp') * XZp
7
8  dag(Zm)' * X * Zp
9  inner(Zm', X, Zp)

```

```

1  XZp = apply(X, Zp)
2  inner(Zm, XZp)

```

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

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

$$\begin{aligned} \boxed{Z_-} \text{---} \overset{i'}{\boxed{X}} \text{---} \overset{i}{\boxed{Z_+}} &= 1 \\ \boxed{Z_+} \text{---} \overset{i'}{\boxed{X}} \text{---} \overset{i}{\boxed{Z_+}} &= 0 \end{aligned}$$

$$\begin{aligned} &= \text{noprime}(X * Zp) \\ &\approx 1 \end{aligned}$$

Tutorial: One-site operators

```

1  XZp = X * Zp
2
3  dag(Zm) * XZp
4
5  dag(Zm') * XZp
6  dag(Zp') * XZp
7
8  dag(Zm)' * X * Zp
9  inner(Zm', X, Zp)

```

```

1  XZp = apply(X, Zp)
2  inner(Zm, XZp)

```

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

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

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

$$\boxed{Z+} \text{---}^{i'} \boxed{X} \text{---}^i \boxed{Z+} = 0$$

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

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
```

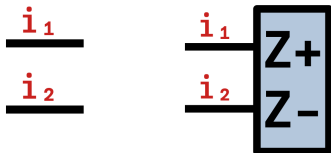
(dim=2|id=505|"S=1/2")
(dim=2|id=576|"S=1/2")

false

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

Tutorial: Two-site states

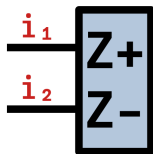
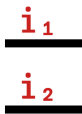
```
1 i1 = Index(2, "S=1/2")
2 i2 = Index(2, "S=1/2")
3
4 i1 == i2
5
6 ZpZm = ITensor(i1, i2)
7 ZpZm[i1=>1, i2=>2] = 1
```



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
8 ZmZp = Zm1 * Zp2
```



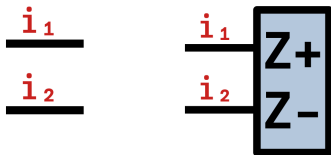
$$|Z+\rangle_1$$
$$|Z+\rangle_2$$

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

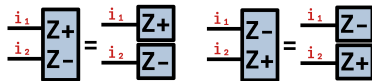
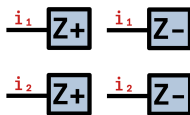
$$|Z+Z-\rangle = |Z+\rangle_1 |Z-\rangle_2$$
$$|Z-Z+\rangle = |Z-\rangle_1 |Z+\rangle_2$$

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
8 ZmZp = Zm1 * Zp2
```



Tutorial: Two-site states

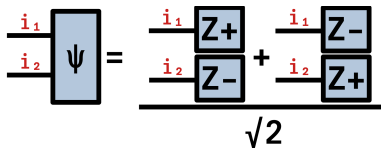
```
1   $\psi = \text{ITensor}(i1, i2)$ 
2   $\psi[i1=>1, i2=>2] = 1/\sqrt{2}$ 
3   $\psi[i1=>2, i2=>1] = 1/\sqrt{2}$ 
4
5   $\psi = (Z_{p1} * Z_{m2} +$ 
6       $Z_{m1} * Z_{p2})/\sqrt{2}$ 
```

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

From single-site states

Tutorial: Two-site states

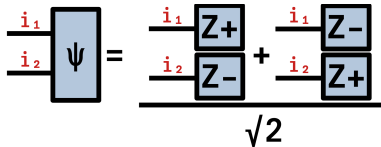
```
1   $\psi = \text{ITensor}(i1, i2)$ 
2   $\psi[i1=>1, i2=>2] = 1/\sqrt{2}$ 
3   $\psi[i1=>2, i2=>1] = 1/\sqrt{2}$ 
4
5   $\psi = (\text{Zp1} * \text{Zm2} +$ 
6          $\text{Zm1} * \text{Zp2})/\sqrt{2}$ 
```



