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

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Center for Computational Quantum Physics

Who am I?

- PhD from Caltech with **John Preskill** and **Steve White** (UCI) in 2018.

mtfishman.github.io

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

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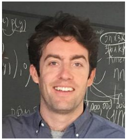
- Stands for "Intelligent Tensor".



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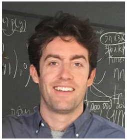

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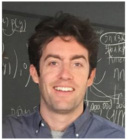
ITENSOR



julia

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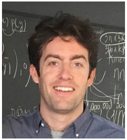

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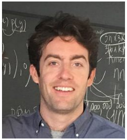

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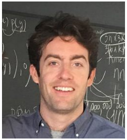

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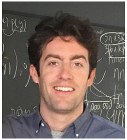

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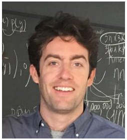

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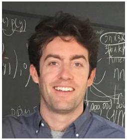

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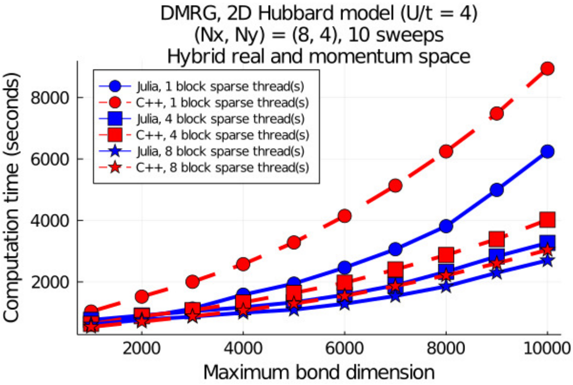

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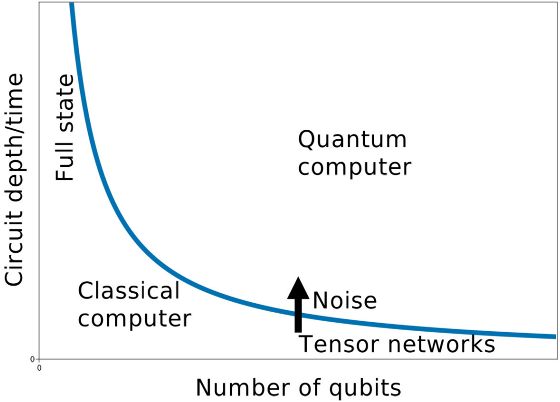
  - Find out more: github.com/GTorlai/PastaQ.jl

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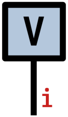
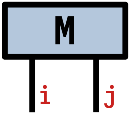
  - This is not the focus of ITensor and PastaQ at the moment, specialized libraries like Yao.jl may be faster.
- Tensor networks are a common, general language for reasoning about quantum many-body systems (for example, quantum circuits).

What are tensor networks?

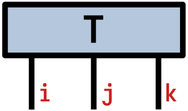
Vector V_i
Order-1 tensor



Matrix M_{ij}
Order-2 tensor



Tensor T_{ijk}
Order-3 tensor



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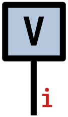
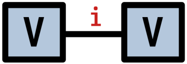


$$\langle V|V\rangle = V_i V_i$$



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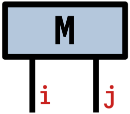

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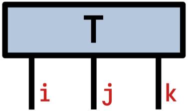

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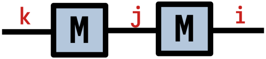

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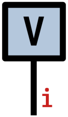

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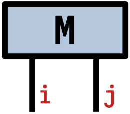

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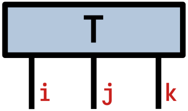

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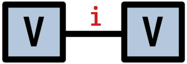

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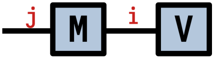
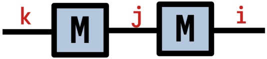
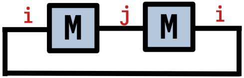


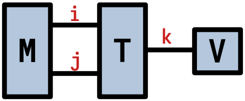
$MM = M_{kj} M_{ji}$



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



$M_{ij} T_{ijk} V_k$



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3. Type the following commands:

```
julia> using Pkg

julia> Pkg.add("ITensors")
[...]

julia> Pkg.add("PastaQ")
[...]
```

How do I install ITensor/PastaQ?

Now you can use ITensors and PastaQ:

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julia> using ITensors

julia> i = Index(2);

julia> A = ITensor(i);
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julia> using PastaQ

julia> gates = [("X", 1), ("CX", (1, 3))];

julia> ψ = runcircuit(gates);
```

Tutorial: One-site state basics

```
using ITensors

i = Index(2)


```

Load ITensor

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

Tutorial: One-site state basics

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Tutorial: One-site state basics

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Zp = ITensor(i)
Zp[i=>1] = 1

Zp = ITensor([1, 0], i)
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$$|Z+\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Construct from a Vector

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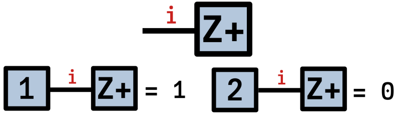

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Zp = ITensor([1, 0], i)
Zm = ITensor([0, 1], i)
Xp = ITensor([1, 1]/√2, i)
Xm = ITensor([1, -1]/√2, i)
```
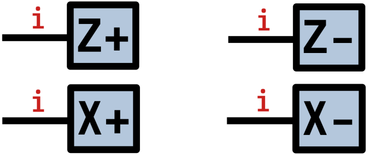

$$|Z+\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \qquad |Z-\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$|X+\rangle = \begin{bmatrix} 1 \\ 1 \end{bmatrix} / \sqrt{2}, \; |X-\rangle = \begin{bmatrix} 1 \\ -1 \end{bmatrix} / \sqrt{2}$$

