Analyzing Quantum Many-Body Systems with ITensor and PastaQ

Matthew Fishman
Center for Computational Quantum Physics (CCQ)
Flatiron Institute, NY
mtfishman.github.io
github.com/mtfishman/ITensorTutorials.jl

June 19, 2022

Flatiron Institute
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Who am I?

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

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

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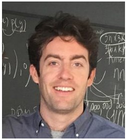

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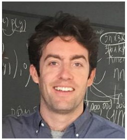

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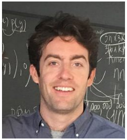

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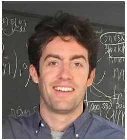

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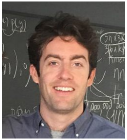

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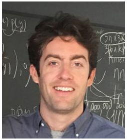

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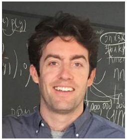

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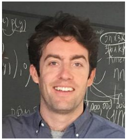

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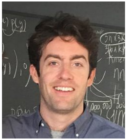

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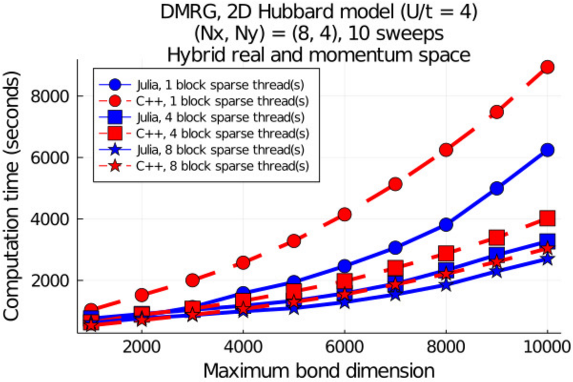
- Great numerical libraries, code ended up faster.



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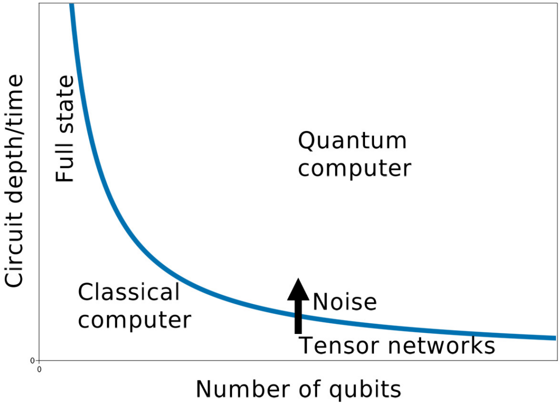
- Find out more: github.com/GTorlai/PastaQ.jl

When should I use tensor networks?

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



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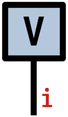
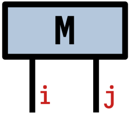
  - ITensor and PastaQ handle this seamlessly.
  - This is not the focus of ITensor and PastaQ at the moment, specialized libraries like Yao.jl may be faster.
- Tensor networks are a common, general language for reasoning about quantum many-body systems (for example, quantum circuits).

What are tensor networks?

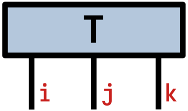
Vector V_i
Order-1 tensor



Matrix M_{ij}
Order-2 tensor



Tensor T_{ijk}
Order-3 tensor



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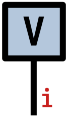
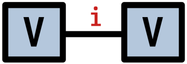


$\langle V|V\rangle = V_i V_i$



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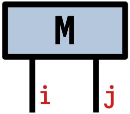

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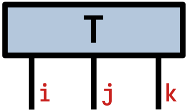

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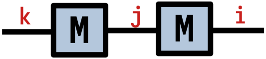

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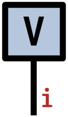

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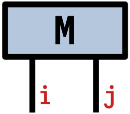

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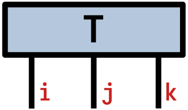

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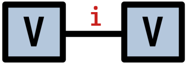

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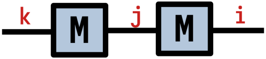
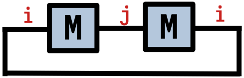
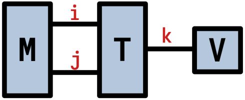


