# 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 1, 2022

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

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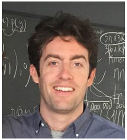

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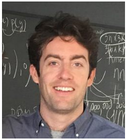

julia

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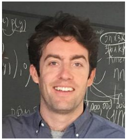

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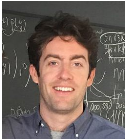

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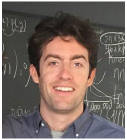

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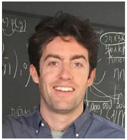

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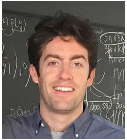

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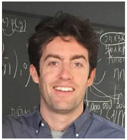

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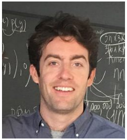

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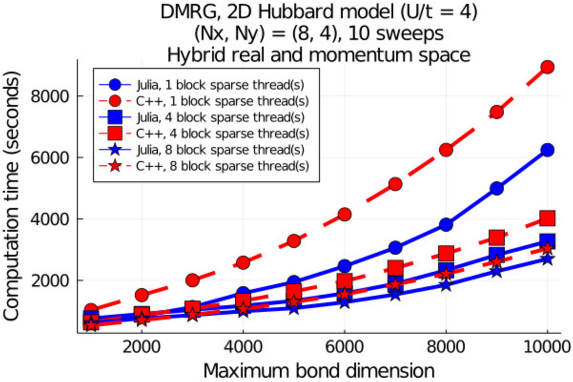

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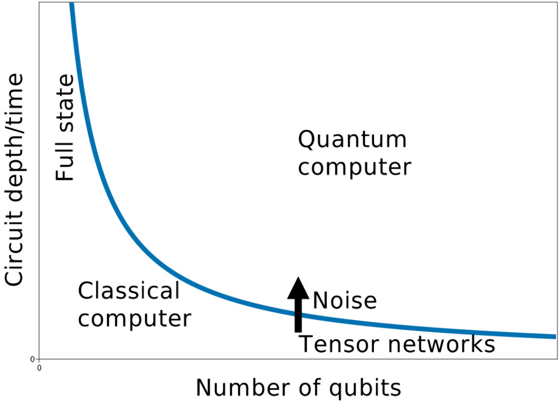
  - Find out more: [github.com/GTorlai/PastaQ.jl](https://github.com/GTorlai/PastaQ.jl)

## *When should I use tensor networks?*

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



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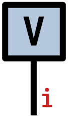
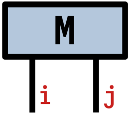
  - This is not the focus of ITensor and PastaQ at the moment, specialized libraries like Yao.jl may be faster.
- Tensor networks are a common, general language for reasoning about quantum many-body systems (for example, quantum circuits).

## *What are tensor networks?*

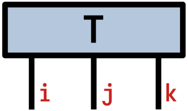
Vector $V_i$
Order-1 tensor




Matrix $M_{ij}$
Order-2 tensor




Tensor $T_{ijk}$
Order-3 tensor



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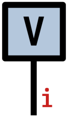
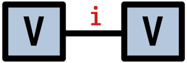



$\langle V|V\rangle = V_i V_i$

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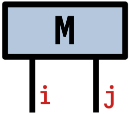


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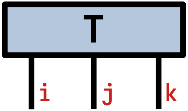


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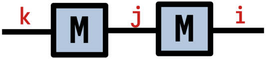

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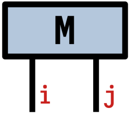


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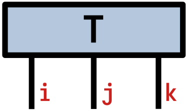


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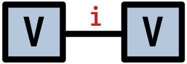


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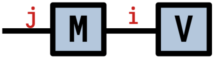
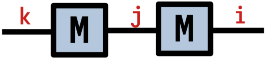
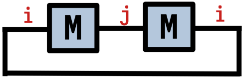