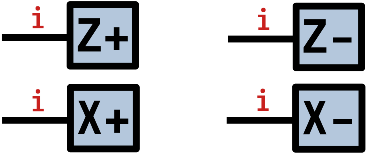
Tutorial: One-site state basics

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



Tutorial: One-site state basics

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



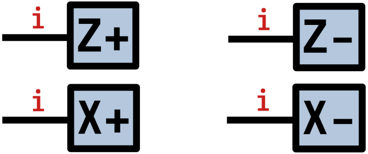

```
Xp = (Zp + Zm)/√2



dag(Zp) * Xp
inner(Zp, Xp)
```

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

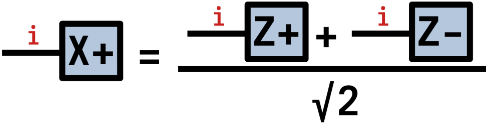
$$\langle Z + |X+\rangle \approx 1/\sqrt{2}$$

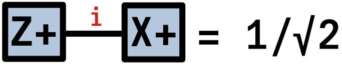
Tutorial: One-site state basics

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



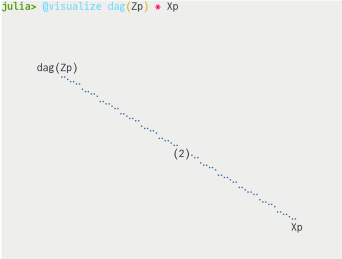

```
Xp = (Zp + Zm)/√2



dag(Zp) * Xp
inner(Zp, Xp)
```





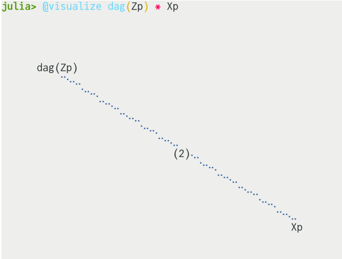
Tutorial: One-site state basics

```julia
using ITensorUnicodePlots

@visualize dag(Zp) * Xp
```

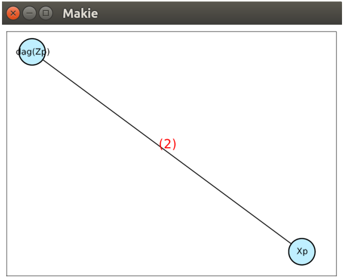


Tutorial: One-site state basics

```
using ITensorUnicodePlots

@visualize dag(Zp) * Xp
```




```
using ITensorGLMakie

@visualize dag(Zp) * Xp
```



Tutorial: One-site states

```
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

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

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

"S=1/2" defines an operator basis

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

```
Zp = state("Z+", i)
Zm = state("Z-", i)
Xp = state("X+", i)
Xm = state("X-", i)
```

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

Tutorial: Custom one-site states

```julia
import ITensors: state


function state(
  ::StateName"iX-",
  ::SiteType"S=1/2"
)
  return [im -im]/√2
end
```

Overload ITensors.jl behavior

Define a state with the name “iX-”

Tutorial: Custom one-site states

```julia
import ITensors: state


function state(
  ::StateName"iX-",
  ::SiteType"S=1/2"
)
  return [im -im]/√2
end
```

Overload ITensors.jl behavior

Define a state with the name "iX-"

```julia
iXm = state("iX-", i)


inner(Zm, iXm)
```

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

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

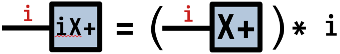
Tutorial: Custom one-site states

```
import ITensors: state


function state(
  ::StateName"iX-",
  ::SiteType"S=1/2"
)
  return [im -im]/√2
end
```

```
iXm = state("iX-", i)


inner(Zm, iXm)
```

Overload ITensors.jl behavior

Define a state with the name "iX-"



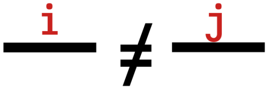
Tutorial: Priming

```
i = Index(2)
j = Index(2)

i ≠ j
```

(dim=2|id=837)
(dim=2|id=899)

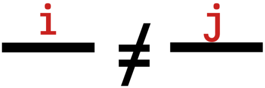
Tutorial: Priming

```
i = Index(2)
j = Index(2)

i ≠ j
```



Tutorial: Priming

```
i = Index(2)
j = Index(2)

i ≠ j
```




```
i = Index(2)

prime(i) == i'

i ≠ i'
noprime(i') == i
```

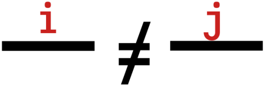
(dim=2|id=837)

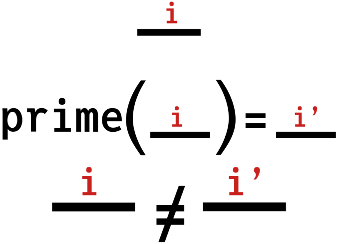
(dim=2|id=837)'

Tutorial: Priming

```
i = Index(2)
j = Index(2)

i ≠ j
```

```
i = Index(2)

prime(i) == i'

i ≠ i'
noprime(i') == i
```





Tutorial: One-site operators

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

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

Tutorial: One-site operators

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

Tutorial: One-site operators

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


```
z = [
  1 0
  0 -1
]
Z = ITensor(z, i', i)


Z = op("Z", i)
```

Matrix representation Z

Convert to ITensor

Use predefined definition

Tutorial: One-site operators

```
Z = op("Z", i)
X = op("X", i)