$tr(MM) = M_{ij} M_{ji}$



$M_{ij} T_{ijk} V_k$



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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

```julia
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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```julia
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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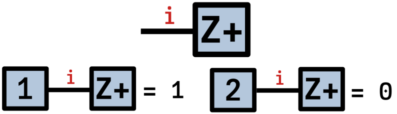


Tutorial: One-site state basics

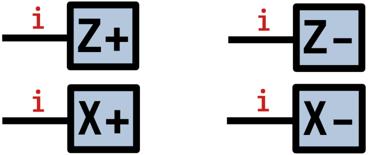
```
Zp=ITensor([1,0],i)
Zm=ITensor([0,1],i)
Xp=ITensor([1,1]/√2,i)
Xm=ITensor([1,-1]/√2,i)
```

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

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

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)
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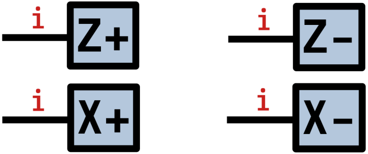
```




```
Xp = (Zp + Zm)/√2



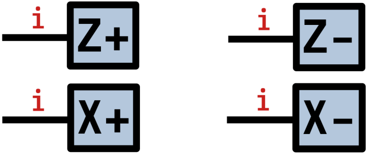
(dag(Zp) * Xp)[]
inner(Zp, Xp)
```

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

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

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)
```

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inner(Zp, Xp)
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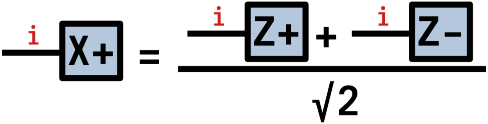
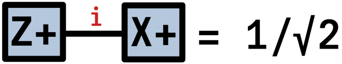
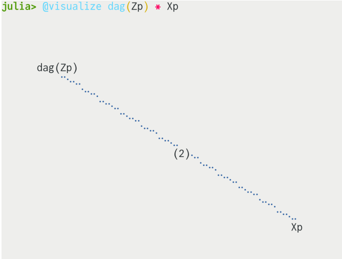




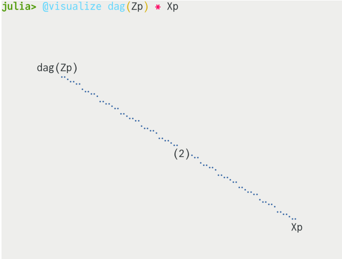
Tutorial: One-site state basics

```julia
using ITensorUnicodePlots

@visualize dag(Zp) * Xp
```

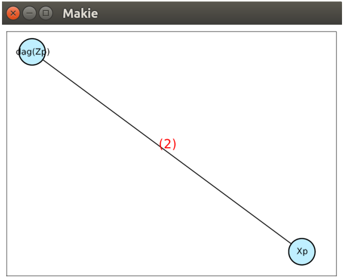


Tutorial: One-site state basics

```julia
using ITensorUnicodePlots

@visualize dag(Zp) * Xp
```




```julia
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("Zp",i)
Zm=state("Zm",i)
Xp=state("Xp",i)
Xm=state("Xm",i)
```

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

Tutorial: Custom one-site states

```
import ITensors: state


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

Overload ITensors.jl behavior

Define a state with the name “iX-”

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


inner(Zm, iXm)
```

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

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

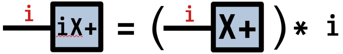
Tutorial: Custom one-site states

```
import ITensors: state


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

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


inner(Zm, iXm)
```

Overload ITensors.jl behavior

Define a state with the name “iX-”



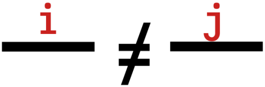
Tutorial: Priming

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

i != j
```

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

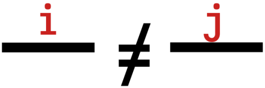
Tutorial: Priming

```
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
```

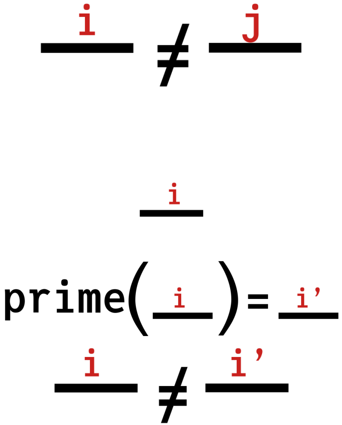
(dim=2|id=837)

(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

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

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

Tutorial: One-site operators

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


```julia
z = [1 0; 0 -1]
```

Matrix representation Z

```julia
Z = ITensor(z, i', i)
```

Convert to ITensor

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

Use predefined definition

Tutorial: One-site operators

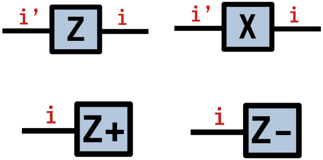
```
Z = op("Z", i)
X = op("X", i)

Zp = state("Zp", i)
Zm = state("Zm", i)
```