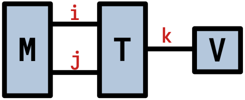

$$MM = M_{kj} M_{ji}$$




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




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



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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*

```julia
using ITensors

i = Index(2)


```

Load ITensor

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

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

Construct from a Vector

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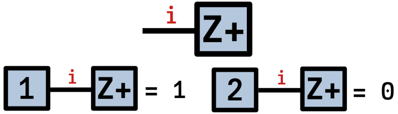


# *Tutorial: One-site state basics*

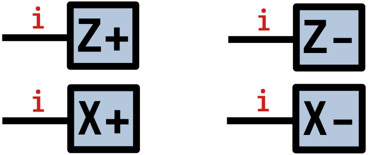
```
Zp = ITensor([1, 0], i)
Zm = ITensor([0, 1], i)
Xp = ITensor([1, 1]/√2, i)
Xm = ITensor([1, -1]/√2, i)
```

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

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

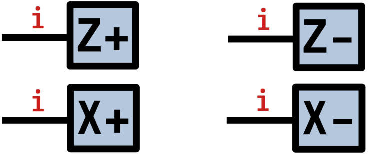
# *Tutorial: One-site state basics*

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



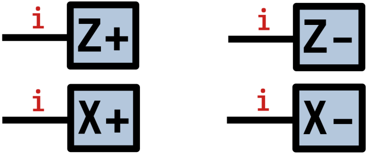

```
Xp = (Zp + Zm)/√2



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

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

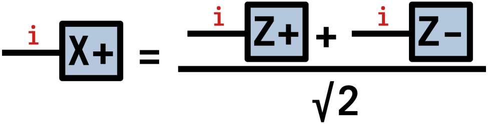
$$\langle Z+|X+\rangle \approx 1/\sqrt{2}$$
$$\langle Z+|X+\rangle \approx 1/\sqrt{2}$$

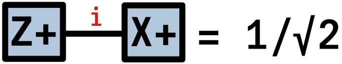
# *Tutorial: One-site state basics*

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



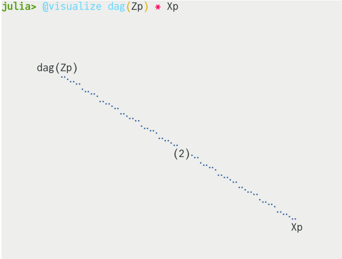

```
Xp = (Zp + Zm)/√2



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



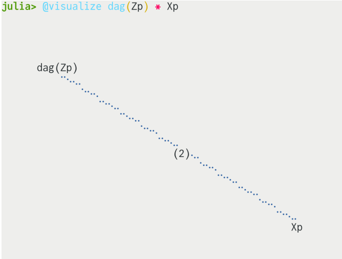
# *Tutorial: One-site state basics*

```julia
using ITensorUnicodePlots

@visualize dag(Zp) * Xp
```

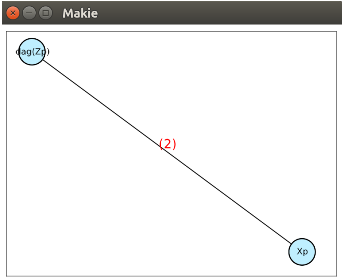


# *Tutorial: One-site state basics*

```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("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*

```
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)
```

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

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

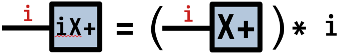
# *Tutorial: Custom one-site states*

```julia
import ITensors: state


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

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


inner(Zm, iXm)
```

Overload ITensors.jl behavior

Define a state with the name "iX-"



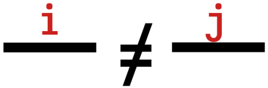
# *Tutorial: Priming*

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

i ≠ j
```

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

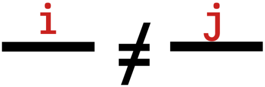
# *Tutorial: Priming*

```
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
```

