Analyzing Quantum Many-Body Systems with ITensor and PastaQ

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

March 1, 2022

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Who am I?

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mtfishman.github.io

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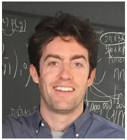

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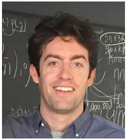

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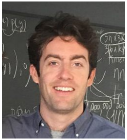

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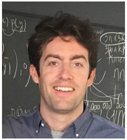

julia

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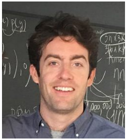

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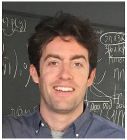

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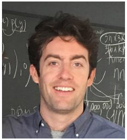

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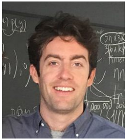

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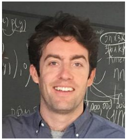

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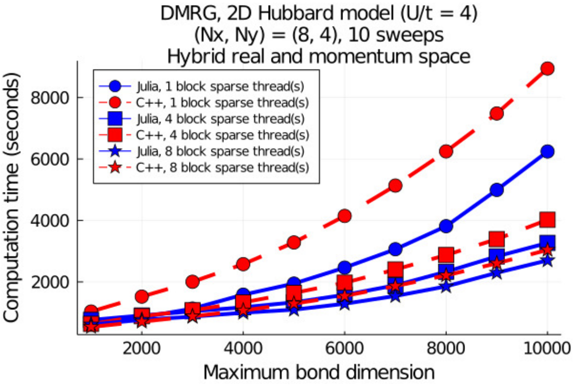
- Great numerical libraries, code ended up faster.



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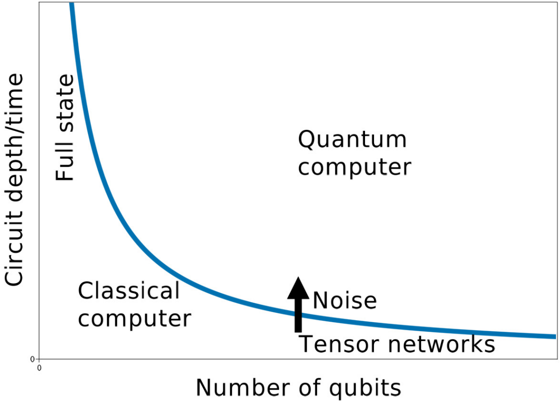
  - Find out more: github.com/GTorlai/PastaQ.jl

When should I use tensor networks?

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



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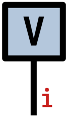
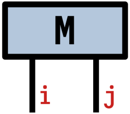
  - ITensor and PastaQ handle this seamlessly.
  - This is not the focus of ITensor and PastaQ at the moment, specialized libraries like Yao.jl may be faster.
- Tensor networks are a common, general language for reasoning about quantum many-body systems (for example, quantum circuits).

What are tensor networks?

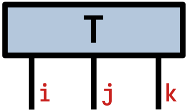
Vector V_i
Order-1 tensor



Matrix M_{ij}
Order-2 tensor



Tensor T_{ijk}
Order-3 tensor



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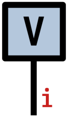
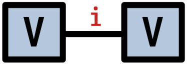


$$\langle V|V\rangle = V_i V_i$$



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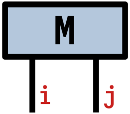

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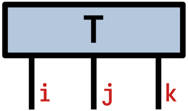

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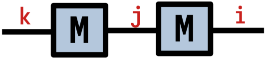

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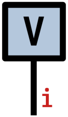

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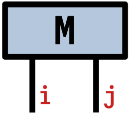

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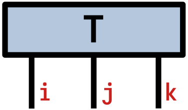

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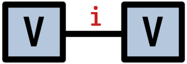

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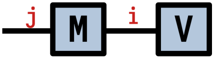

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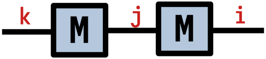
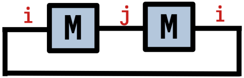
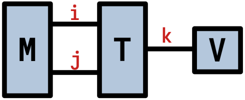


$tr(MM) = M_{ij} M_{ji}$



$M_{ij} T_{ijk} V_k$



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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

```
using ITensors

i = Index(2)


```

Load ITensor

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

Tutorial: One-site state basics

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Tutorial: One-site state basics