Z
X

|Z+⟩
|Z-⟩

Tutorial: One-site operators

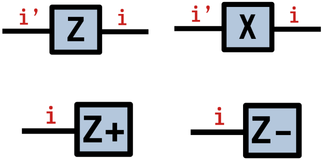
```
Z = op("Z", i)
X = op("X", i)

Zp = state("Zp", i)
Zm = state("Zm", i)
```



Tutorial: One-site operators

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

Zp = state("Zp", i)
Zm = state("Zm", i)
```

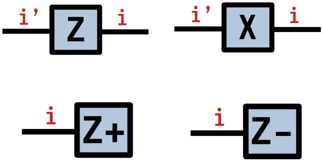
```
X * Zp == Zm'
noprime(X * Zp) == Zm
```



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

Tutorial: One-site operators

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

Zp = state("Zp", i)
Zm = state("Zm", i)
```




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

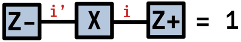
Tutorial: One-site operators

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

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

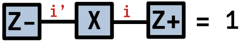
Tutorial: One-site operators

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



Tutorial: One-site operators

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



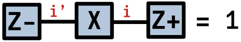

```
apply(X, Zp) ==
  noprime(X * Zp)



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

$$X|Z+\rangle$$

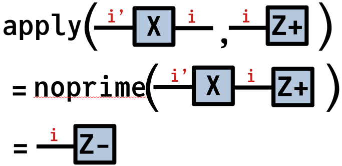
$$\langle Z-|X|Z+\rangle \approx 1$$

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(
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  return [0 im; im 0]
end
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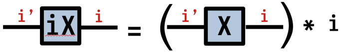
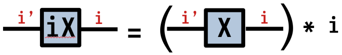


Tutorial: Custom one-site operators

```julia
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

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function op(
  ::OpName"iX",
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op("iX", i)
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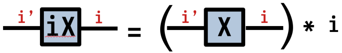



```julia
X * im
```

Tutorial: Two-site states

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

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”)

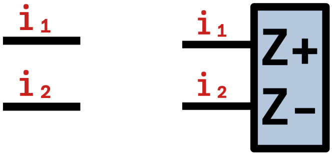
$$|\text{Z+}\rangle_1 |\text{Z-}\rangle_2 = |\text{Z+Z-}\rangle$$

Tutorial: Two-site states

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

i1 != i2

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



Tutorial: Two-site states

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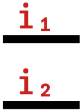
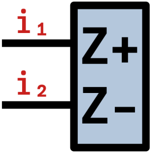
```






```
Zp1=state("Zp",i1)
Zp2=state("Zp",i2)
Zm1=state("Zm",i1)
Zm2=state("Zm",i2)


ZpZm = Zp1 * Zm2
```

$|\mathrm{Z+}\rangle_1$

$|\mathrm{Z+}\rangle_2$

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

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

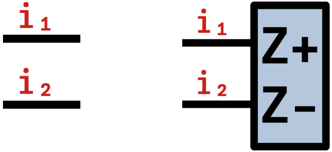
$$|\mathrm{Z+Z\text{-}}\rangle = |\mathrm{Z+}\rangle_1 |\mathrm{Z\text{-}}\rangle_2$$

Tutorial: Two-site states

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

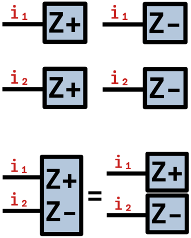
i1 != i2

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




```
Zp1=state("Zp",i1)
Zp2=state("Zp",i2)
Zm1=state("Zm",i1)
Zm2=state("Zm",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
```

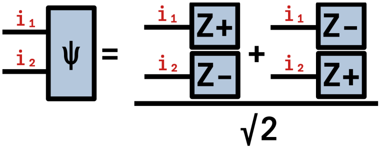
$$(|\mathrm{Z}+\rangle|\mathrm{Z}\text{-}\rangle + |\mathrm{Z}\text{-}\rangle|\mathrm{Z}+\rangle)/\sqrt{2}$$

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

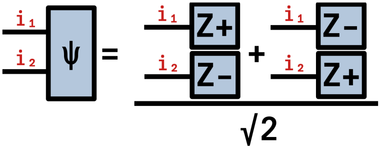
ψ = (Zp1 * Zm2 +
     Zm1 * Zp2)/√2
```