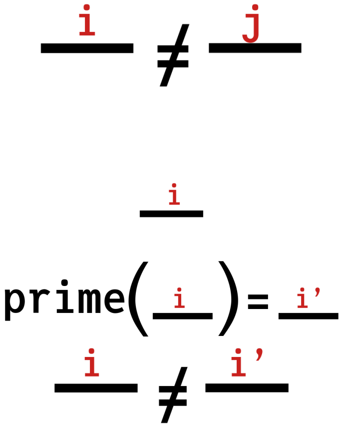
(dim=2|id=837)

(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', dag(i))


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

Matrix representation Z

Convert to ITensor

Use predefined definition

# *Tutorial: One-site operators*

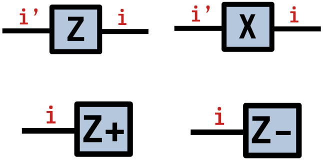
```
Z = op("Z", i)
X = op("X", i)

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

Z
X

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

# *Tutorial: One-site operators*

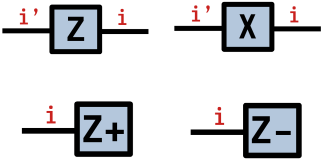
```
Z = op("Z", i)
X = op("X", i)

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
```

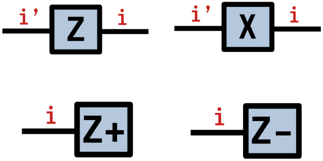



$$X|\text{Z+}\rangle = |\text{Z-}\rangle$$

# *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
```



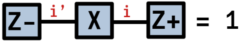

## *Tutorial: One-site operators*

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

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

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

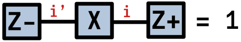
# *Tutorial: One-site operators*

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

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



# *Tutorial: One-site operators*

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

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



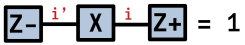

```
apply(X, Zp) ==
  noprime(X * Zp)



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

$$X|Z+\rangle$$

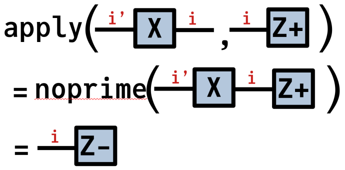
$$\langle Z-|X|Z+\rangle \approx 1$$

# *Tutorial: One-site operators*

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

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




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



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



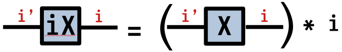
## *Tutorial: Custom one-site operators*

```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*

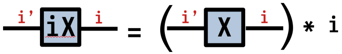
```julia
import ITensors: op

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



# *Tutorial: Custom one-site operators*

```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*

```julia
import ITensors: op

function op(
  ::OpName"iX",
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)
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    im 0
  ]
end
```
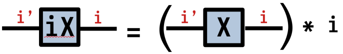




```julia
op("iX", i)
```

```julia
X * im
```

# *Tutorial: Two-site states*

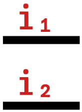
```julia
i1 = Index(2, "S=1/2")
i2 = Index(2, "S=1/2")

i1 ≠ i2

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

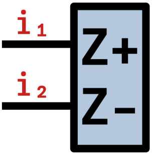
(dim=2|id=505|"S=1/2")
(dim=2|id=576|"S=1/2")

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

# *Tutorial: Two-site states*

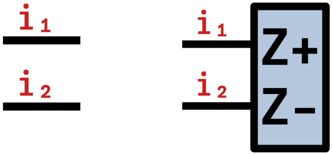
```
i1 = Index(2, "S=1/2")
i2 = Index(2, "S=1/2")