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

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

Construct from a Vector

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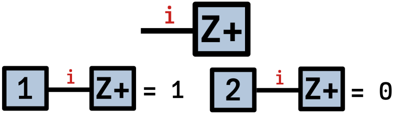

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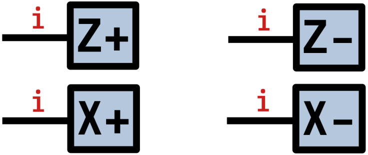
```
Zp = ITensor([1, 0], i)
Zm = ITensor([0, 1], i)
Xp = ITensor([1, 1]/√2, i)
Xm = ITensor([1, -1]/√2, i)
```

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

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

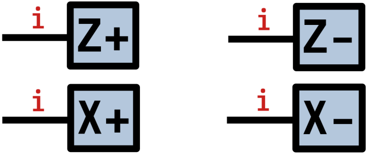
Tutorial: One-site state basics

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



Tutorial: One-site state basics

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




```
Xp = (Zp + Zm)/√2



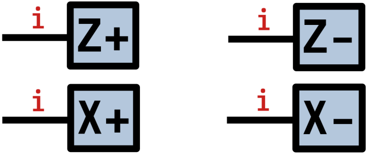
dag(Zp) * Xp
inner(Zp, Xp)
```

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

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

Tutorial: One-site state basics

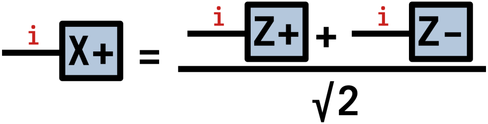
```
Zp = ITensor([1, 0], i)
Zm = ITensor([0, 1], i)
Xp = ITensor([1, 1]/√2, i)
Xm = ITensor([1, -1]/√2, i)
```

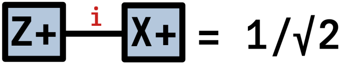



```
Xp = (Zp + Zm)/√2



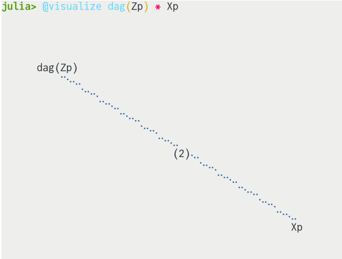
dag(Zp) * Xp
inner(Zp, Xp)
```





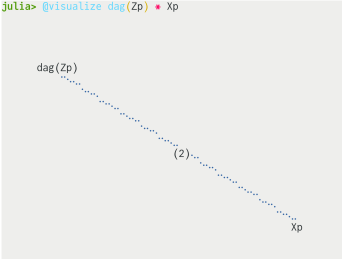
Tutorial: One-site state basics

```julia
using ITensorUnicodePlots

@visualize dag(Zp) * Xp
```

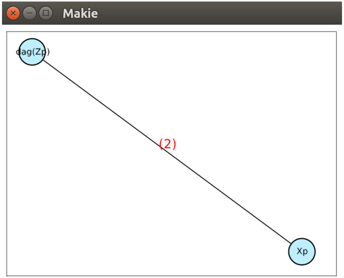


Tutorial: One-site state basics

```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

```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

```
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-"

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


inner(Zm, iXm)
```

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

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

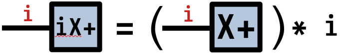
Tutorial: Custom one-site states

```julia
import ITensors: state


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

Overload ITensors.jl behavior

Define a state with the name “iX-”

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


inner(Zm, iXm)
```



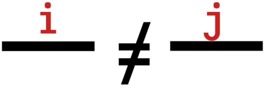
Tutorial: Priming

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

i ≠ j
```

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

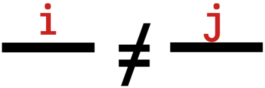
Tutorial: Priming

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

i ≠ j
```