Tutorial: Two-site states

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

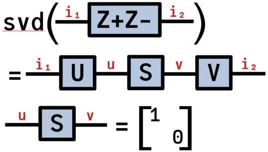
ψ = (Zp1 * Zm2 +
      Zm1 * Zp2)/√2
```




```
inner(ZpZm, ψ) == 1/√2


_, S, _ = svd(ZpZm, i1);
diag(S) == [1, 0]

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



Tutorial: Two-site states

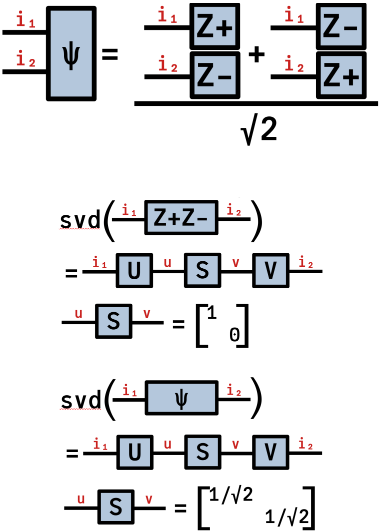
```
ψ = ITensor(i1, i2)
ψ[i1=>1, i2=>2] = 1/√2
ψ[i1=>2, i2=>1] = 1/√2

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

```
inner(ZpZm, ψ) == 1/√2


_, S, _ = svd(ZpZm, i1);
diag(S) == [1, 0]

_, S, _ = 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 ($n = 2$)

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

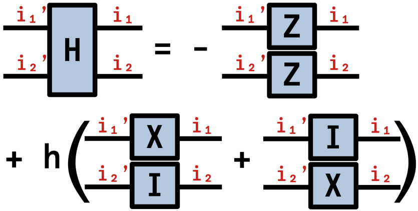
Tutorial: Two-site operators

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

```julia
Id1 = op("Id", i1)
Z1 = op("Z", i1)
X1 = op("X", i1)
Id2 = op("Id", i2)
Z2 = op("Z", i2)
X2 = op("X", i2)

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

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

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

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



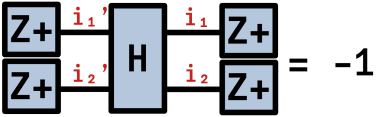
Tutorial: Two-site operators

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

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

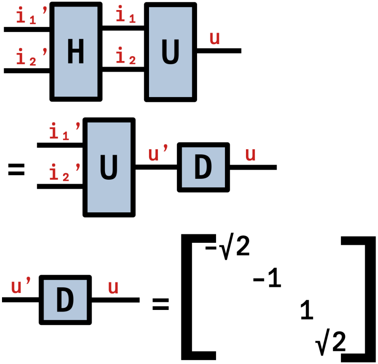
Tutorial: Two-site operators

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



Tutorial: Two-site operators

```
D, _ = eigen(H);
diag(D) ≈ [-√2, -1, 1, √2]
```



Tutorial: Custom two-site operators

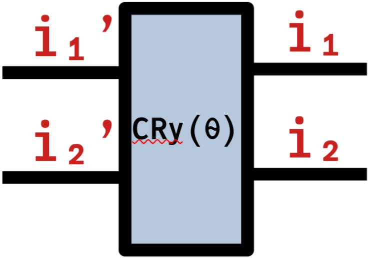
```julia
import ITensors: op

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

$\mathrm{CRy}(\theta)$

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
```



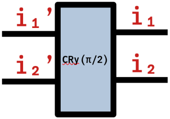
Tutorial: Custom two-site operators

```
CRy = op("CRy", i1, i2; θ=π/2)
```

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

Tutorial: Custom two-site operators

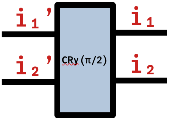
```
CRy = op("CRy", i1, i2; θ=π/2)
```



Tutorial: Custom two-site operators

```
CRy = op("CRy", i1, i2; θ=π/2)
```

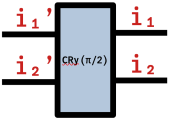
```
Xp1=state("Xp",i1)
Xm1=state("Xm",i1)
Xp2=state("Xp",i2)
Xm2=state("Xm",i2)

apply(CRy, Zm1 * Zp2) ≈
        Zm1 * Xp2
```



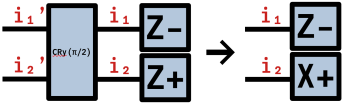
$$\mathrm{CRy}(\pi/2)|\text{Z-Z+}\rangle = |\text{Z-X+}\rangle$$

Tutorial: Custom two-site operators

