Analyzing Quantum Many-Body Systems with ITensor and PastaQ

Matthew Fishman
Center for Computational Quantum Physics (CCQ)
Flatiron Institute, NY
https://mtfishman.github.io/

February 26, 2022

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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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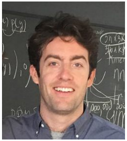
- Stands for “Intelligent Tensor”.

ITensor



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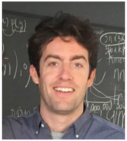

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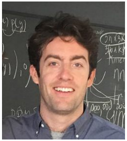

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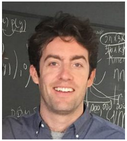

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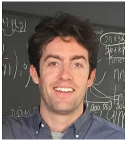

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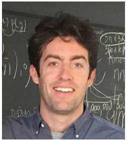

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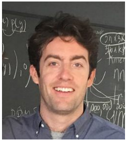

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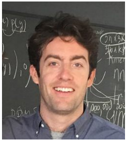

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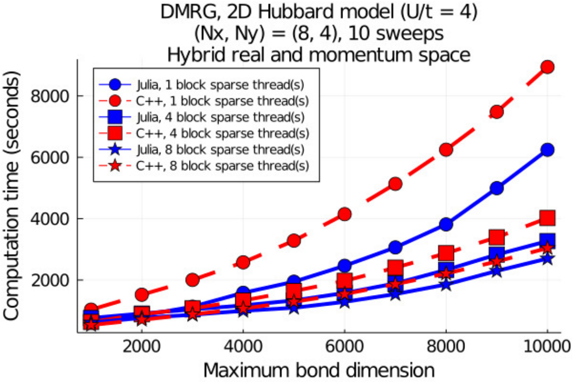

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- Find out more: github.com/GTorlai/PastaQ.jl

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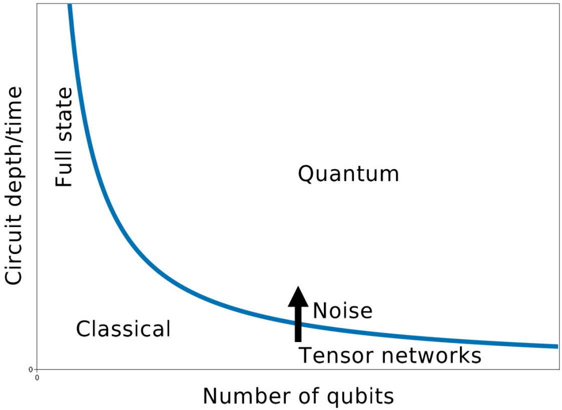
- Tensor networks are a common, general language for reasoning about quantum many-body systems (for example, quantum circuits).

When should I use tensor networks?

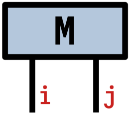
- In my opinion, tensor networks are the best general purpose tool we have right now for studying quantum many-body systems (while we wait for a general purpose quantum computer).



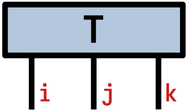
What are tensor networks?

Vector V_i
Order-1 tensor

Matrix M_{ij}
Order-2 tensor



Tensor T_{ijk}
Order-3 tensor



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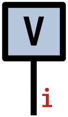

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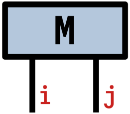

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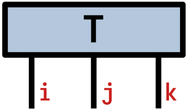
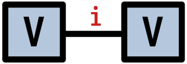
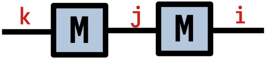


Vector inner product



Matrix-vector multiplication

Matrix-matrix multiplication



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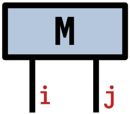

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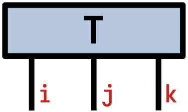

Vector inner
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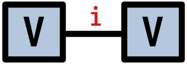
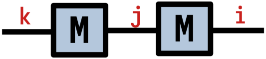
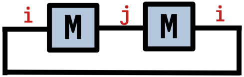


Matrix-vector
multiplication

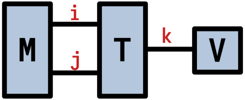
Matrix-matrix
multiplication



Trace of matrix-matrix
multiplication



General tensor
network



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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:

```julia
julia> using ITensors

julia> i = Index(2);

julia> A = ITensor(i);

julia> using PastaQ

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

julia> $\psi$ = 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