Tutorial: Priming

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

i ≠ j
```



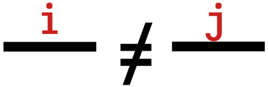

```
i = Index(2)

prime(i) == i'

i ≠ i'
noprime(i') == i
```

(dim=2|id=837)

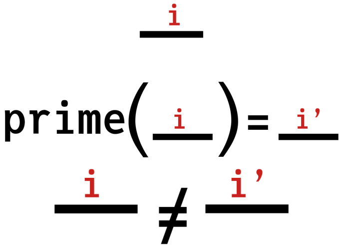
(dim=2|id=837)'

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

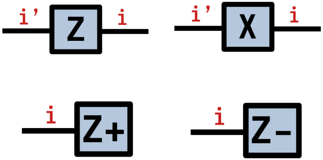
X

$|\text{Z+}\rangle$

$|\text{Z-}\rangle$

Tutorial: One-site operators

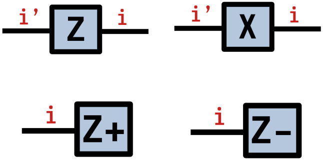
```
Z = op("Z", i)
X = op("X", i)

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



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
```

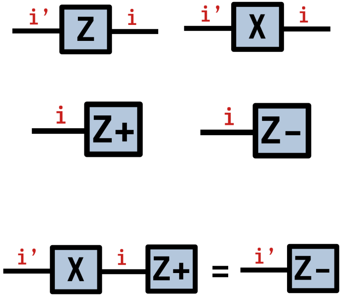


$$X|Z+\rangle = |Z\text{-}\rangle$$

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

```
XZp = X * Zp

dag(Zm) * XZp

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

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

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

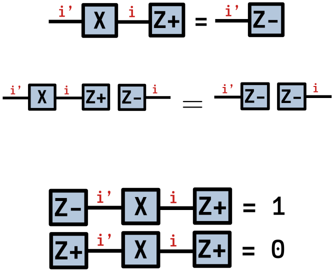
$$|\mathrm{Z}-\rangle\langle \mathrm{Z}+|X$$

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

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

Tutorial: One-site operators

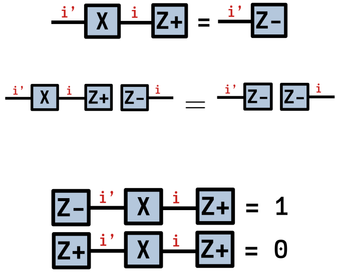
```
XZp = X * Zp

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)
```

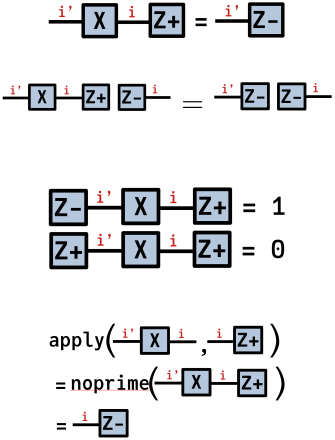


$= \text{noprime}(X * Zp)$
≈ 1

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)
```



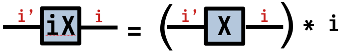
Tutorial: Custom one-site operators

```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

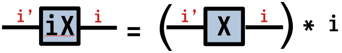
```julia
import ITensors: op

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



Tutorial: Custom one-site operators

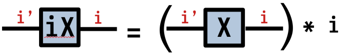
```
import ITensors: op

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

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



Tutorial: Custom one-site operators

```
import ITensors: op

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




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

```
X * im
```

Tutorial: Two-site states

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

i1 == i2

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

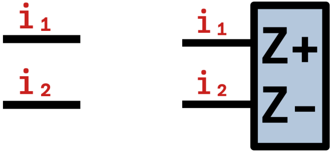
(dim=2|id=505|“S=1/2”)
(dim=2|id=576|“S=1/2”)

false

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

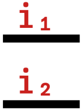
Tutorial: Two-site states

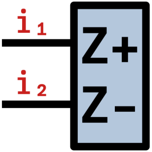
```
i1 = Index(2, "S=1/2")
i2 = Index(2, "S=1/2")

i1 == i2

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



Tutorial: Two-site states

```
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
```

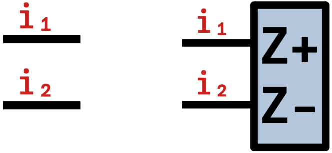
$|\text{Z+}\rangle_1$
$|\text{Z+}\rangle_2$