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  $\text{inner}(\psi, \psi)$ 
2  $\text{inner}(\text{ZpZm}, \psi)$ 
3
4  $\text{U}, \text{S}, \text{V} = \text{svd}(\text{ZmZp}, i1)$ 
5  $\text{s} = \text{diag}(\text{S})$ 
6
7  $\text{U}, \text{S}, \text{V} = \text{svd}(\psi, i1)$ 
8  $\text{s} = \text{diag}(\text{S})$ 
```



$$\approx 1$$
$$\approx 1/\sqrt{2}$$

$$\approx [1, 0]$$

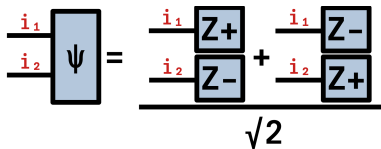
$$\approx [1/\sqrt{2}, 1/\sqrt{2}]$$

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       $\text{Zm1} * \text{Zp2})/\sqrt{2}$ 

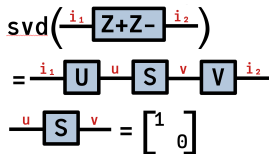
```



```

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

```



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   $\text{inner}(\psi, \psi)$ 
2   $\text{inner}(\text{ZpZm}, \psi)$ 
3
4   $U, S, V = \text{svd}(\text{ZmZp}, i1)$ 
5   $s = \text{diag}(S)$ 
6
7   $U, S, V = \text{svd}(\psi, i1)$ 
8   $s = \text{diag}(S)$ 

```

$$\begin{array}{c} i_1 \\ i_2 \end{array} \left[\Psi \right] = \frac{1}{\sqrt{2}} \left(\begin{array}{c} i_1 \\ i_2 \end{array} \left[\begin{array}{c} Z+ \\ Z- \end{array} \right] + \begin{array}{c} i_1 \\ i_2 \end{array} \left[\begin{array}{c} Z- \\ Z+ \end{array} \right] \right)$$

$$\begin{aligned} & \text{svd} \left(\begin{array}{c} i_1 \\ i_2 \end{array} \left[\begin{array}{c} Z+Z- \\ Z- \\ Z+ \end{array} \right] \right) \\ &= \begin{array}{c} i_1 \\ i_2 \end{array} \left[\begin{array}{c} U \\ S \\ V \end{array} \right] \begin{array}{c} u \\ v \end{array} \left[\begin{array}{c} 1 \\ 0 \end{array} \right] \end{aligned}$$

$$\begin{aligned} & \text{svd} \left(\begin{array}{c} i_1 \\ i_2 \end{array} \left[\Psi \right] \right) \\ &= \begin{array}{c} i_1 \\ i_2 \end{array} \left[\begin{array}{c} U \\ S \\ V \end{array} \right] \begin{array}{c} u \\ v \end{array} \left[\begin{array}{c} 1/\sqrt{2} \\ 1/\sqrt{2} \end{array} \right] \end{aligned}$$

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 # ...
```

Make a Hamiltonian:

Transverse field Ising ($n = 2$)

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

```
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)
```

Alternative:

Build from single-site operators.

(Less error-prone.)

Tutorial: Two-site operators

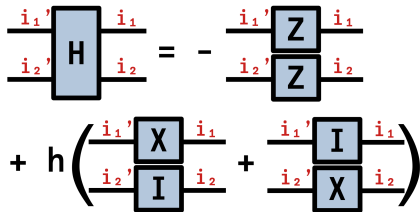
```
1 H = ITensor(i1', i2', i1, i2)
2 H[i1'=>2, i2'=>1,
3   i1=>2, i2=>1] = -1
4 # ...
```

```
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  ZpZp = Zp1 * Zp2
2
3
4
5  (dag(ZpZp)' * H * ZpZp)[]
6  inner(ZpZp', H, ZpZp)
7  inner(ZpZp, apply(H, ZpZp))
```

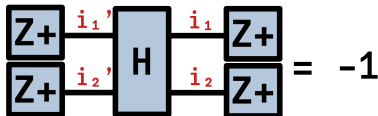
Expectation value:

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

$$\approx -1$$

Tutorial: Two-site operators

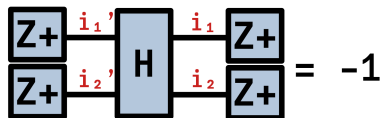
```
1  ZpZp = Zp1 * Zp2
2
3
4
5  (dag(ZpZp)' * H * ZpZp)[]
6  inner(ZpZp', H, ZpZp)
7  inner(ZpZp, apply(H, ZpZp))
```



Tutorial: Two-site operators

```
1 ZpZp = Zp1 * Zp2
2
3
4
5 (dag(ZpZp)' * H * ZpZp)[]
6 inner(ZpZp', H, ZpZp)
7 inner(ZpZp, apply(H, ZpZp))
```

```
1 D, U = eigen(H)
2 diag(D)
```

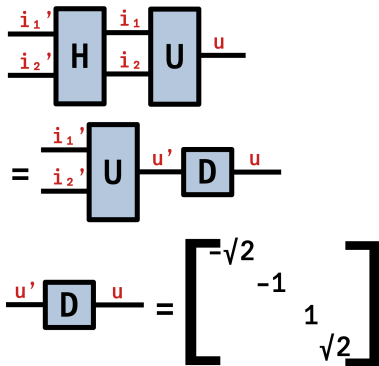


$$\approx [-\sqrt{2}, -1, 1, \sqrt{2}]$$

Tutorial: Two-site operators

```
1 ZpZp = Zp1 * Zp2
2
3
4
5 (dag(ZpZp)' * H * ZpZp)[]
6 inner(ZpZp', H, ZpZp)
7 inner(ZpZp, apply(H, ZpZp))
```

```
1 D, U = eigen(H)
2 diag(D)
```



Tutorial: Custom two-site operators

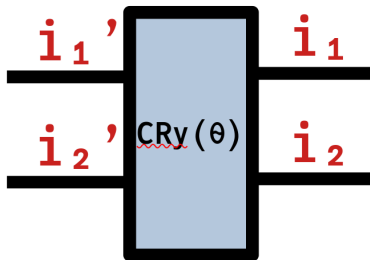
```
1  import ITensors: op
2
3  function op(
4      ::OpName"CRy",
5      ::SiteType"S=1/2";
6       $\theta$ 
7  )
8      c = cos( $\theta/2$ )
9      s = sin( $\theta/2$ )
10     return [
11         1 0 0 0
12         0 1 0 0
13         0 0 c -s
14         0 0 s  c
15     ]
16 end
```

Controlled-Ry (CRy)
rotation gate

$\text{CRy}(\theta)$

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
```



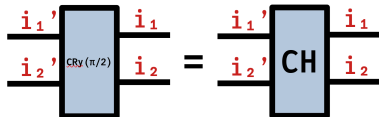
Tutorial: Custom two-site operators

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

Controlled-Hadamard gate
 $\text{CH} = \text{CRy}(\theta=\pi/2)$

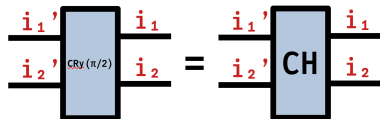
Tutorial: Custom two-site operators

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



Tutorial: Custom two-site operators

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



```
1 ZpZm = Zp1 * Zm2  
2  
3 CH_Xm = apply(CH, ZpZm)  
4  
5 CH_Xm  $\approx$  Zp1 * Xm2
```

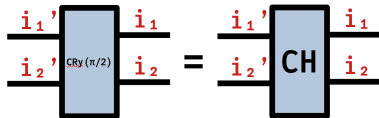
$$|Z+Z-\rangle = |Z+\rangle_1 |Z-\rangle_2$$

$$\text{CH}|Z+Z-\rangle = |Z+X-\rangle$$

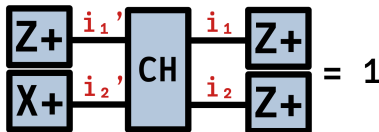
true

Tutorial: Custom two-site operators

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



```
1 ZpZm = Zp1 * Zm2  
2  
3 CH_Xm = apply(CH, ZpZm)  
4  
5 CH_Xm  $\approx$  Zp1 * Xm2
```



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
```

Function to minimize:
Expectation value of the
energy.