```
using ITensors

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Tutorial: One-site state basics

```julia
using ITensors

i = Index(2)


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

Zp = ITensor([1, 0], i)
```

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

Construct from a Vector

Tutorial: One-site state basics

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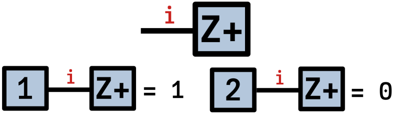

Tutorial: One-site state basics

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

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

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

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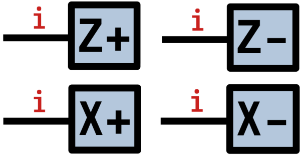

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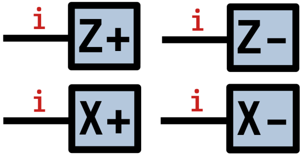


```
(Zp + Zm)/√2
dag(Zp) * Xp
(dag(Zp) * Xp)[]
inner(Zp, Xp)
norm(Xp)
```

$\approx$ Xp

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

$\approx 1/\sqrt{2}$

$\approx 1/\sqrt{2}$

≈ 1

Tutorial: One-site state basics

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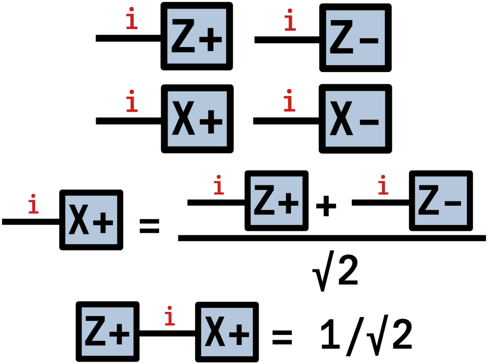
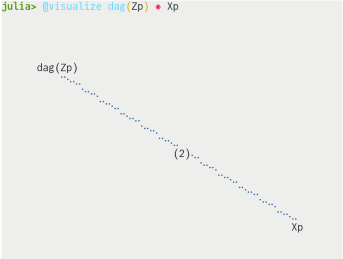


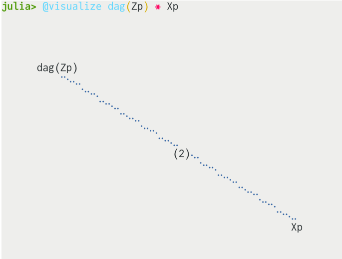
Tutorial: One-site state basics

```julia
using ITensorUnicodePlots

@visualize dag(Zp) * Xp
```

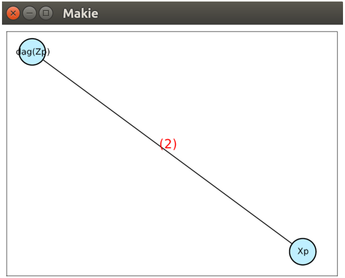


Tutorial: One-site state basics

```julia
using ITensorUnicodePlots

@visualize dag(Zp) * Xp
```




```julia
using ITensorGLMakie

@visualize dag(Zp) * Xp
```



Tutorial: One-site states

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

"S=1/2" defines an operator basis

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

Tutorial: One-site states

```
i = Index(2, "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)
(Zp + Zm)/√2
(Zp - Zm)/√2
```

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

$\approx$ im * Xm

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

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

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-”

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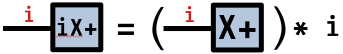
iXm = state("iX-", i)

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



Tutorial: Priming

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

i == j
```

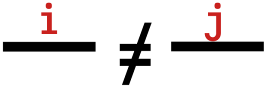
(dim=2|id=837)
(dim=2|id=899)

false

Tutorial: Priming

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

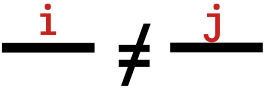
i == j
```



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)'
(dim=2|id=837)'
true
true

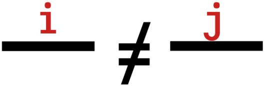
Tutorial: Priming

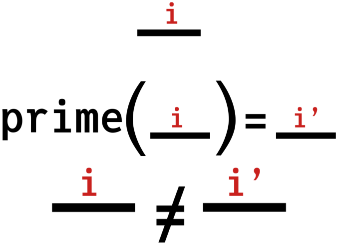
```
i = Index(2)
j = Index(2)

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)
```