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

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

Tutorial: Two-site states

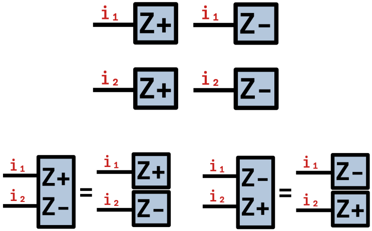
```julia
i1 = Index(2, "S=1/2")
i2 = Index(2, "S=1/2")

i1 == i2

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




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

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

ZpZm = Zp1 * Zm2
ZmZp = Zm1 * Zp2
```



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
```

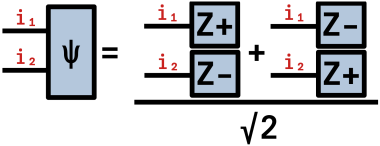
$(|\mathrm{Z+}\rangle|\mathrm{Z-}\rangle + |\mathrm{Z-}\rangle|\mathrm{Z+}\rangle)/\sqrt{2}$

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

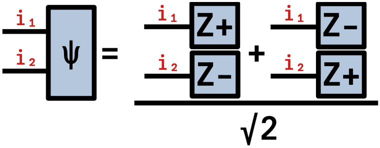
ψ = (Zp1 * Zm2 +
        Zm1 * Zp2)/√2
```



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

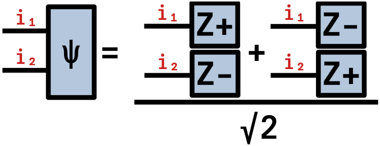
```
ψ = ITensor(i1, i2)
ψ[i1=>1, i2=>2] = 1/√2
ψ[i1=>2, i2=>1] = 1/√2

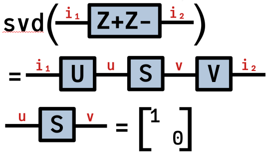
ψ = (Zp1 * Zm2 +
        Zm1 * Zp2)/√2
```

```
inner(ψ, ψ)
inner(ZpZm, ψ)

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

U, S, V = svd(ψ, i1)
s = diag(S)
```





Tutorial: Two-site states

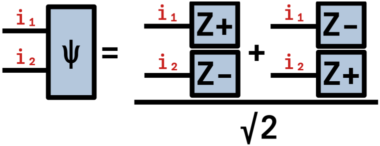
```
ψ = ITensor(i1, i2)
ψ[i1=>1, i2=>2] = 1/√2
ψ[i1=>2, i2=>1] = 1/√2

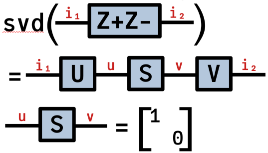
ψ = (Zp1 * Zm2 +
        Zm1 * Zp2)/√2
```

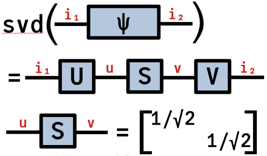
```
inner(ψ, ψ)
inner(ZpZm, ψ)

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
# ...
```

```
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
# ...
```

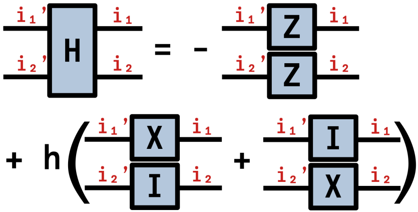
```
Id1 = op("Id", i1)
Z1 = op("Z", i1)
X1 = op("X", i1)
# ...

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



(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))
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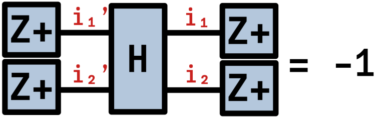
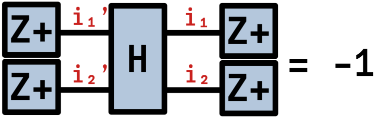


Tutorial: Two-site operators

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




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

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

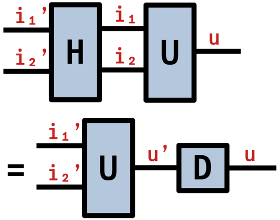
Tutorial: Two-site operators

```
ZpZp = Zp1 * Zp2



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

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



$$= \begin{bmatrix} -\sqrt{2} & & & \\ & -1 & & \\ & & 1 & \\ & & & \sqrt{2} \end{bmatrix}$$