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

Tutorial: Two-site state optimization

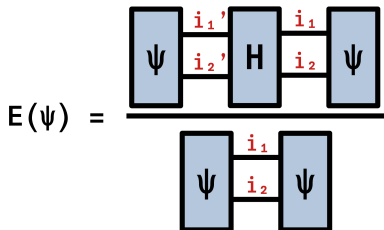
```
1 function E( $\psi$ )  
2    $\psi H \psi = \text{inner}(\psi', H, \psi)$   
3    $\psi \psi = \text{inner}(\psi, \psi)$   
4   return  $\psi H \psi / \psi \psi$   
5 end
```

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

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
```



Simple gradient descent.
Must provide function $f(x)$
to minimize and $\partial f(x)$,
the gradient of f at x .
 γ is the gradient
descent 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
```

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

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

Tutorial: Two-site state optimization

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

$$|\psi_0\rangle = (|Z+Z+\rangle + |Z-Z-\rangle)/\sqrt{2}$$

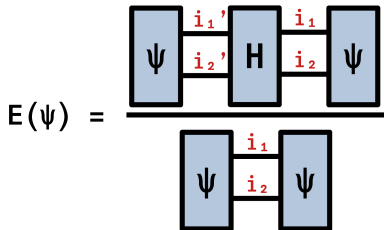
$$\approx -1$$

Using Zygote for automatic differentiation of the energy.

$$\approx 2$$

Tutorial: Two-site state optimization

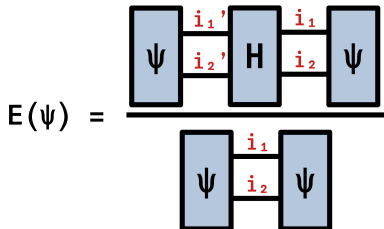
```
1  $\psi_0 = (Z_{p1} * Z_{m2} +$   
2  $Z_{m1} * Z_{p2})/\sqrt{2}$   
3  
4  $E(\psi_0)$   
5  
6 using Zygote: gradient  
7  $\partial E(\psi) = \text{gradient}(E, \psi)[1]$   
8  
9  $\text{norm}(\partial E(\psi_0))$ 
```



Tutorial: Two-site state optimization

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

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



Minimize over ψ :

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

$$(-1, 2)$$

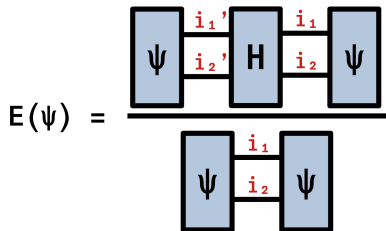
$$(-1.4142131, 0.0010865277)$$

$$\approx (-\sqrt{2}, 0)$$

Tutorial: Two-site state optimization

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

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



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

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
```

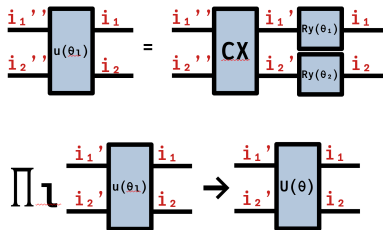
Tutorial: Two-site circuit optimization

```
1 # 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
```

```
# PastaQ notation:
u( $\theta$ , j1, j2) = [
    ("Ry", j1, (;  $\theta$ = $\theta$ [1])),
    ("Ry", j2, (;  $\theta$ = $\theta$ [2])),
    ("CNOT", j1, j2),
    ("Ry", j1, (;  $\theta$ = $\theta$ [3])),
    ("Ry", j2, (;  $\theta$ = $\theta$ [4])),
]
U( $\theta$ , i1, i2) =
    buildcircuit(u( $\theta$ , 1, 2), [i1, i2])
```


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

References state:

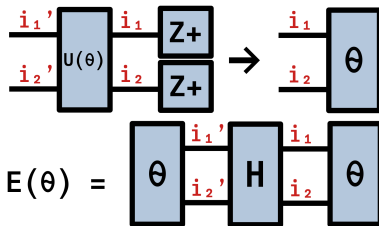
$$|0\rangle = |Z+Z+\rangle$$

Find θ that minimizes:

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

Tutorial: Two-site circuit optimization

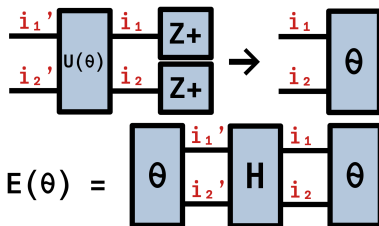
```
1  $\psi_0 = Z_{p1} * Z_{p2}$ 
2
3
4 function E( $\theta$ )
5    $\psi_\theta = \text{apply}(U(\theta), \psi_0)$ 
6   return inner( $\psi_\theta'$ , H,  $\psi_\theta$ )
7 end
```



Tutorial: Two-site circuit optimization

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

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

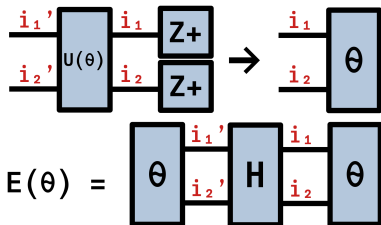


$$\min_{\theta} E(\theta) \quad \partial_{\theta} E(\theta)$$

Tutorial: Two-site circuit optimization

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