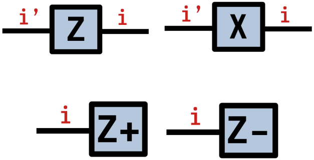
Z
X

|Z+⟩
|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)
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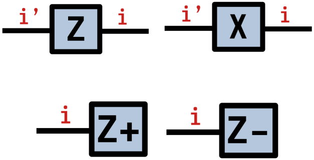
```




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

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

false

true

true

Tutorial: One-site operators

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

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

```
XZp = X * Zp
XZp == Zm
XZp == Zm'
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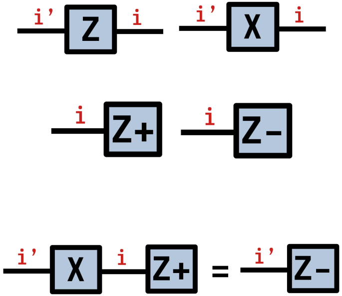


Tutorial: One-site operators

```
XZp = X * Zp

dag(Zm) * XZp

dag(Zm') * XZp
dag(Zp') * XZp

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

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

$$|\mathrm{Z}-\rangle\langle \mathrm{Z}+|X$$

$$\langle \mathrm{Z}-|X|\mathrm{Z}+\rangle \approx 1$$
$$\langle \mathrm{Z}+|X|\mathrm{Z}+\rangle \approx 0$$

$$\langle \mathrm{Z}-|X|\mathrm{Z}+\rangle \approx 1$$
$$\langle \mathrm{Z}-|X|\mathrm{Z}+\rangle \approx 1$$

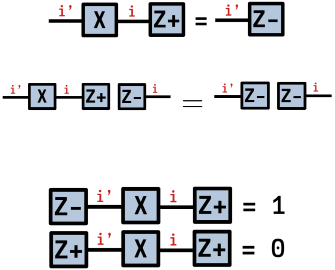
Tutorial: One-site operators

```
XZp = X * Zp

dag(Zm) * XZp

dag(Zm') * XZp
dag(Zp') * XZp

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



Tutorial: One-site operators

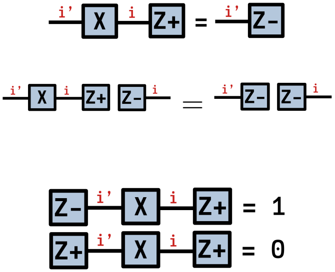
```
XZp = X * Zp

dag(Zm) * XZp

dag(Zm') * XZp
dag(Zp') * XZp

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

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



= noprime(X * Zp)

≈ 1

Tutorial: One-site operators

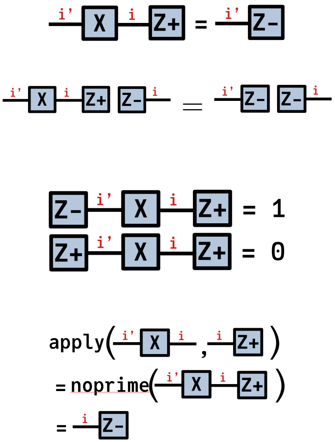
```
XZp = X * Zp

dag(Zm) * XZp

dag(Zm') * XZp
dag(Zp') * XZp

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

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



Tutorial: Custom one-site operators

```julia
import ITensors: op

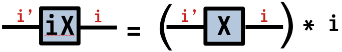
function op(
  ::OpName"iX",
  ::SiteType"S=1/2"
)
  return [
    0 im
    im 0
  ]
end
```

Overload ITensors.jl behavior

Tutorial: Custom one-site operators

```
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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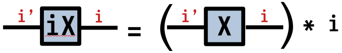
import ITensors: op

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

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



Tutorial: Custom one-site operators

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import ITensors: op

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)
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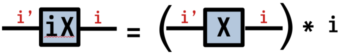
    im 0
  ]
end
```




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

```julia
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")

false

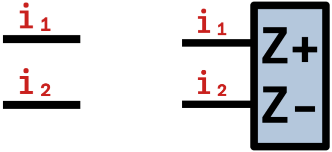
$|Z+\rangle_1 |Z\text{-}\rangle_2 = |Z{+}Z\text{-}\rangle$

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

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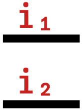
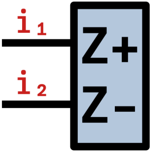
i1 = Index(2, "S=1/2")
i2 = Index(2, "S=1/2")

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
ZmZp = Zm1 * Zp2
```