```
CRy = op("CRy", i1, i2; θ=π/2)
```




```
Xp1=state("Xp",i1)
Xm1=state("Xm",i1)
Xp2=state("Xp",i2)
Xm2=state("Xm",i2)

apply(CRy, Zm1 * Zp2) ≈
      Zm1 * Xp2
```



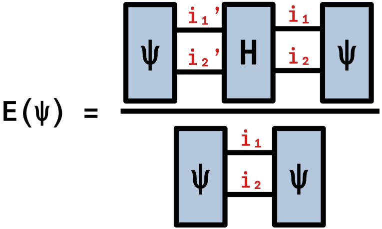
Tutorial: Two-site state optimization

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

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

Tutorial: Two-site state optimization

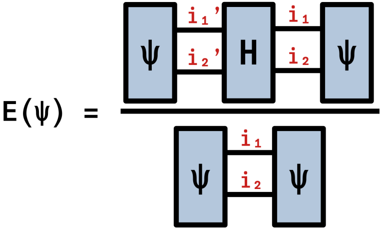
```julia
function E(ψ)
  ψHψ = inner(ψ', H, ψ)
  ψψ = inner(ψ, ψ)
  return ψHψ / ψψ
end
```



Tutorial: Two-site state optimization

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

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



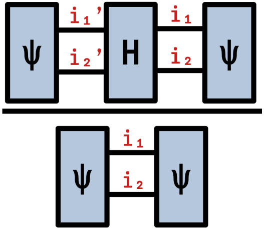
Gradient descent.

$f(x)$: function to minimize.
$\partial\mathrm{f}(\mathrm{x})$: gradient of f.
γ: step size.

Tutorial: Two-site state optimization

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

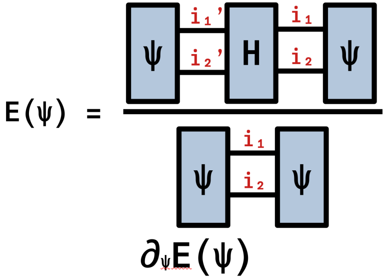
```julia
function minimize(f, ∂f, x;
                  nsteps, γ)
  for n in 1:nsteps
    x = x - γ * ∂f(x)
    println("Step = $(n),
          f(x) = $(f(x))")
  end
  return x
end
```

$E(\psi) =$ 

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

Tutorial: Two-site state optimization

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

E(ψ0) == -1

using Zygote # autodiff
∂E(ψ) = gradient(E, ψ)[1]

norm(∂E(ψ0)) == 2
```

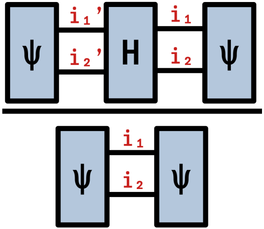


Tutorial: Two-site state optimization

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

E(ψ0) == -1

using Zygote # autodiff
∂E(ψ) = gradient(E, ψ)[1]

norm(∂E(ψ0)) == 2
```

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

E(ψ0) == -1
E(ψ) # ≈ -1.4142131 ≈ -√2

```

$E(\psi) =$

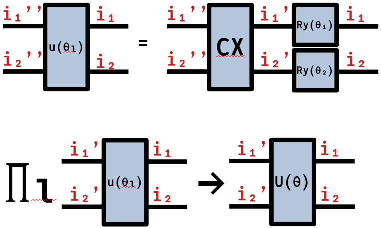


$\partial_\psi E(\psi)$

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

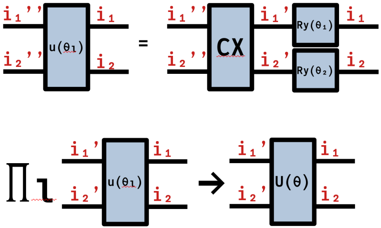
Tutorial: Two-site circuit optimization

```
# 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

```
# 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([i1,i2],u(θ))
```



Tutorial: Two-site circuit optimization