Zp = state("Z+", i)
Zm = state("Z-", i)
```

Z

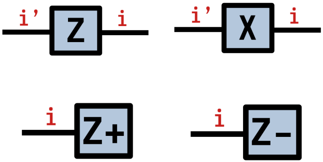
X

|Z+⟩

|Z-⟩

Tutorial: One-site operators

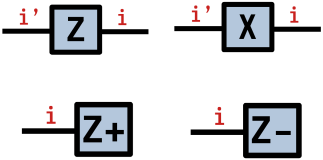
```
Z = op("Z", i)
X = op("X", i)

Zp = state("Z+", i)
Zm = state("Z-", i)
```



Tutorial: One-site operators

```
Z = op("Z", i)
X = op("X", i)

Zp = state("Z+", i)
Zm = state("Z-", i)
```

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

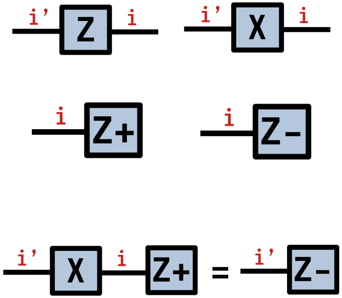


$$X|\text{Z+}\rangle = |\text{Z-}\rangle$$

Tutorial: One-site operators

```
Z = op("Z", i)
X = op("X", i)

Zp = state("Z+", i)
Zm = state("Z-", i)
```

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



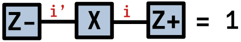
Tutorial: One-site operators

```
dag(Zm)' * X * Zp
inner(Zm', X, Zp)
```

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

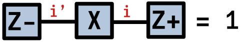
Tutorial: One-site operators

```
dag(Zm)' * X * Zp
inner(Zm', X, Zp)
```



Tutorial: One-site operators

```
dag(Zm)' * X * Zp
inner(Zm', X, Zp)
```



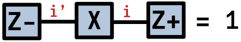

```
apply(X, Zp) ==
  noprime(X * Zp)



inner(Zm, apply(X, Zp))
```

$$X|Z+\rangle$$

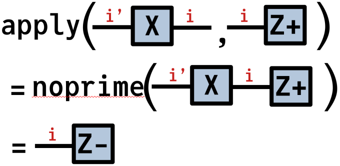
$$\langle Z - |X|Z+\rangle \approx 1$$

Tutorial: One-site operators

```
dag(Zm)' * X * Zp
inner(Zm', X, Zp)
```




```
apply(X, Zp) ==
  noprime(X * Zp)



inner(Zm, apply(X, Zp))
```



Tutorial: Custom one-site operators

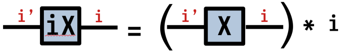
```julia
import ITensors: op

function op(
  ::OpName"iX",
  ::SiteType"S=1/2"
)
  return [
    0 im
    im 0
  ]
end
```

Overload ITensors.jl behavior

Tutorial: Custom one-site operators

```julia
import ITensors: op

function op(
  ::OpName"iX",
  ::SiteType"S=1/2"
)
  return [
    0 im
    im 0
  ]
end
```



Tutorial: Custom one-site operators

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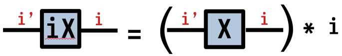
import ITensors: op

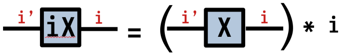
function op(
  ::OpName"iX",
  ::SiteType"S=1/2"
)
  return [
    0 im
    im 0
  ]
end
```

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



Tutorial: Custom one-site operators

```
import ITensors: op

function op(
  ::OpName"iX",
  ::SiteType"S=1/2"
)
  return [
    0 im
    im 0
  ]
end
```




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

```
X * im
```

Tutorial: Two-site states

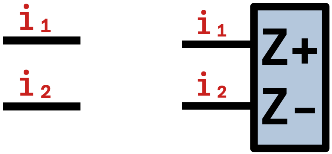
```
i1 = Index(2, "S=1/2")
i2 = Index(2, "S=1/2")

i1 ≠ i2

ZpZm = ITensor(i1, i2)
ZpZm[i1=>1, i2=>2] = 1
```

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

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

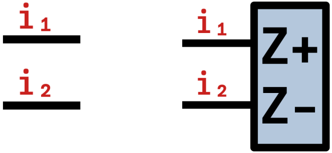
Tutorial: Two-site states

```
i1 = Index(2, "S=1/2")
i2 = Index(2, "S=1/2")

i1 ≠ i2

ZpZm = ITensor(i1, i2)
ZpZm[i1=>1, i2=>2] = 1
```



Tutorial: Two-site states

```
i1 = Index(2, "S=1/2")
i2 = Index(2, "S=1/2")

i1 ≠ i2

ZpZm = ITensor(i1, i2)
ZpZm[i1=>1, i2=>2] = 1
```




```
Zp1 = state("Z+", i1)
Zp2 = state("Z+", i2)

Zm1 = state("Z-", i1)
Zm2 = state("Z-", i2)

ZpZm = Zp1 * Zm2
```

$|\mathrm{Z+}\rangle_1$

$|\mathrm{Z+}\rangle_2$

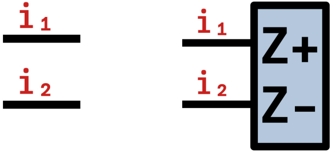
$|\mathrm{Z\text{-}}\rangle_1$

$|\mathrm{Z\text{-}}\rangle_2$

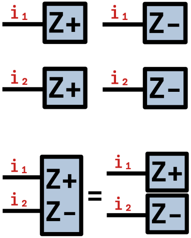
$$|\mathrm{Z+Z\text{-}}\rangle = |\mathrm{Z+}\rangle_1 |\mathrm{Z\text{-}}\rangle_2$$

Tutorial: Two-site states

```
i1 = Index(2, "S=1/2")
i2 = Index(2, "S=1/2")

i1 ≠ i2

ZpZm = ITensor(i1, i2)
ZpZm[i1=>1, i2=>2] = 1
```




```
Zp1 = state("Z+", i1)
Zp2 = state("Z+", i2)

Zm1 = state("Z-", i1)
Zm2 = state("Z-", i2)

ZpZm = Zp1 * Zm2
```