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
```

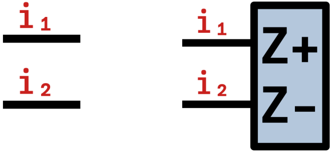
$|Z+\rangle_1$
$|Z+\rangle_2$

$|Z\text{-}\rangle_1$
$|Z\text{-}\rangle_2$

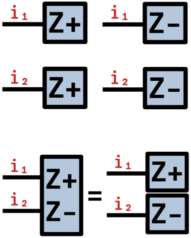
$$|Z{+}Z\text{-}\rangle = |Z+\rangle_1 |Z\text{-}\rangle_2$$

# *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*

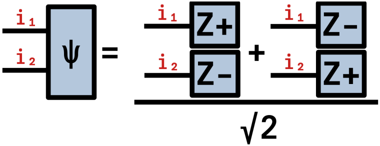
```
ψ = ITensor(i1, i2)
ψ[i1=>1, i2=>2] = 1/√2
ψ[i1=>2, i2=>1] = 1/√2

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

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

From single-site states

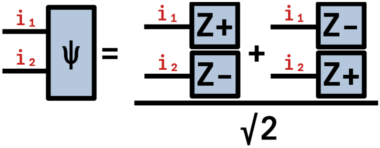
# *Tutorial: Two-site states*

```
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)


U, S, V = svd(ZmZp, i1)
s = diag(S)

U, S, V = svd(ψ, i1)
s = diag(S)
```

$\approx 1$

$\approx 1/\sqrt{2}$

$\approx [1,\ 0]$

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

# *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)


U, S, V = svd(ZmZp, i1)
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U, S, V = svd(ψ, i1)
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```
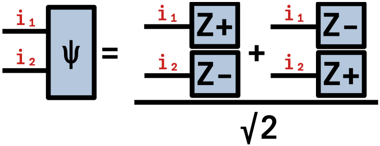
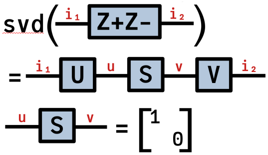
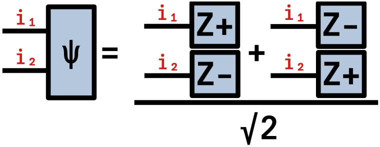



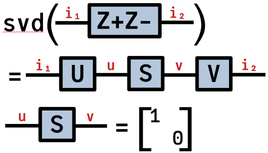



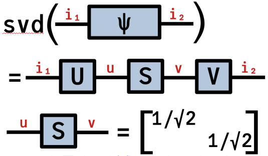
# *Tutorial: Two-site states*

```
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)


U, S, V = svd(ZmZp, i1)
s = diag(S)

U, S, V = svd(ψ, i1)
s = diag(S)
```



# *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 ($n = 2$)

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

Alternative:
Build from single-site operators.
(Less error-prone.)

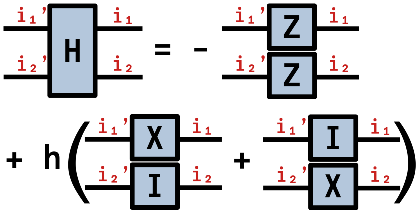
# *Tutorial: Two-site operators*

```
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 ($n = 2$)

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



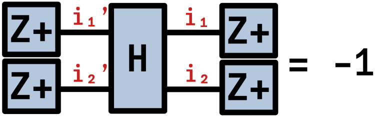
# *Tutorial: Two-site operators*

```
ZpZp = Zp1 * Zp2

inner(ZpZp', H, ZpZp)
```

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

## *Tutorial: Two-site operators*

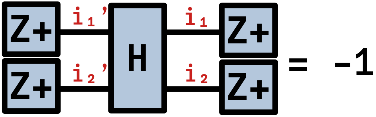
```
ZpZp = Zp1 * Zp2

inner(ZpZp', H, ZpZp)
```



# *Tutorial: Two-site operators*

```
ZpZp = Zp1 * Zp2

inner(ZpZp', H, ZpZp)
```

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

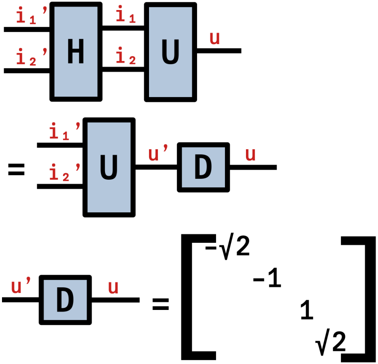



$\approx$ [-√2, -1, 1, √2]

# *Tutorial: Two-site operators*