```
ψ0 = Zp1 * Zp2


function E(θ)
  ψθ = apply(U(θ,i1,i2),ψ0)
  return inner(ψθ',H,ψθ)
end
∂E(θ) = gradient(E, θ)[1]
```

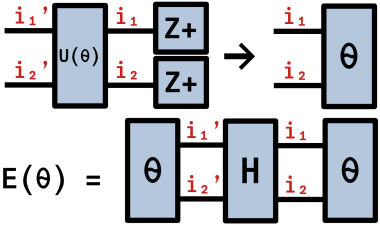
References state:

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

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

Tutorial: Two-site circuit optimization

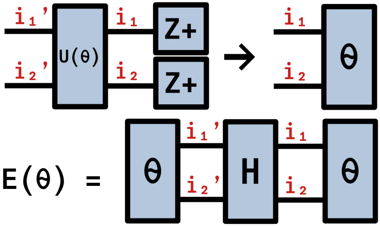
```julia
ψ0 = Zp1 * Zp2


function E(θ)
  ψθ = apply(U(θ,i1,i2),ψ0)
  return inner(ψθ',H,ψθ)
end
∂E(θ) = gradient(E, θ)[1]
```



Tutorial: Two-site circuit optimization

```
ψ0 = Zp1 * Zp2


function E(θ)
  ψθ = apply(U(θ,i1,i2),ψ0)
  return inner(ψθ',H,ψθ)
end
∂E(θ) = gradient(E, θ)[1]
```

```
θ0 = [0, 0, 0, 0]
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 = (Zp1*Zp2 + Zm1*Zm2)/√2



function F(θ)
  ψθ = apply(U(θ,i1,i2),ψ0)
  return -abs2(inner(ψ,ψθ))
end
∂F(θ) = gradient(F, θ)[1]
```

Reference state:

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

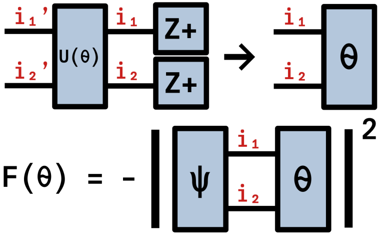
Target state:

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

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

Tutorial: Two-site fidelity optimization

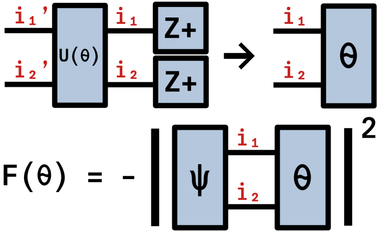
```
ψ0 = Zp1*Zp2
ψ = (Zp1*Zp2 + Zm1*Zm2)/√2
function F(θ)
  ψθ = apply(U(θ,i1,i2),ψ0)
  return -abs2(inner(ψ,ψθ))
end
∂F(θ) = gradient(F, θ)[1]
```



Tutorial: Two-site fidelity optimization

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



function F(θ)
  ψθ = apply(U(θ,i1,i2),ψ0)
  return -abs2(inner(ψ,ψθ))
end
∂F(θ) = gradient(F, θ)[1]
```

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

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



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

Tutorial: n-site states with MPS

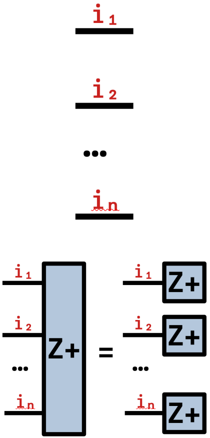
```julia
n = 30
i = [Index(2, "S=1/2")
     for j in 1:n];


Zp = MPS(i, "Zp");
Zm = MPS(i, "Zm");

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, "Zp");
Zm = MPS(i, "Zm");

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



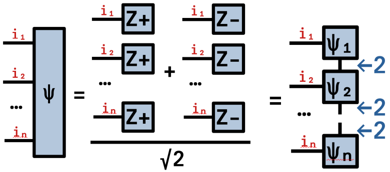
Tutorial: n-site states with MPS

```
ψ = (Zp + Zm)/√2;


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

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

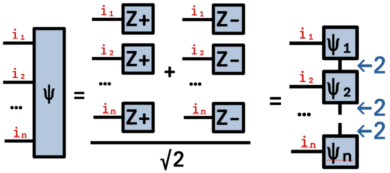
Tutorial: n-site states with MPS

```
ψ = (Zp + Zm)/√2;


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



Tutorial: n-site states with MPS

```
ψ = (Zp + Zm)/√2;


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



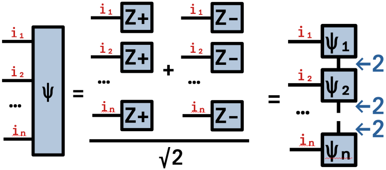

```
  inner(Zp, Zp) ≈ 1


  inner(Zp, ψ) ≈ 1/√2
```