Tutorial: Two-site states

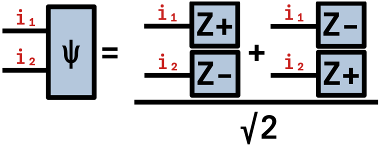
```
ψ = ITensor(i1, i2)
ψ[i1=>1, i2=>2] = 1/√2
ψ[i1=>2, i2=>1] = 1/√2

ψ = (Zp1 * Zm2 +
        Zm1 * Zp2)/√2
```

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

From single-site states

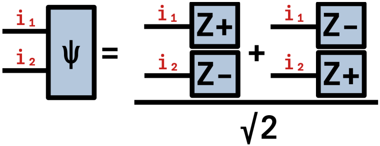
Tutorial: Two-site states

```
ψ = ITensor(i1, i2)
ψ[i1=>1, i2=>2] = 1/√2
ψ[i1=>2, i2=>1] = 1/√2

ψ = (Zp1 * Zm2 +
          Zm1 * Zp2)/√2
```

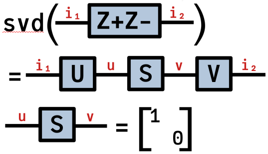


Tutorial: Two-site states

```
ψ = ITensor(i1, i2)
ψ[i1=>1, i2=>2] = 1/√2
ψ[i1=>2, i2=>1] = 1/√2

ψ = (Zp1 * Zm2 +
        Zm1 * Zp2)/√2
```



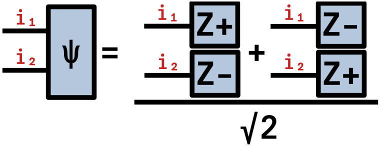

```
inner(ZpZm, ψ) == 1/√2


U, S, V = svd(ZmZp, i1)
diag(S) == [1, 0]

U, S, V = svd(ψ, i1)
diag(S) == [1/√2, 1/√2]
```

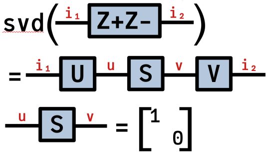


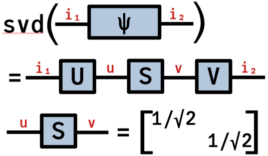
Tutorial: Two-site states

```
ψ = ITensor(i1, i2)
ψ[i1=>1, i2=>2] = 1/√2
ψ[i1=>2, i2=>1] = 1/√2

ψ = (Zp1 * Zm2 +
        Zm1 * Zp2)/√2
```

```
inner(ZpZm, ψ) == 1/√2


U, S, V = svd(ZmZp, i1)
diag(S) == [1, 0]

U, S, V = svd(ψ, i1)
diag(S) == [1/√2, 1/√2]
```







Tutorial: Two-site operators

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

Make a Hamiltonian:
Transverse field Ising ($n = 2$)

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

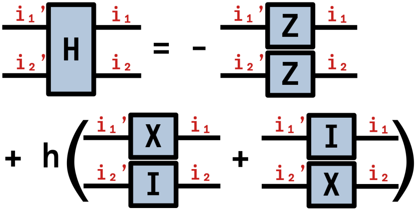
Tutorial: Two-site operators

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

```
Id1 = op("Id", i1)
Z1 = op("Z", i1)
X1 = op("X", i1)
# ...

ZZ = Z1 * Z2
XI = X1 * Id2
IX = Id1 * X2

h = 0.5
H = -ZZ + h * (XI + IX)
```

Make a Hamiltonian:
Transverse field Ising ($n = 2$)

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



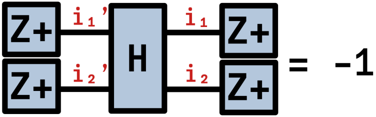
Tutorial: Two-site operators

```
inner(Zp' * Zp', H, Zp * Zp)
```

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

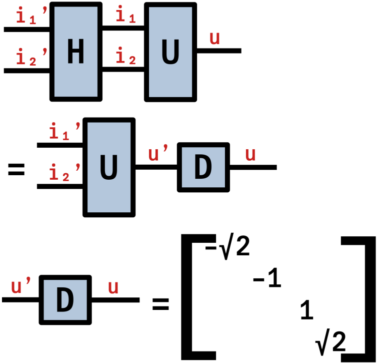
Tutorial: Two-site operators

```
inner(Zp' * Zp', H, Zp * Zp)
```



Tutorial: Two-site operators

```
D, U = eigen(H)
diag(D) == [-√2, -1, 1, √2]
```



Tutorial: Custom two-site operators

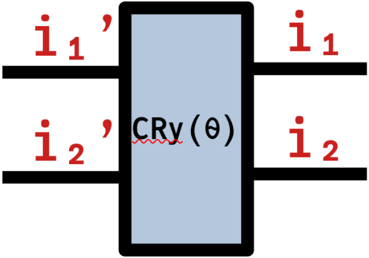
```julia
import ITensors: op

function op(
  ::OpName"CRy",
  ::SiteType"S=1/2";
  θ
)
  c = cos(θ/2)
  s = sin(θ/2)
  return [
    1 0 0  0
    0 1 0  0
    0 0 c -s
    0 0 s  c
  ]
end
```

Controlled-Ry (CRy) rotation gate

CRy(θ)

Tutorial: Custom two-site operators

```
import ITensors: op

function op(
  ::OpName"CRy",
  ::SiteType"S=1/2";
  θ
)
  c = cos(θ/2)
  s = sin(θ/2)
  return [
    1 0 0  0
    0 1 0  0
    0 0 c -s
    0 0 s  c
  ]
end
```