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

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

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

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)

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ZpZm = Zp1 * Zm2
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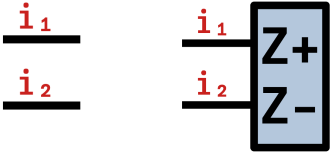
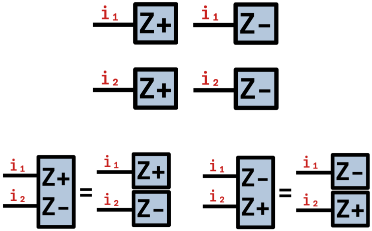




Tutorial: Two-site states

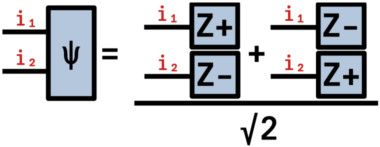
```
ψ = ITensor(i1, i2)
ψ[i1=>1, i2=>2] = 1/√2
ψ[i1=>2, i2=>1] = 1/√2

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

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

From single-site states

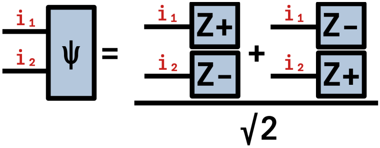
Tutorial: Two-site states

```
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(ψ, ψ)
inner(ZpZm, ψ)

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

U, S, V = svd(ψ, i1)
s = diag(S)
```

≈ 1

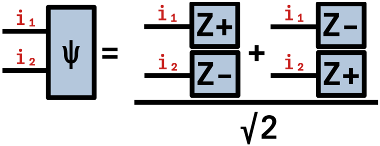
$\approx 1/\sqrt{2}$

$\approx [1, 0]$

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

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

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s = diag(S)
```
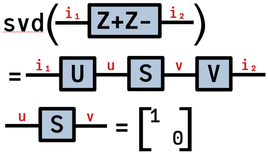
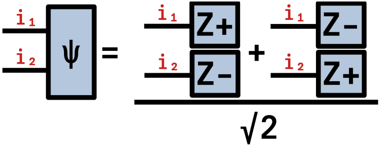
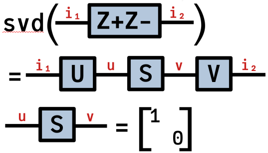



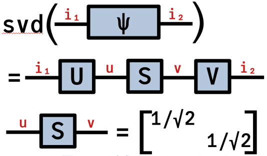
Tutorial: Two-site states

```
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(ψ, ψ)
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
# ...
```

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

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

```
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)
```

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

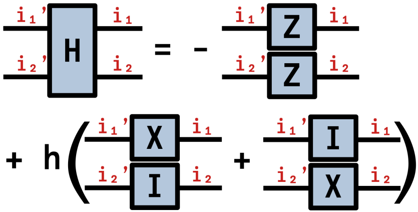
Tutorial: Two-site operators

```
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

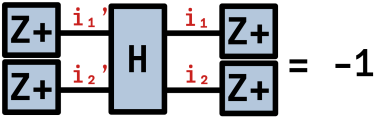
```
ZpZp = Zp1 * Zp2
(dag(ZpZp)' * H * ZpZp)[]
inner(ZpZp', H, ZpZp)
inner(ZpZp, apply(H, ZpZp))
```

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

$\approx$ -1

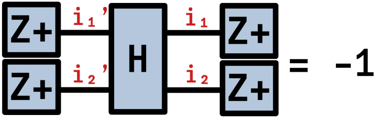
Tutorial: Two-site operators

```
ZpZp = Zp1 * Zp2



(dag(ZpZp)' * H * ZpZp)[]
inner(ZpZp', H, ZpZp)
inner(ZpZp, apply(H, ZpZp))
```



Tutorial: Two-site operators

```
ZpZp = Zp1 * Zp2



(dag(ZpZp)' * H * ZpZp)[]
inner(ZpZp', H, ZpZp)
inner(ZpZp, apply(H, ZpZp))
```



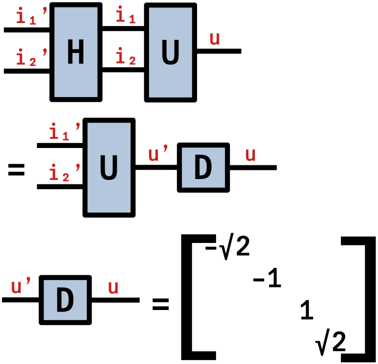