Tutorial: Custom two-site operators

```julia
import ITensors: op

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

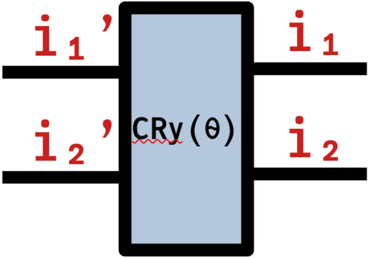
Controlled-Ry (CRy) rotation gate

CRy(θ)

Tutorial: Custom two-site operators

```
import ITensors: op

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



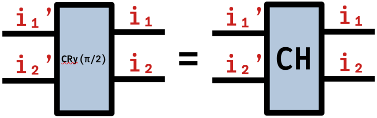
Tutorial: Custom two-site operators

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

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

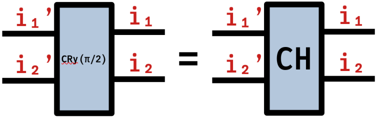
Tutorial: Custom two-site operators

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



Tutorial: Custom two-site operators

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




```
ZpZm = Zp1 * Zm2

CH_Xm = apply(CH, ZpZm)

CH_Xm ≈ Zp1 * Xm2
```

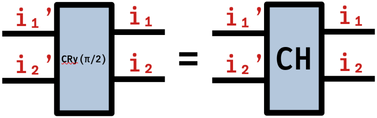
$|\text{Z+Z-}\rangle = |\text{Z+}\rangle_1 |\text{Z-}\rangle_2$

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

true

Tutorial: Custom two-site operators

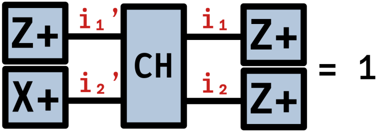
```
CH = op("CRy", i1, i2;
        θ=π/2)
```




```
ZpZm = Zp1 * Zm2

CH_Xm = apply(CH, ZpZm)

CH_Xm ≈ Zp1 * Xm2
```



Tutorial: Two-site state optimization

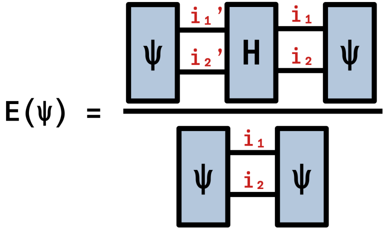
```
function E(ψ)
  ψHψ = inner(ψ', H, ψ)
  ψψ = inner(ψ, ψ)
  return ψHψ / ψψ
end
```

Function to minimize:
Expectation value of the energy.

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

Tutorial: Two-site state optimization

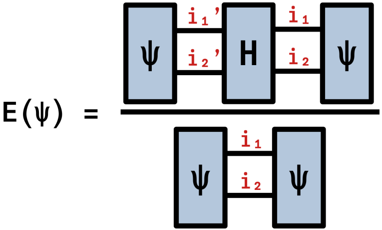
```
function E(ψ)
  ψHψ = inner(ψ', H, ψ)
  ψψ = inner(ψ, ψ)
  return ψHψ / ψψ
end
```



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
```



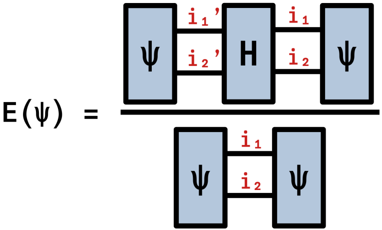
Simple gradient descent. Must provide function f(x) to minimize and ∂f(x), the gradient of f at x.

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

```julia
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.

≈ 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))
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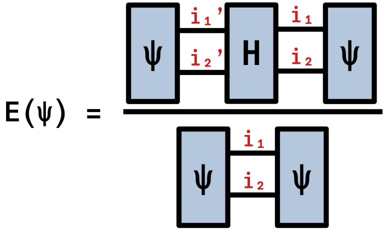
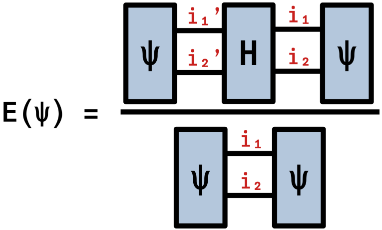


Tutorial: Two-site state optimization

```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))
```



Minimize over ψ:

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

(-1, 2)