```
1  $\theta_0 = [0, 0, 0, 0]$ 
2  $\theta = \text{minimize}(\mathbf{E}, \partial\mathbf{E}, \theta_0;$ 
3   nsteps=40,  $\gamma=0.5$ )
4
5  $\mathbf{E}(\theta_0)$ ,  $\text{norm}(\partial\mathbf{E}(\theta_0))$ 
6  $\mathbf{E}(\theta)$ ,  $\text{norm}(\partial\mathbf{E}(\theta))$ 
7
```



$$\begin{aligned} &(-1, \sqrt{3}/2) \\ &(-1.4142077, 0.0017584116) \\ &\approx (-\sqrt{2}, 0) \end{aligned}$$

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:

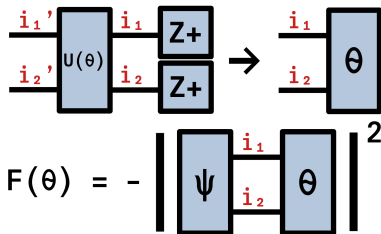
$$|\psi\rangle = (|Z+Z+\rangle + |Z-Z-\rangle)/\sqrt{2}$$

Find θ that minimizes:

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

Tutorial: Two-site fidelity optimization

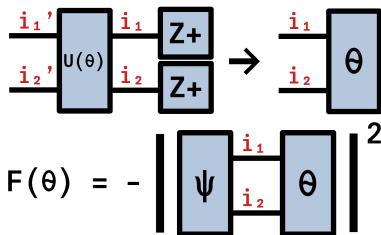
```
1  $\psi_0 = Z_{p1} * Z_{p2}$ 
2  $\psi = (Z_p Z_p + Z_m Z_m) / \sqrt{2}$ 
3
4
5
6 function F( $\theta$ )
7    $\psi_\theta = \text{apply}(U(\theta, i_1, i_2), \psi_0)$ 
8   return  $-\text{abs}(\text{inner}(\psi, \psi_\theta))^2$ 
9 end
```



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
```

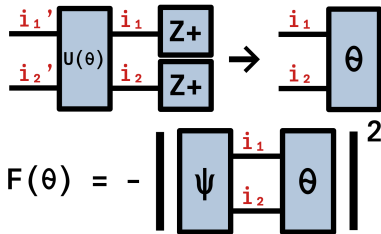
```
1  $\theta_0 = [0, 0, 0, 0]$ 
2  $\theta = \text{minimize}(F, \partial F, \theta_0;$ 
3     nsteps=50,  $\gamma=0.1$ )
4
5  $F(\theta_0), \text{norm}(\partial F(\theta_0))$ 
6  $F(\theta), \text{norm}(\partial F(\theta))$ 
7
```