```
ZpZp = Zp1 * Zp2

inner(ZpZp', H, ZpZp)
```

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



# *Tutorial: Custom two-site operators*

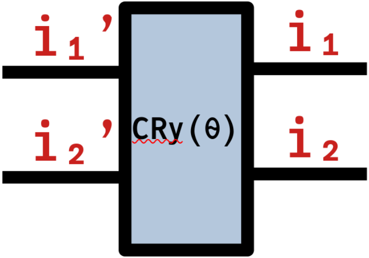
```julia
import ITensors: op

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*

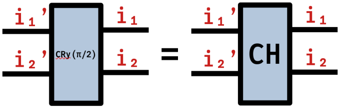
```
CH = op("CRy", i1, i2; θ=π/2)
```

Controlled-Hadamard gate

$\mathrm{CH} = \mathrm{CRy}(\theta{=}\pi/2)$

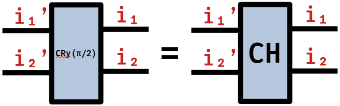
# *Tutorial: Custom two-site operators*

```
CH = op("CRy", i1, i2; θ=π/2)
```



# *Tutorial: Custom two-site operators*

```
CH = op("CRy", i1, i2; θ=π/2)
```

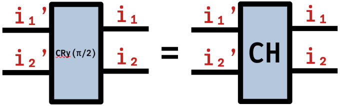



```
apply(CH, Zp * Zm) ==
  Zp1 * Xm2
```

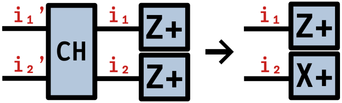
$$\text{CH}|\text{Z+Z-}\rangle = |\text{Z+X-}\rangle$$

# *Tutorial: Custom two-site operators*

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




```julia
apply(CH, Zp * Zm) ==
  Zp1 * Xm2
```



## *Tutorial: Two-site state optimization*

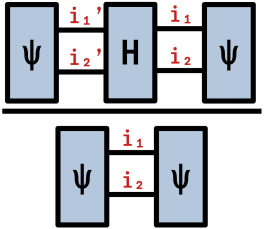
```
function E(ψ)
  ψHψ = inner(ψ', H, ψ)
  ψψ = inner(ψ, ψ)
  return ψHψ / ψψ
end
```

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

# *Tutorial: Two-site state optimization*

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

E(ψ) =

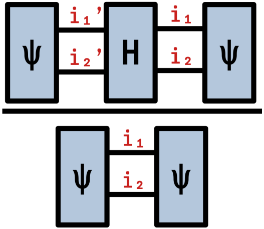


# *Tutorial: Two-site state optimization*

```
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
```

E(ψ) =



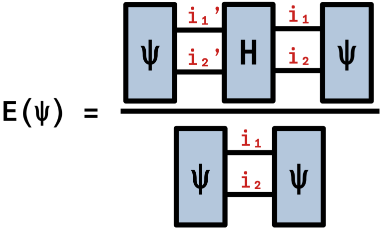

Gradient descent.