```
D, U = eigen(H)
diag(D)
```

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

Tutorial: Two-site operators

```
ZpZp = Zp1 * Zp2



(dag(ZpZp)' * H * ZpZp)[]
inner(ZpZp', H, ZpZp)
inner(ZpZp, apply(H, ZpZp))
```

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



Tutorial: Custom two-site operators

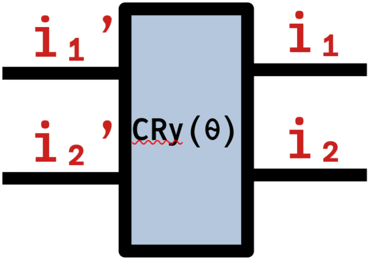
```julia
import ITensors: op

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

CRy(θ)

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
```



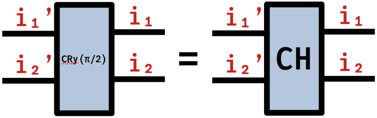
Tutorial: Custom two-site operators

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

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

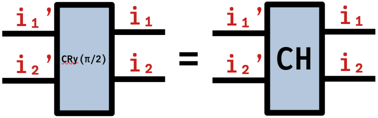
Tutorial: Custom two-site operators

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



Tutorial: Custom two-site operators

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




```
ZpZm = Zp1 * Zm2

CH_Xm = apply(CH, ZpZm)

CH_Xm ≈ Zp1 * Xm2
```

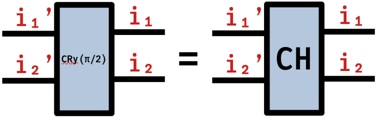
$|Z{+}Z{-}\rangle = |Z{+}\rangle_1 |Z{-}\rangle_2$

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

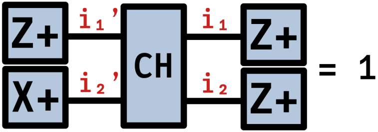
true

Tutorial: Custom two-site operators

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




```
ZpZm = Zp1 * Zm2

CH_Xm = apply(CH, ZpZm)

CH_Xm ≈ Zp1 * Xm2
```



Tutorial: Two-site state optimization

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

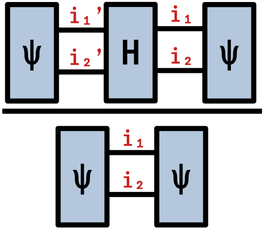
Function to minimize: Expectation value of the energy.

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

Tutorial: Two-site state optimization

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

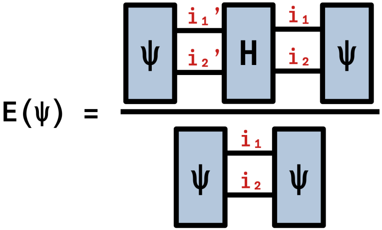
E(ψ) =



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
```

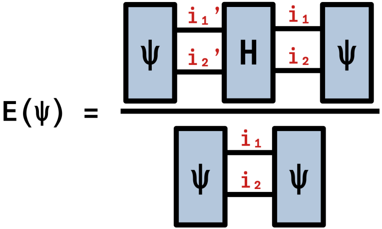


Simple gradient descent.
Must provide function f(x)
to minimize and ∂f(x),
the gradient of f at x.
γ is the gradient
descent step size.

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)

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

norm(∂E(ψ0))
```

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

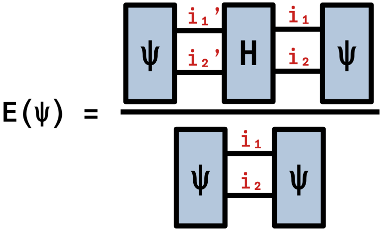
$\approx$ -1

Using Zygote for automatic differentation of the energy.

$\approx$ 2

Tutorial: Two-site state optimization

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

E(ψ0)

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

norm(∂E(ψ0))
```