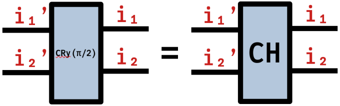
Tutorial: Custom two-site operators

```
CH = op("CRy", i1, i2; θ=π/2)
```

Controlled-Hadamard gate
CH = CRy(θ=$\pi/2$)

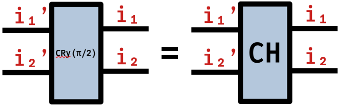
Tutorial: Custom two-site operators

```
CH = op("CRy", i1, i2; θ=π/2)
```



Tutorial: Custom two-site operators

```
CH = op("CRy", i1, i2; θ=π/2)
```

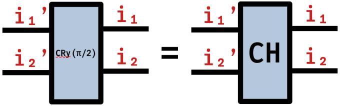



```
apply(CH, Zp1 * Zp2) ==
      Zp1 * Xp2
```

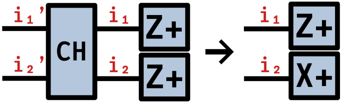
$$\mathrm{CH}|\mathrm{Z+Z+}\rangle = |\mathrm{Z+X+}\rangle$$

Tutorial: Custom two-site operators

```
CH = op("CRy", i1, i2; θ=π/2)
```




```
apply(CH, Zp1 * Zp2) ==
      Zp1 * Xp2
```



Tutorial: Two-site state optimization

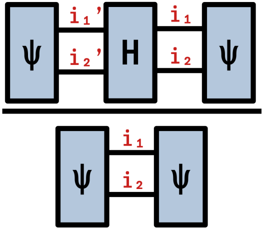
```
function E(ψ)
  ψHψ = inner(ψ', H, ψ)
  ψψ = inner(ψ, ψ)
  return ψHψ / ψψ
end
```

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

Tutorial: Two-site state optimization

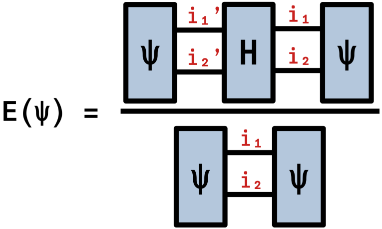
```
function E(ψ)
  ψHψ = inner(ψ', H, ψ)
  ψψ = inner(ψ, ψ)
  return ψHψ / ψψ
end
```

E(ψ) =



Tutorial: Two-site state optimization

```
function E(ψ)
  ψHψ = inner(ψ', H, ψ)
  ψψ = inner(ψ, ψ)
  return ψHψ / ψψ
end
```




```
function minimize(f, ∂f, x;
  nsteps, γ)
  for n in 1:nsteps
    x = x - γ * ∂f(x)
  end
  return x
end
```

Gradient descent.

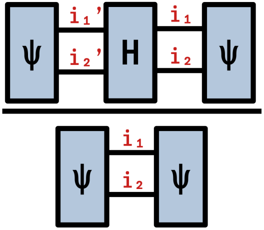
$f(x)$: function to minimize.
∂f(x): gradient of f.
γ: step size.

Tutorial: Two-site state optimization

```
function E(ψ)
  ψHψ = inner(ψ', H, ψ)
  ψψ = inner(ψ, ψ)
  return ψHψ / ψψ
end
```

```
function minimize(f, ∂f, x;
  nsteps, γ)
  for n in 1:nsteps
    x = x - γ * ∂f(x)
  end
  return x
end
```

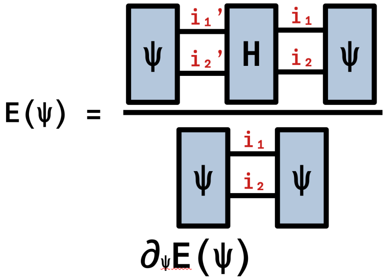
$E(\psi) =$



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

Tutorial: Two-site state optimization

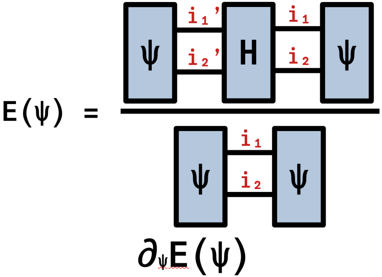
```
ψ₀ = (Zp1 * Zm2 +
        Zm1 * Zp2)/√2

E(ψ₀) == -1

using Zygote # autodiff

∂E(ψ) = gradient(E, ψ)[1]
norm(∂E(ψ₀)) == 2
```



Tutorial: Two-site state optimization

```julia
ψ0 = (Zp1 * Zm2 +
        Zm1 * Zp2)/√2

E(ψ0) == -1

using Zygote # autodiff

∂E(ψ) = gradient(E, ψ)[1]
norm(∂E(ψ0)) == 2
```

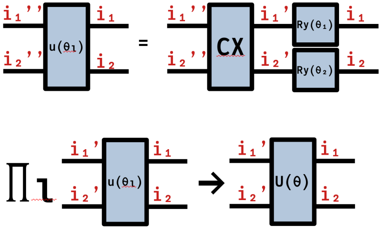
```julia
ψ = minimize(E, ∂E, ψ0;
       nsteps=10, γ=0.1)

E(ψ0) == -1
E(ψ) == -1.4142131 ≈ -√2
```



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

Tutorial: Two-site circuit optimization

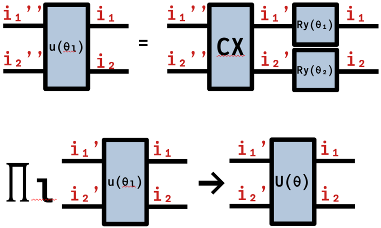
```
# Circuit as a vector of gates:
U(θ, i1, i2) = [
  op("Ry", i1; θ=θ[1]),
  op("Ry", i2; θ=θ[2]),
  op("CX", i1, i2),
  op("Ry", i1; θ=θ[3]),
  op("Ry", i2; θ=θ[4]),
]
```