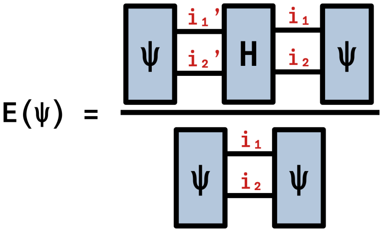
(-1.4142131, 0.0010865277)

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

Tutorial: Two-site state optimization

```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))
```



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

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]),
]
```

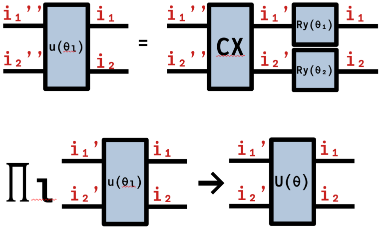
Tutorial: Two-site circuit optimization

```
# 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]),
]
```

```
# 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:

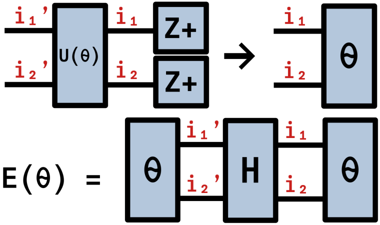
$|0\rangle = |\mathrm{Z+Z+}\rangle$

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

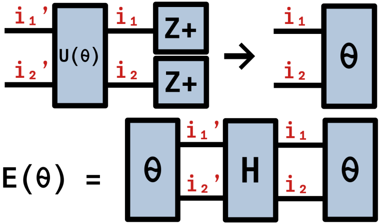
```
ψ0 = Zp1 * Zp2


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
```

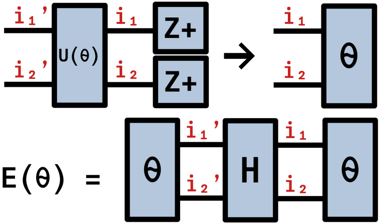
```
θ0 = [0, 0, 0, 0]
θ = minimize(E, ∂E, θ0;
        nsteps=40, γ=0.5)

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
```

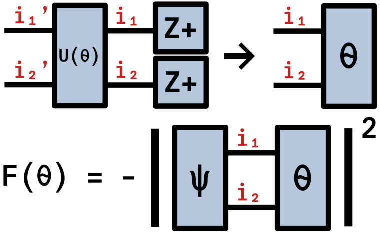
Reference state:
$|0\rangle = |Z{+}Z{+}\rangle$

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

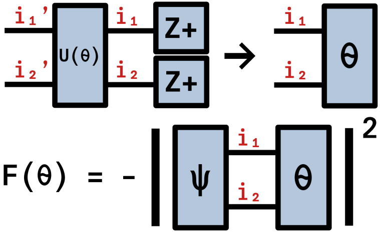
```
ψ0 = Zp1 * Zp2
ψ = (ZpZp + ZmZm) / √2



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))

```



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

Tutorial: Two-site fidelity optimization

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



function F(θ)
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  return -abs(inner(ψ, ψθ))^2
end
```
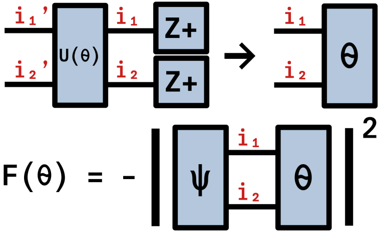




```
θ0 = [0, 0, 0, 0]
θ = minimize(F, ∂F, θ0;
        nsteps=50, γ=0.1)

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-")

maxlinkdim(Zp)
```

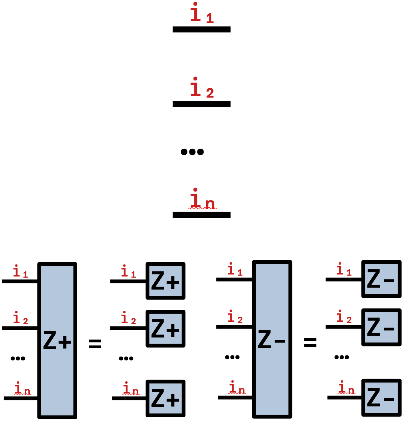
n-site state

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

1 (product state)

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-")

maxlinkdim(Zp)
```



Tutorial: n-site states with MPS

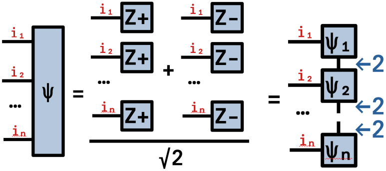
```
ψ = (Zp + Zm)/√2


maxlinkdim(ψ)
```