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

# *Tutorial: Two-site state optimization*

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

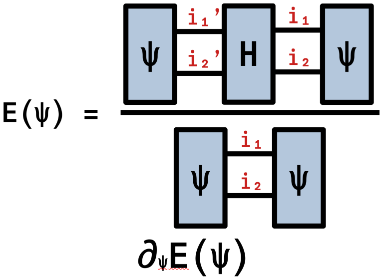
```
function minimize(f, ∂f, x;
  nsteps, γ)
  for n in 1:nsteps
    x = x - γ * ∂f(x)
  end
  return x
end
```




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

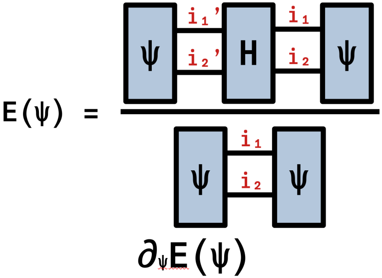
# *Tutorial: Two-site state optimization*

```
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*

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

E(ψ0) == -1

using Zygote # autodiff

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



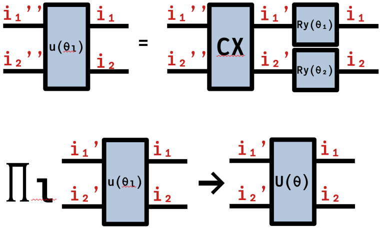

```
ψ = minimize(E, ∂E, ψ0;
       nsteps=10, γ=0.1)

E(ψ0), norm(∂E(ψ0))
E(ψ), norm(∂E(ψ))
```

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

(-1, 2)
(-1.4142131, 0.0010865277)
$\quad \approx$ (-$\sqrt{2}$, 0)

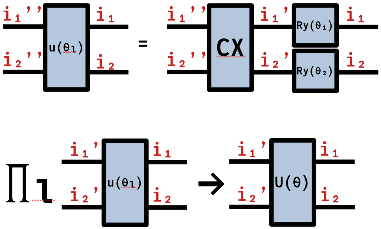
# *Tutorial: Two-site circuit optimization*

```
# 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, j1, j2) = [
  ("Ry", j1, (; θ=θ[1])),
  ("Ry", j2, (; θ=θ[2])),
  ("CNOT", j1, j2),
  ("Ry", j1, (; θ=θ[3])),
  ("Ry", j2, (; θ=θ[4])),
]

U(θ, i1, i2) =
  buildcircuit(u(θ, 1, 2), [i1, i2])
```



# *Tutorial: Two-site circuit optimization*

```
ψ0 = Zp1 * Zp2


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

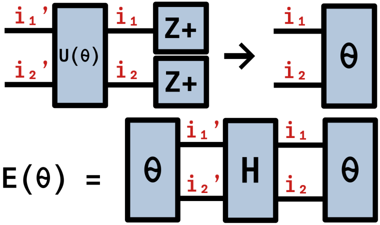
References state:

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

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

# *Tutorial: Two-site circuit optimization*

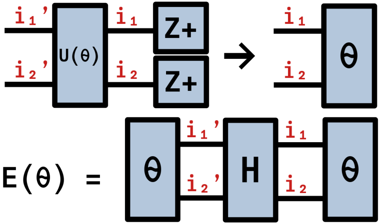
```
ψ0 = Zp1 * Zp2


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



# *Tutorial: Two-site circuit optimization*

```
ψ0 = Zp1 * Zp2


function E(θ)
  ψθ = apply(U(θ), 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
```

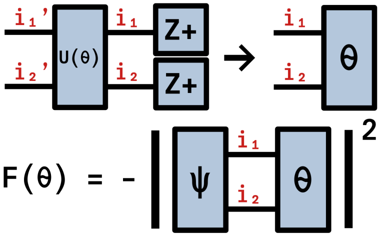
Reference state:
$|0\rangle = |Z{+}Z{+}\rangle$

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

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

# *Tutorial: Two-site fidelity optimization*

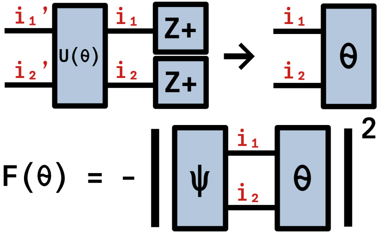
```
ψ0 = Zp1 * Zp2
ψ = (ZpZp + ZmZm) / √2