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

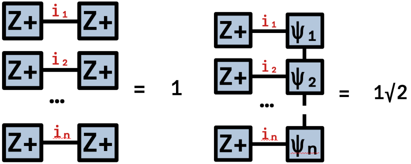
$$\langle Z+|\psi\rangle = 1/\sqrt{2}$$

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

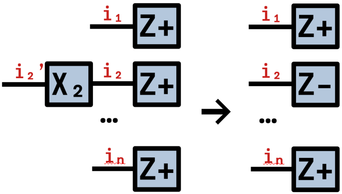
```
j = n ÷ 2
Xj = op("X", i[j])

XjZp = apply(Xj, Zp);


st = [k == j ? "Zm" : "Zp"
      for k in 1:n];
XjZp = MPS(i, st);
```

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

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

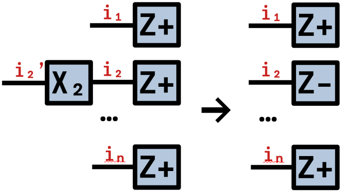
Tutorial: n-site states with MPS

```
j = n ÷ 2
Xj = op("X", i[j])

XjZp = apply(Xj, Zp);


st = [k == j ? "Zm" : "Zp"
      for k in 1:n];
XjZp = MPS(i, st);
```



Tutorial: n-site states with MPS

```
j = n ÷ 2
Xj = op("X", i[j])

XjZp = apply(Xj, Zp);


st = [k == j ? "Zm" : "Zp"
      for k in 1:n];
XjZp = MPS(i, st);
```




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

Tutorial: n-site operators with MPO

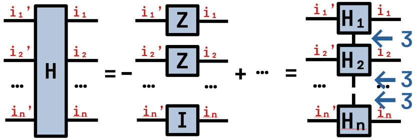
```julia
function ising(n; h)
  H = OpSum()
  for j in 1:(n - 1)
    H -= "Z", j, "Z", j + 1
  end
  for j in 1:n
    H += h, "X", j
  end
  return H
end

h = 0.5 # field
H = MPO(ising(n; 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

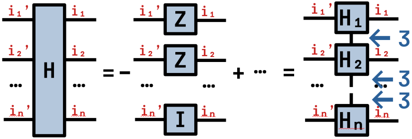
```julia
function ising(n; h)
  H = OpSum()
  for j in 1:(n - 1)
    H -= "Z", j, "Z", j + 1
  end
  for j in 1:n
    H += h, "X", j
  end
  return H
end

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

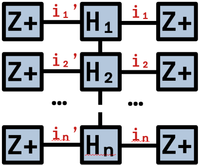


Tutorial: n-site operators with MPO

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

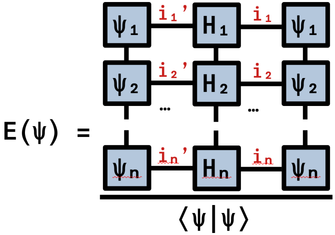
```julia
Zp = MPS(i, "Zp");
inner(Zp', H, Zp) ≈ -(n-1)

```





Tutorial: n-site state optimization

```julia
function E(ψ)
  ψHψ = inner(ψ', H, ψ)
  ψψ = inner(ψ, ψ)
  return ψHψ / ψψ
end
∂E(ψ) = gradient(E, ψ)[1]
```



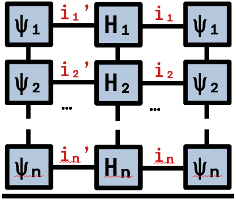
$$\min_{\psi} E(\psi) \qquad \partial_{\psi} E(\psi)$$

Tutorial: n-site state optimization

```julia
function minimize(f, ∂f, x;
                  nsteps,γ,
                  kwargs...)
  for n in 1:nsteps
    x=-(x,γ*∂f(x);kwargs...)
    println("Step = $(n),
          f(x) = $(f(x))")
  end
  return x
end
```

```julia
ψ0 = MPS(i, "Zp");
ψ = minimize(E, ∂E, ψ0;
      nsteps=50,γ=0.1,
      cutoff=1e-5);
ψ /= norm(ψ);

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

E(ψ) =



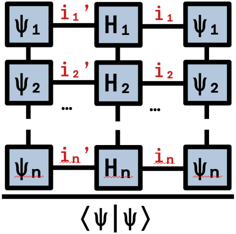
⟨ψ|ψ⟩

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

Tutorial: n-site state optimization