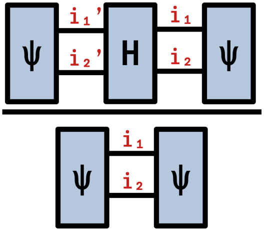


Tutorial: Two-site state optimization

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

E(ψ0)

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

norm(∂E(ψ0))
```

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

E(ψ0), norm(∂E(ψ0))
E(ψ), norm(∂E(ψ))

```

E(ψ) =



Minimize over ψ:

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

(-1, 2)

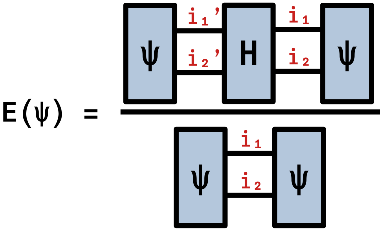
(-1.4142131, 0.0010865277)

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

Tutorial: Two-site state optimization

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

E(ψ0)

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

norm(∂E(ψ0))
```

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

E(ψ0), norm(∂E(ψ0))
E(ψ), norm(∂E(ψ))

```



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

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]),
]
```

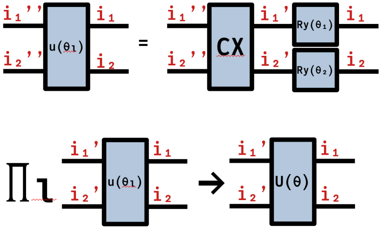
Tutorial: Two-site circuit optimization

```julia
# 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]),
]
```

```julia
# 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

```
# 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

```
ψ0 = Zp1 * Zp2


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

References state:

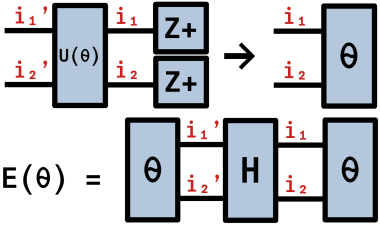
$|0\rangle = |\mathrm{Z{+}Z{+}}\rangle$

Find θ that minimizes:

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

Tutorial: Two-site circuit optimization

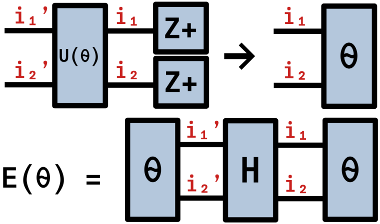
```
ψ0 = Zp1 * Zp2


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]
θ = minimize(E, ∂E, θ0;
        nsteps=40, γ=0.5)

E(θ0), norm(∂E(θ0))
E(θ), norm(∂E(θ))

```

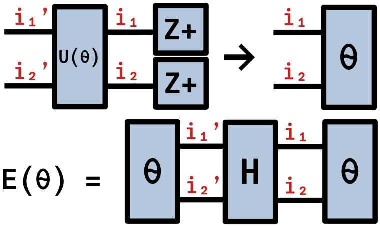


$$\min_{\theta} E(\theta) \qquad \partial_\theta E(\theta)$$

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]
θ = minimize(E, ∂E, θ0;
          nsteps=40, γ=0.5)

E(θ0), norm(∂E(θ0))
E(θ), norm(∂E(θ))

```



$(-1, \sqrt{3}/2)$

$(-1.4142077, 0.0017584116)$

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

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:

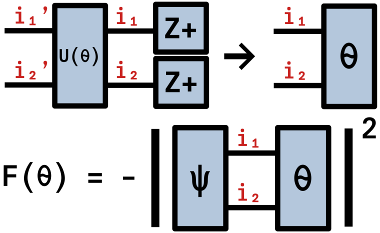
$|\psi\rangle = (|Z{+}Z{+}\rangle + |Z{-}Z{-}\rangle)/\sqrt{2}$

Find θ that minimizes:

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

Tutorial: Two-site fidelity optimization

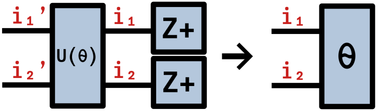
```
ψ0 = Zp1 * Zp2
ψ = (ZpZp + ZmZm) / √2