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
```




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

# *Tutorial: n-site states with MPS*

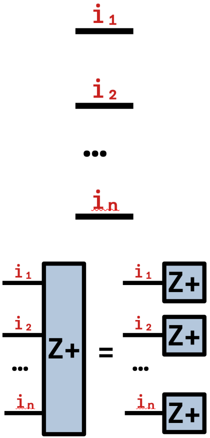
```julia
n = 30
i = [Index(2, "S=1/2")
          for j in 1:n]


Zp = MPS(i, "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
```



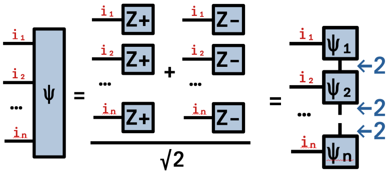
# *Tutorial: n-site states with MPS*

```
ψ = (Zp + Zm)/√2


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

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

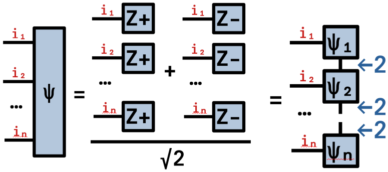
# *Tutorial: n-site states with MPS*

```
ψ = (Zp + Zm)/√2


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



# *Tutorial: n-site states with MPS*

```
ψ = (Zp + Zm)/√2


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



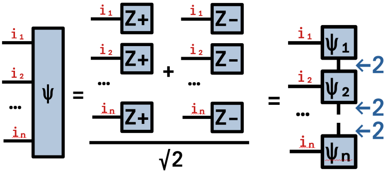

```
inner(Zp, Zp) == 1


inner(Zp, ψ) == 1/√2
```

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

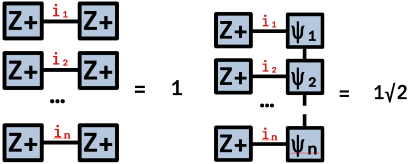
$$\langle Z+|\psi\rangle = 1/\sqrt{2}$$

# *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*

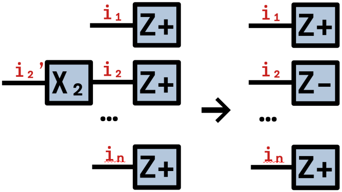
```
j = n ÷ 2
Xⱼ = op("X", i[j])

XⱼZp = apply(Xⱼ, Zp)


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

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

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

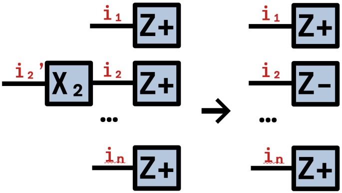
*Tutorial: n-site states with MPS*

```julia
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)
```



# *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*

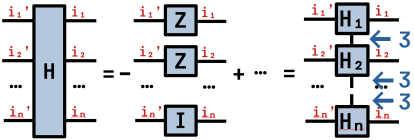
```julia
function ising(n; h)
  H = OpSum()
  for j in 1:(n - 1)
    H -= "Z", j, "Z", j + 1
  end
  for j in 1:n
    H += h, "X", j
  end
  return H
end

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

$n$ sites

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

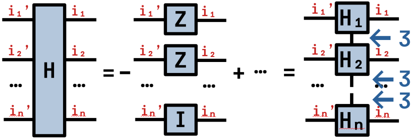
# *Tutorial: n-site operators with MPO*

```
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
```

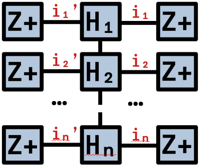


*Tutorial: n-site operators with MPO*

```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)
```