```
function minimize(f, ∂f, x;
                  nsteps,γ,
                  kwargs...)
  for n in 1:nsteps
    x=-(x,γ*∂f(x);kwargs...)
    println("Step = $(n),
            f(x) = $(f(x))")
  end
  return x
end
```

E(ψ) =



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

```
ψ0 = MPS(i, "Zp");
ψ = minimize(E, ∂E, ψ0;
      nsteps=50,γ=0.1,
      cutoff=1e-5);
ψ /= norm(ψ);

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

```
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)
  Uθ = ITensor[]
  for l in 1:(nlayers-1)
    θl=θ[(1:n) .+ l*n]
    Uθ=[Uθ;Ry_layer(θl,i)]
    Uθ=[Uθ;CX_layer(i)]
  end
  return Uθ
end
```

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

Tutorial: n-site circuit optimization

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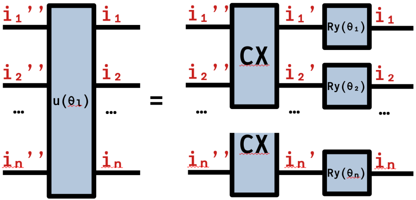
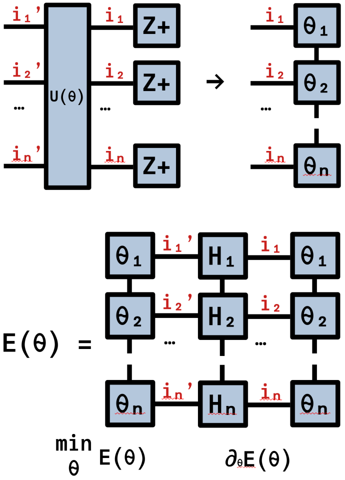


$$\prod_l u(\theta_l) \rightarrow U(\theta)$$

Tutorial: n-site states with MPS

```julia
ψ0 = MPS(i, "Zp");
nlayers = 6
function E(θ)
  ψθ = apply(U(θ,i;nlayers),ψ0)
  return inner(ψθ',H,ψθ)
end
∂E(θ) = gradient(E, θ)[1]

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



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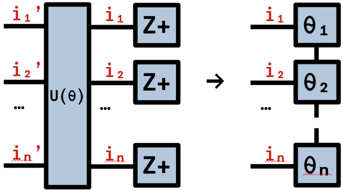
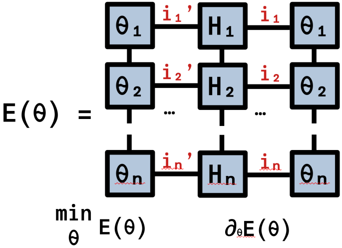
```

```julia
ψθ = apply(U(θ,i;nlayers),ψ0);
maxlinkdim(ψ0) == 1
maxlinkdim(ψθ) == 3
E(θ0) # ≈ -29
E(θ) # ≈ -31.017062
```

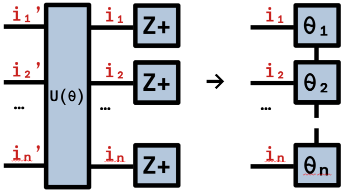


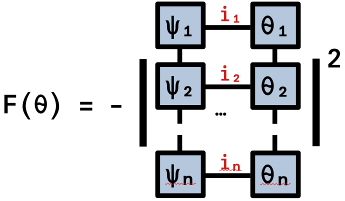


Tutorial: n-site states with MPS

```
ψ0 = MPS(i, "Zp");
nlayers = 6
function F(θ)
  ψθ=apply(U(θ,i;nlayers),ψ0)
  return -abs2(inner(ψ,ψθ))
end
∂F(θ) = gradient(F, θ)[1]

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





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

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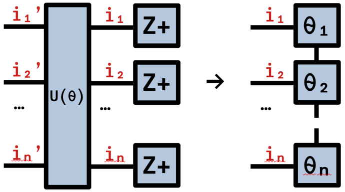
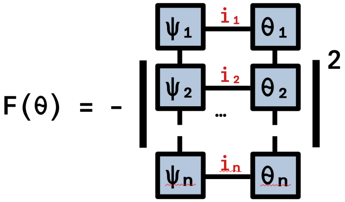
```

```julia
maxlinkdim(ψ0) == 1
maxlinkdim(ψθ) == 2
F(θ0) # ≈ -0.556066
F(θ) # ≈ -0.989336
```





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Other features not mentioned

- Noisy state and process simulation (PastaQ).
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- More that I am probably forgetting... Ask Giacomo and me for more details.

Future directions/in progress

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

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