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

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



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

$\approx (-0.5, 0.5)$
 $\approx (-0.9938992, 0.07786879)$
 $\approx (-1, 0)$

Tutorial: n -site states with MPS

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

n -site state

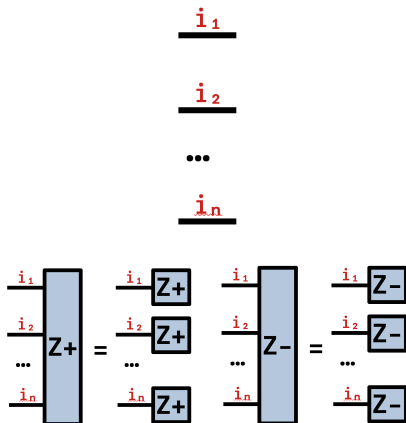
$|Z + Z + \dots Z + \rangle$

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

1 (product state)

Tutorial: n -site states with MPS

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



Tutorial: n-site states with MPS

1 $\psi = (Z_p + Z_m)/\sqrt{2}$

2

3

4 $\text{maxlinkdim}(\psi)$

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

2 (entangled state)

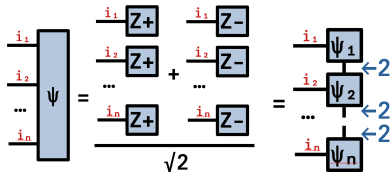
Tutorial: n -site states with MPS

$$1 \quad \psi = (Z_p + Z_m)/\sqrt{2}$$

2

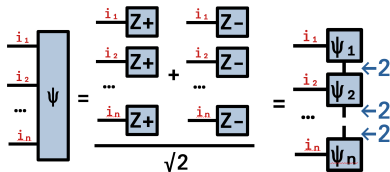
3

$$4 \quad \text{maxlinkdim}(\psi)$$



Tutorial: n -site states with MPS

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

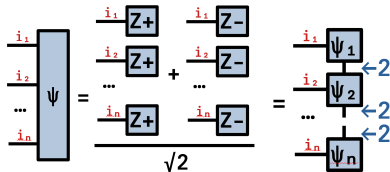


- 1 $\text{inner}(Z_p, Z_p)$
- 2 $\text{inner}(Z_m, Z_p)$
- 3 $\text{norm}(\psi)$
- 4 $\text{inner}(Z_p, \psi)$

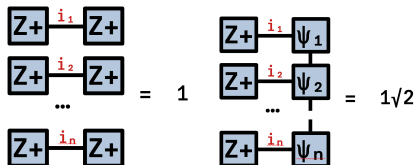
$$\begin{aligned} \langle Z+ | Z+ \rangle &\approx 1 \\ \langle Z- | Z+ \rangle &\approx 0 \\ ||\psi\rangle| &\approx 1 \\ \langle Z+ | \psi \rangle &\approx 1/\sqrt{2} \end{aligned}$$

Tutorial: n -site states with MPS

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



- 1 $\text{inner}(Z_p, Z_p)$
- 2 $\text{inner}(Z_m, Z_p)$
- 3 $\text{norm}(\psi)$
- 4 $\text{inner}(Z_p, \psi)$



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)
```

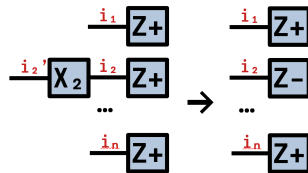
$j = n \div 2$
 X_j

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

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

Tutorial: n -site states with MPS

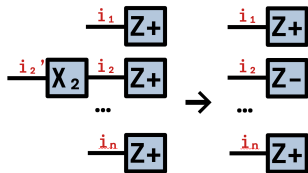
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```

```
1  maxlinkdim(XjZp)
2  inner(Zp, XjZp)
3  inner(XjZp, apply(Xj, Zp))
```



1 (product state)

≈ 0

≈ 1

Tutorial: n-site operators with MPO

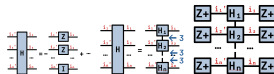
```
1 function ising(n; h)
2   H = OpSum()
3   for j in 1:(n - 1)
4     H -= "Z", j, "Z", j + 1
5   end
6   for j in 1:n
7     H += h, "X", j
8   end
9   return H
10 end
```

n sites

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

Tutorial: n -site operators with MPO

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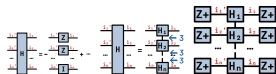


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7      H += h, "X", j
8    end
9    return H
10 end

```



= 3 (local Hamiltonian)

```

1  h = 0.5
2  H = MPO(ising(n; h=h), i)
3  maxlinkdim(H)
4  Zp = MPS(i, "Z+")
5  inner(Zp', H, Zp)
6