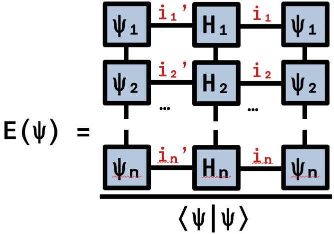


# *Tutorial: n-site state optimization*

```
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)
```




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

# *Tutorial: n-site state optimization*

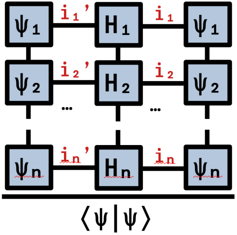
```
ψ0 = MPS(i, "Z+")

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)
```

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

E(ψ) =




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

# *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*

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```

```
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
```

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

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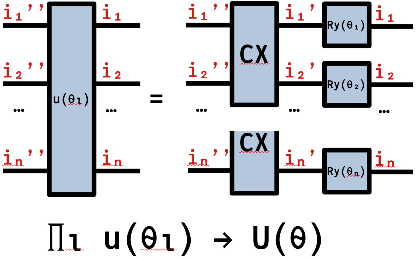
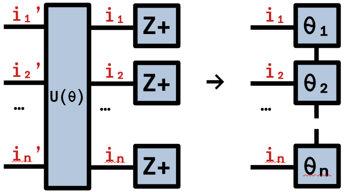
end
```

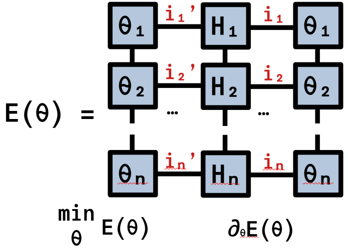


# *Tutorial: n-site states with MPS*

```
ψ_0 = MPS(i, "Z+")
nlayers = 6
function E(θ)
  ψ_θ = apply(U(θ, i; nlayers), ψ_0)
  return inner(ψ_θ', H, ψ_θ)
end

θ_0 = zeros(nlayers * n)
θ = minimize(E, ∂E, θ_0;
        nsteps=20, γ=0.1)
```



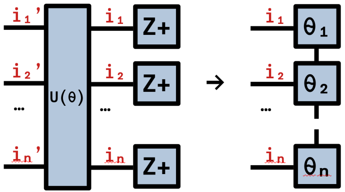



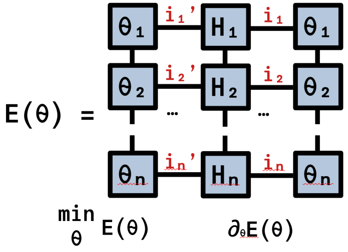
# *Tutorial: n-site states with MPS*

```
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)
```

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

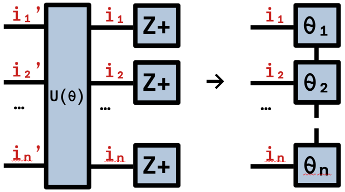


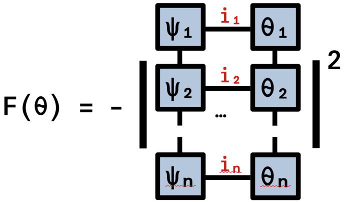



# *Tutorial: n-site states with MPS*

```
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)
```




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

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θ = minimize(F, ∂F, θ₀;
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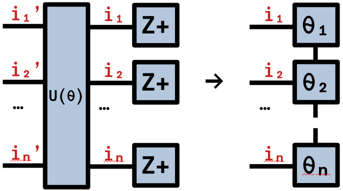
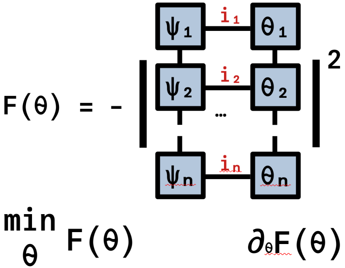
```

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



## *Other features not mentioned*

- Noisy state and process simulation (PastaQ). AD/optimization support in progress.

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

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- Infinite MPS and tensor network tools like VUMPS and TDVP.
- Improved MPO compression for time evolving operators.
- 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!