Tutorial: Two-site circuit optimization

```julia
# PastaQ notation:
u(θ) = [
  ("Ry", 1, (; θ=θ[1])),
  ("Ry", 2, (; θ=θ[2])),
  ("CNOT", 1, 2),
  ("Ry", 1, (; θ=θ[3])),
  ("Ry", 2, (; θ=θ[4])),
]

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



Tutorial: Two-site circuit optimization

```
ψ0 = Zp1 * Zp2


function E(θ)
  ψθ = apply(U(θ, i1, i2), ψ0)
  return inner(ψθ', H, ψθ)
end
```

References state:

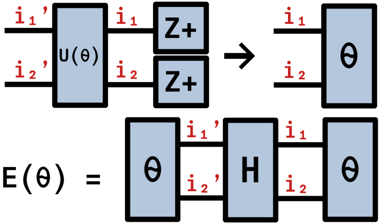
$|0\rangle = |Z{+}Z{+}\rangle$

$$\min_\theta \mathrm{E}(\theta)$$
$$= \min_\theta \langle 0|\mathrm{U}(\theta)^\dagger \, \mathrm{H} \, \mathrm{U}(\theta)|0\rangle$$
$$= \min_\theta \langle \theta|\mathrm{H}|\theta\rangle$$

Tutorial: Two-site circuit optimization

```
ψ0 = Zp1 * Zp2


function E(θ)
  ψθ = apply(U(θ, i1, i2), ψ0)
  return inner(ψθ', H, ψθ)
end
```



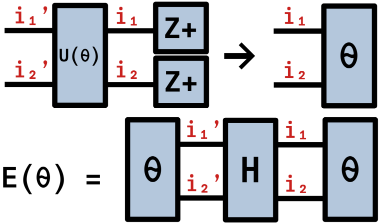
Tutorial: Two-site circuit optimization

```
ψ0 = Zp1 * Zp2


function E(θ)
  ψθ = apply(U(θ, i1, i2), ψ0)
  return inner(ψθ', H, ψθ)
end
```

```
θ0 = [0, 0, 0, 0]
∂E(θ) = gradient(E, θ)[1]
θ = minimize(E, ∂E, θ0;
        nsteps=40, γ=0.5)

E(θ0) == -1
E(θ) == -1.4142077 ≈ -√2
```



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

Tutorial: Two-site fidelity optimization

```
ψ0 = Zp1 * Zp2
ψ = (ZpZp + ZmZm) / √2
function F(θ)
  ψθ = apply(U(θ, i1, i2), ψ0)
  return -abs(inner(ψ, ψθ))^2
end
```

Reference state:
$|0\rangle = |Z{+}Z{+}\rangle$

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

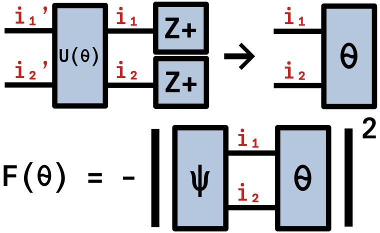
$$\min_\theta \mathrm{F}(\theta) = \min_\theta -|\langle\psi|\mathrm{U}(\theta)|0\rangle|^2$$

Tutorial: Two-site fidelity optimization

```
ψ0 = Zp1 * Zp2
ψ = (ZpZp + ZmZm) / √2



function F(θ)
  ψθ = apply(U(θ, i1, i2), ψ0)
  return -abs(inner(ψ, ψθ))^2
end
```



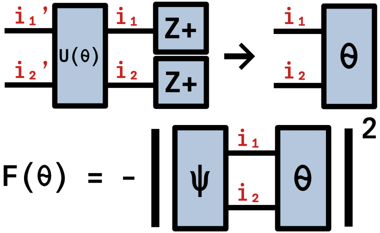
Tutorial: Two-site fidelity optimization

```
ψ0 = Zp1 * Zp2
ψ = (ZpZp + ZmZm) / √2


function F(θ)
  ψθ = apply(U(θ, i1, i2), ψ0)
  return -abs(inner(ψ, ψθ))^2
end
```

```
θ0 = [0, 0, 0, 0]
∂F(θ) = gradient(F, θ)[1]
θ = minimize(F, ∂F, θ0;
          nsteps=50, γ=0.1)

F(θ0) == -0.5
F(θ) == -0.9938992 ≈ -1
```



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

Tutorial: n-site states with MPS

```
n = 30
i = [Index(2, "S=1/2")
        for j in 1:n]


Zp = MPS(i, "Z+")

maxlinkdim(Zp) == 1 # product state
```

n-site state

$$|Z+Z+\ldots Z+\rangle$$

Tutorial: n-site states with MPS

```
n = 30
i = [Index(2, "S=1/2")
         for j in 1:n]


Zp = MPS(i, "Z+")

maxlinkdim(Zp) == 1 # product state
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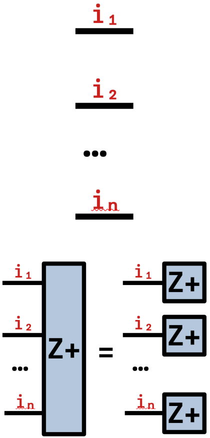


Tutorial: n-site states with MPS

```
ψ = (Zp + Zm)/√2

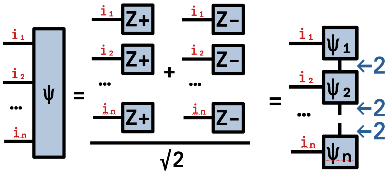

maxlinkdim(ψ) == 2 # entangled state
```