```

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

$$\approx -(n - 1) = -29$$

Tutorial: n -site state optimization

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

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

Minimize over ψ :

$$\langle\psi|\mathbf{H}|\psi\rangle / \langle\psi|\psi\rangle$$

DMRG solves:

$$\mathbf{H}|\psi\rangle \approx |\psi\rangle$$

Tutorial: n -site state optimization

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```



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

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```

```

1   $\text{maxlinkdim}(\psi_0)$ 
2   $\text{maxlinkdim}(\psi)$ 
3   $\text{maxlinkdim}(\psi_{\text{dmrg}})$ 
4   $\mathbf{E}(\psi_0), \text{norm}(\partial(\psi_0))$ 
5   $\mathbf{E}(\psi), \text{norm}(\partial\mathbf{E}(\psi))$ 
6   $\mathbf{E}(\psi_{\text{dmrg}}), \text{norm}(\partial\mathbf{E}(\psi_{\text{dmrg}}))$ 

```

$$E(\psi) = \sum_{\alpha, \beta} \langle \psi | \psi \rangle$$

$\min_{\psi} E(\psi) \quad \partial E(\psi)$
 $= 1$ (product state)
 $= 3$ (entangled state)
 $= 2$ (entangled state)
 $\approx (-29, 5.4772256)$
 $\approx (-31.0317917, 0.06673780)$
 $\approx (-31.0356110, 0.02413237)$

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

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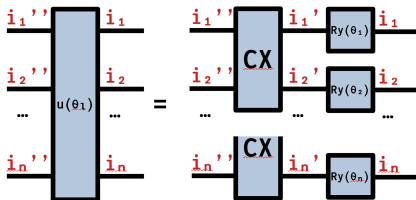
```
1 function U( $\theta$ , i; nlayers)
2   n = length(i)
3    $U_\theta = \text{Ry\_layer}(\theta[1:n], i)$ 
4   for l in 1:(nlayers - 1)
5      $\theta_l = \theta[(1:n) .+ l * n]$ 
6      $U_\theta = [U_\theta; \text{CX\_layer}(i)]$ 
7      $U_\theta = [U_\theta; \text{Ry\_layer}(\theta_l, i)]$ 
8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

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

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



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

Tutorial: n -site states with MPS

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

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

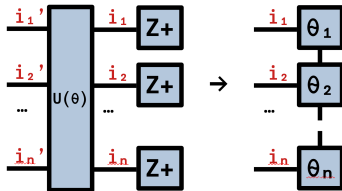
Minimize over θ :

$$|\theta\rangle = U(\theta)|0\rangle$$

$$E(\theta) = \langle \theta | H | \theta \rangle$$

Tutorial: n -site states with MPS

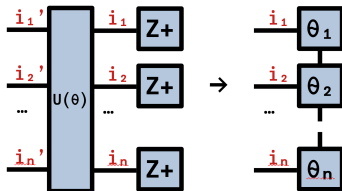
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1  $\psi_0 = \text{MPS}(i, \text{"Z+"})$ 
2 nlayers = 6
3 function E( $\theta$ )
4    $\psi_\theta = \text{apply}(U(\theta, i; \text{nlayers}), \psi_0)$ 
5   return inner( $\psi_\theta'$ , H,  $\psi_\theta$ )
6 end
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```

```
1 maxlinkdim( $\psi_0$ )
2 maxlinkdim( $\psi_\theta$ )
3 E( $\theta_0$ ), norm( $\partial \text{E}(\theta_0)$ )
4 E( $\theta$ ), norm( $\partial \text{E}(\theta)$ )
```



1 (product state)
2 (entangled state)
(-29, 5.773335)
(-31.017062, 0.000759)

Tutorial: n -site states with MPS

```

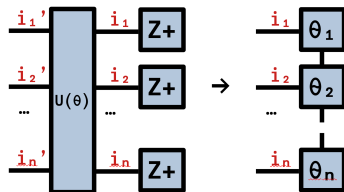
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```

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4  E( $\theta$ ), norm( $\partial \text{E}(\theta)$ )

```



$$E(\theta) =$$

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

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