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

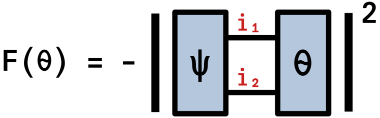


Tutorial: Two-site fidelity optimization

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

F(θ0), norm(∂F(θ0))
F(θ), norm(∂F(θ))

```

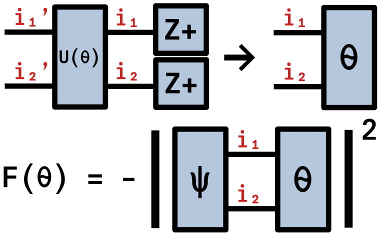




$\min_{\theta} F(\theta)$ $\partial_\theta F(\theta)$

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
```




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

F(θ₀), norm(∂F(θ₀))
F(θ), norm(∂F(θ))

```

$\approx$ (-0.5, 0.5)

$\approx$ (-0.9938992, 0.07786879)

$\approx$ (-1, 0)

Tutorial: n-site states with MPS

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

Zp = MPS(i, "Z+")
Zm = MPS(i, "Z-")

ψ = (Zp + Zm)/√2

```

n-site state

$|\mathrm{Z{+}Z{+}...Z{+}}\rangle$
$|\mathrm{Z{-}Z{-}...Z{-}}\rangle$

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

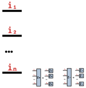
Tutorial: n-site states with MPS

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

Zp = MPS(i, "Z+")
Zm = MPS(i, "Z-")

ψ = (Zp + Zm)/√2

```



Tutorial: n-site states with MPS

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

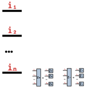
Zp = MPS(i, "Z+")
Zm = MPS(i, "Z-")

ψ = (Zp + Zm)/√2

```

```julia
maxlinkdim(Zp)
maxlinkdim(ψ)
inner(Zp, Zp)
inner(Zm, Zp)
norm(ψ)

inner(Zp, ψ)
```



1 (product state)

2 (entangled state)

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

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

$(\langle Z+| + \langle Z-|)(|Z+\rangle + |Z+\rangle)/2$

≈ 1

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

Tutorial: n-site states with MPS

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

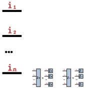
Zp = MPS(i, "Z+")
Zm = MPS(i, "Z-")

ψ = (Zp + Zm)/√2

```

```
maxlinkdim(Zp)
maxlinkdim(ψ)
inner(Zp, Zp)
inner(Zm, Zp)
norm(ψ)

inner(Zp, ψ)
```



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)
```

j = n ÷ 2
X_j

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

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

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]
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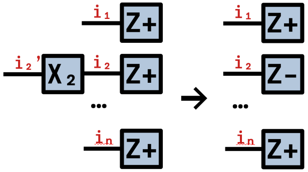


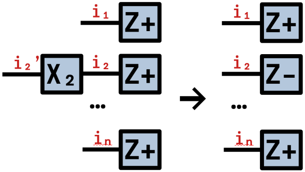
Tutorial: n-site states with MPS

```
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)
inner(Zp, X_jZp)
inner(X_jZp, apply(X_j, Zp))
```



1 (product state)

≈ 0

≈ 1

Tutorial: n-site operators with MPO

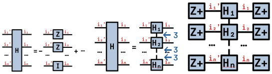
```julia
function ising(n; h)
  H = OpSum()
  for j in 1:(n - 1)
    H -= "Z", j, "Z", j + 1
  end
  for j in 1:n
    H += h, "X", j
  end
  return H
end
```

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
```

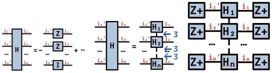


Tutorial: n-site operators with MPO

```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
```

```julia
h = 0.5
H = MPO(ising(n; h=h), i)
maxlinkdim(H)
Zp = MPS(i, "Z+")
inner(Zp', H, Zp)

```



= 3 (local Hamiltonian)

$\langle Z{+}Z{+}\ldots Z{+}|H|Z{+}Z{+}\ldots Z{+}\rangle$
$\approx -(n - 1) = -29$

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)
```

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

Minimize over ψ:
$\langle\psi|\mathrm{H}|\psi\rangle / \langle\psi|\psi\rangle$

DMRG solves:
$\mathrm{H}|\psi\rangle \approx |\psi\rangle$

Tutorial: n-site state optimization

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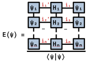

$\min_{\psi} E(\psi)$ $\partial_{\psi} E(\psi)$

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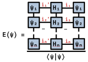

$\min_{\psi} E(\psi)$ $\quad \partial_{\psi} E(\psi)$

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

= 1 (product state)
= 3 (entangled state)
= 2 (entangled state)
≈ (-29, 5.4772256)
≈ (-31.0317917, 0.06673780)
≈ (-31.0356110, 0.02413237)