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

Tutorial: n-site states with MPS

```
ψ = (Zp + Zm)/√2

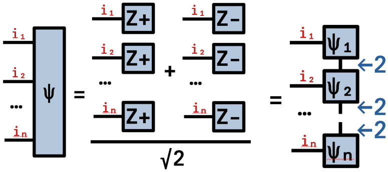

maxlinkdim(ψ) == 2 # entangled state
```



Tutorial: n-site states with MPS

```
ψ = (Zp + Zm)/√2

maxlinkdim(ψ) == 2 # entangled state
```




```
inner(Zp, Zp) == 1

inner(Zp, ψ) == 1/√2
```

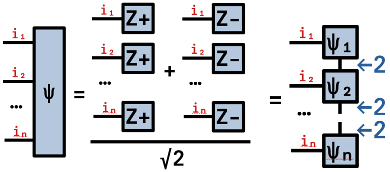
$$\langle Z+|Z+\rangle = 1$$

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

Tutorial: n-site states with MPS

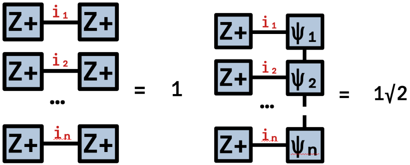
```
ψ = (Zp + Zm)/√2


maxlinkdim(ψ) == 2 # entangled state
```




```
inner(Zp, Zp) == 1


inner(Zp, ψ) == 1/√2
```



Tutorial: n-site states with MPS

```
j = n ÷ 2
Xj = op("X", i[j])

XjZp = apply(Xj, Zp)


state = [k == j ? "Z-" : "Z+"
                        for k in 1:n]
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

```
j = n ÷ 2
Xj = op("X", i[j])

XjZp = apply(Xj, Zp)


state = [k == j ? "Z-" : "Z+"
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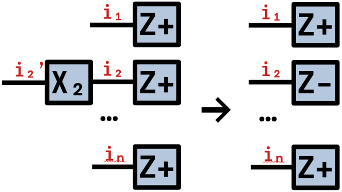
```



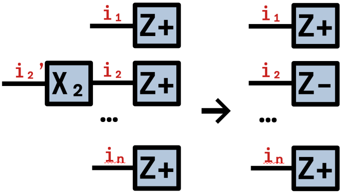
Tutorial: n-site states with MPS

```
j = n ÷ 2
X_j = op("X", i[j])

X_jZp = apply(X_j, Zp)


state = [k == j ? "Z-" : "Z+"
                      for k in 1:n]
X_jZp = MPS(i, state)
```

```
maxlinkdim(X_jZp) == 1
inner(Zp, X_jZp) == 0
```



Tutorial: n-site operators with MPO

```
function ising(n; h)
  H = OpSum()
  for j in 1:(n - 1)
    H -= "Z", j, "Z", j + 1
  end
  for j in 1:n
    H += h, "X", j
  end
  return H
end

h = 0.5
H = MPO(ising(n; h=h), i)
maxlinkdim(H) == 3
```

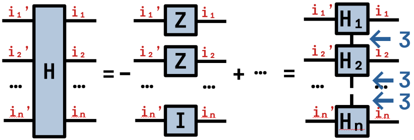
n sites

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

Tutorial: n-site operators with MPO

```julia
function ising(n; h)
  H = OpSum()
  for j in 1:(n - 1)
    H -= "Z", j, "Z", j + 1
  end
  for j in 1:n
    H += h, "X", j
  end
  return H
end

h = 0.5
H = MPO(ising(n; h=h), i)
maxlinkdim(H) == 3
```

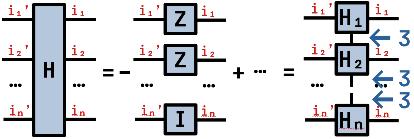


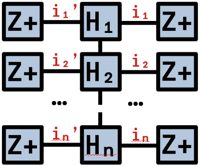
Tutorial: n-site operators with MPO

```julia
function ising(n; h)
  H = OpSum()
  for j in 1:(n - 1)
    H -= "Z", j, "Z", j + 1
  end
  for j in 1:n
    H += h, "X", j
  end
  return H
end

h = 0.5
H = MPO(ising(n; h=h), i)
maxlinkdim(H) == 3
```

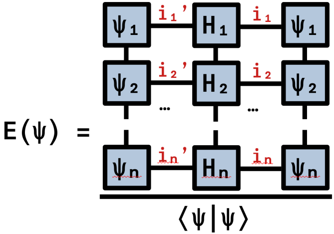
```julia
Zp = MPS(i, "Z+")
inner(Zp', H, Zp) == -(n-1)
```





Tutorial: n-site state optimization

```
function E(ψ)
  ψHψ = inner(ψ', H, ψ)
  ψψ = inner(ψ, ψ)
  return ψHψ / ψψ
end
```



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

Tutorial: n-site state optimization

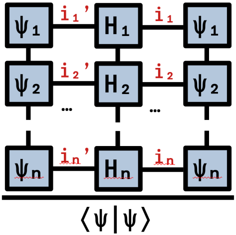
```
function E(ψ)
  ψHψ = inner(ψ', H, ψ)
  ψψ = inner(ψ, ψ)
  return ψHψ / ψψ
end
```

```
ψ₀ = MPS(i, "Z+")

ψ = minimize(E, ∂E, ψ₀;
        nsteps=50, γ=0.1,
        maxdim=10, cutoff=1e-5)

E_dmrg, ψ_dmrg = dmrg(H, ψ₀;
        nsweeps=10,
        maxdim=10, cutoff=1e-5)
```

$E(\psi)$ =



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

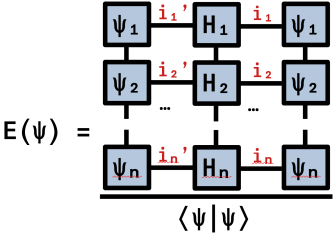
Tutorial: n-site state optimization

```
function E(ψ)
  ψHψ = inner(ψ', H, ψ)
  ψψ = inner(ψ, ψ)
  return ψHψ / ψψ
end
```

```
ψ0 = MPS(i, "Z+")

ψ = minimize(E, ∂E, ψ0;
        nsteps=50, γ=0.1,
        maxdim=10, cutoff=1e-5)

Edmrg, ψdmrg = dmrg(H, ψ0;
        nsweeps=10,
        maxdim=10, cutoff=1e-5)
```



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

```
maxlinkdim(ψ0) == 1
maxlinkdim(ψ) == 3
maxlinkdim(ψdmrg) == 3
E(ψ0) == -29
E(ψ) == -31.0317917
E(ψdmrg) == -31.0356110
```

Tutorial: n-site circuit optimization

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

Tutorial: n-site circuit optimization

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

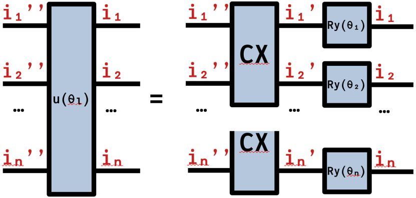
```julia
function U(θ, i; nlayers)
  n = length(i)
  for l in 1:(nlayers - 1)
    θ_l = θ[(1:n) .+ l * n]
    U_θ = [U_θ; Ry_layer(θ_l, i)]
    U_θ = [U_θ; CX_layer(i)]
  end
  return U_θ
end
```

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

Tutorial: n-site circuit optimization

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

```julia
function U(θ, i; nlayers)
  n = length(i)
  for l in 1:(nlayers - 1)
    θ_l = θ[(1:n) .+ l * n]
    U_θ = [U_θ; Ry_layer(θ_l, i)]
    U_θ = [U_θ; CX_layer(i)]
  end
  return U_θ
end
```

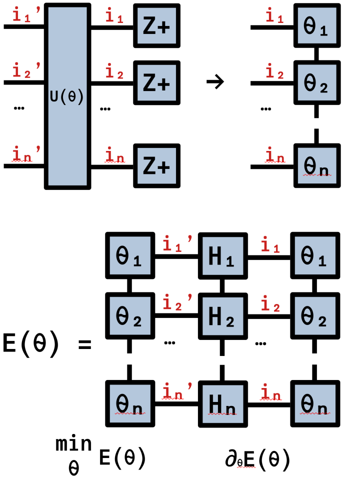


$$\prod_l u(\theta_l) \rightarrow U(\theta)$$

Tutorial: n-site states with MPS

```julia
ψ0 = MPS(i, "Z+")
nlayers = 6
function E(θ)
  ψθ = apply(U(θ, i; nlayers), ψ0)
  return inner(ψθ', H, ψθ)
end

θ0 = zeros(nlayers * n)
θ = minimize(E, ∂E, θ0;
        nsteps=20, γ=0.1)
```



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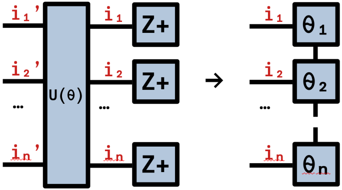
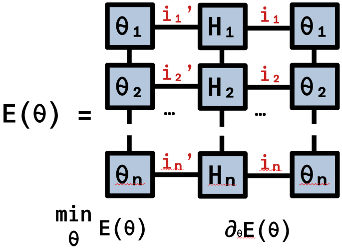
```julia
maxlinkdim(ψ0) = 1
maxlinkdim(ψθ) = 3
E(θ0) == -29
E(θ) == -31.017062
```

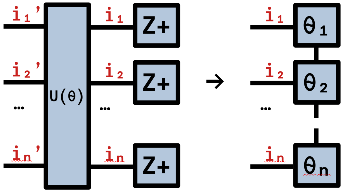


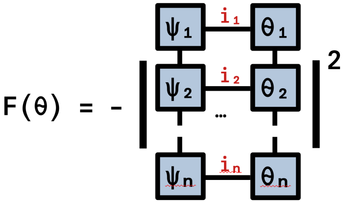


Tutorial: n-site states with MPS

```
ψ₀ = MPS(i, "Z+")
nlayers = 6
function F(θ)
  ψθ = apply(U(θ, i; nlayers), ψ₀)
  return -abs(inner(ψ', ψθ))^2
end

θ₀ = zeros(nlayers * n)
θ = minimize(F, ∂F, θ₀;
        nsteps=20, γ=0.1)
```





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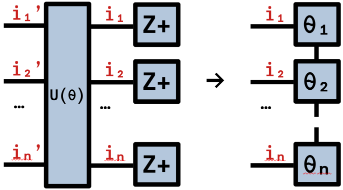
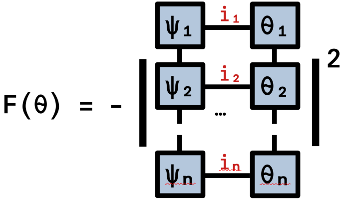
```julia
maxlinkdim(ψ0) == 1
maxlinkdim(ψθ) == 2
F(θ0) == -0.556066
F(θ) == -0.995230
```





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- More that I am probably forgetting... Ask Giacomo and me for more details.

Future directions/in progress

- More AD, make ITensor fully differentiable (have some work to do, like tensor decompositions and general network contractions, more MPS/MPO functions. You will find bugs, please contribute gradient definitions!).

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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!