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

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

$$
\begin{aligned}
U(\theta) = \; & Ry_1(\theta_1) \; ... \; Ry_n(\theta_n) \\
& * \; CX_{1,2} \; ... \; CX_{n-1,n} \\
& * \; Ry_1(\theta_{n+1}) \; ... \; Ry_n(\theta_{2n}) \\
& * \; ...
\end{aligned}
$$

Tutorial: n-site circuit optimization

```julia
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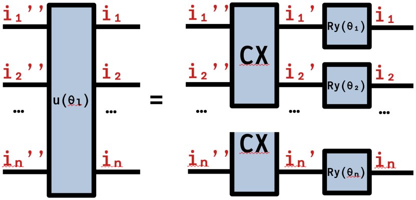
    Uθ = [Uθ; Ry_layer(θl, i)]
  end
  return Uθ
end
```



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

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)
```

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

Minimize over θ:

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

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

Tutorial: n-site states with MPS

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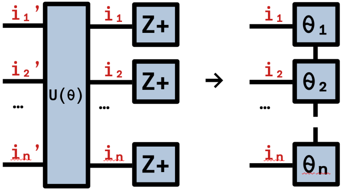

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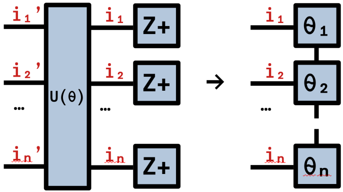
```

```
maxlinkdim(ψ0)
maxlinkdim(ψθ)
E(θ0), norm(∂E(θ0))
E(θ), norm(∂E(θ))
```



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

Tutorial: n-site states with MPS

```
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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;
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```

```
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E(θ0), norm(∂E(θ0))
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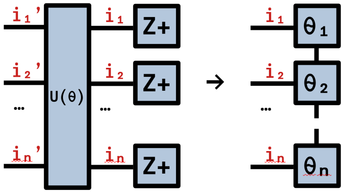

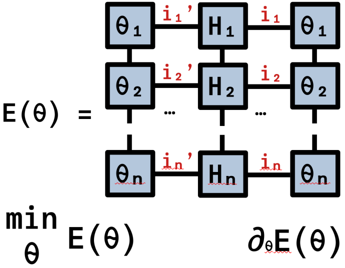

Tutorial: n-site states with MPS

```
ψ_0 = MPS(i, "Z+")
nlayers = 6
function F(θ)
  ψ_θ = apply(U(θ, i; nlayers), ψ_0)
  return -abs(inner(ψ', ψ_θ))^2
end

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

```
# |0⟩ = |Z+Z+...Z+⟩

# Minimize over θ:
# F(θ) = −|⟨ψ|U(θ)|0⟩|^2
#      = −|⟨ψ|θ⟩|2
```

Tutorial: n-site states with MPS

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end

θ0 = zeros(nlayers * n)
θ = minimize(F, ∂F, θ0;
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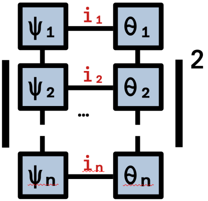
```

$F(\theta) = -$



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

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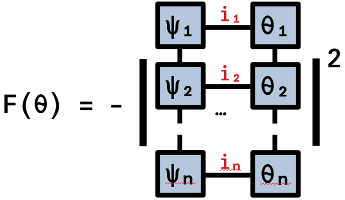

$$\min_{\theta} F(\theta) \qquad \partial_\theta F(\theta)$$

```
maxlinkdim(ψ0)
maxlinkdim(ψθ)
F(θ0), norm(∂F(θ0))
F(θ), norm(∂F(θ))
```

```
# 1 (product state)
# 2 (entangled state)
# (−0.556066, 0.895717)
# (−0.995230, 0.048939)
```

Future directions

- 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!).

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- Many ongoing projects and directions: quantum chemistry (for example UCC), real space parallel DMRG, TDVP, and TEBD, MPO compression tools, general approximate contraction techniques for unstructured networks, contracting and optimizing general tensor networks with AD, infinite MPS and tensor network tools like VUMPS and TDVP, trying out different network topologies for noisy circuit tomography, simulation and optimization.

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