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

2 (entangled state)

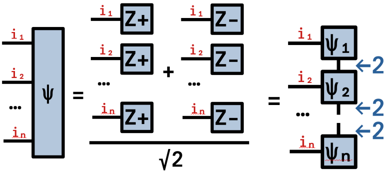
Tutorial: n-site states with MPS

```
ψ = (Zp + Zm)/√2


maxlinkdim(ψ)
```



Tutorial: n-site states with MPS

```
ψ = (Zp + Zm)/√2


maxlinkdim(ψ)
```

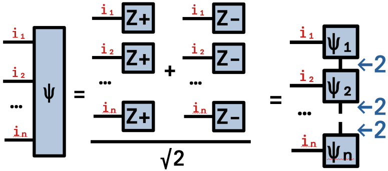



```
inner(Zp, Zp)
inner(Zm, Zp)
norm(ψ)
inner(Zp, ψ)
```

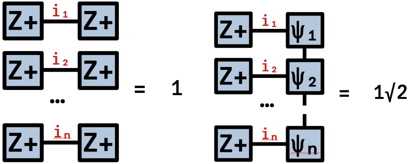
$$\langle Z+|Z+\rangle \approx 1$$
$$\langle Z-|Z+\rangle \approx 0$$
$$||\psi\rangle| \approx 1$$
$$\langle Z+|\psi\rangle \approx 1/\sqrt{2}$$

Tutorial: n-site states with MPS

```
ψ = (Zp + Zm)/√2


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)
```

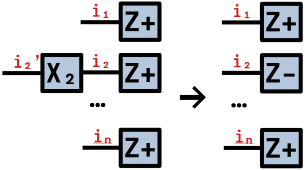
$j = n/2$
X_j

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

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

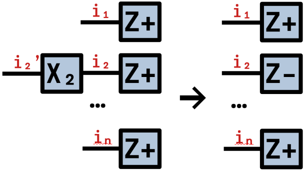
Tutorial: n-site states with MPS

```
j = n ÷ 2
Xⱼ = op("X", i[j])

XⱼZp = apply(Xⱼ, Zp)


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)
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

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

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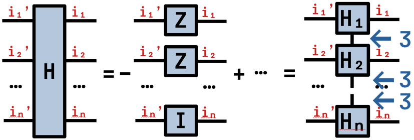

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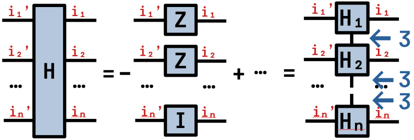
    H += h, "X", j
  end
  return H
end
```

```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 operators with MPO

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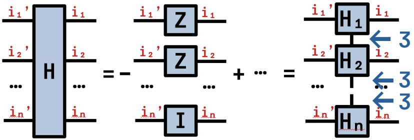
```

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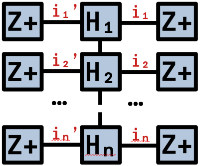

Tutorial: n-site state optimization

```
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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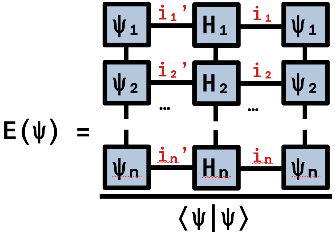

$\min_{\psi} E(\psi)$ $\partial_{\psi} E(\psi)$

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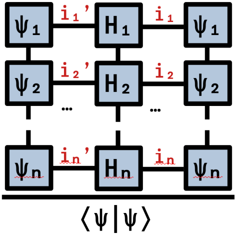
```

$E(\psi) =$ 

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

maxlinkdim(ψ_0)	$= 1$ (product state)
maxlinkdim(ψ)	$= 3$ (entangled state)
maxlinkdim(ψ_{dmrg})	$= 2$ (entangled state)
E(ψ_0), norm(∂(ψ_0))	$\approx$ (-29, 5.4772256)
E(ψ), norm(∂E(ψ))	$\approx$ (-31.0317917, 0.06673780)
E(ψ_{dmrg}), norm(∂E(ψ_{dmrg}))	$\approx$ (-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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```

```
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
```

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

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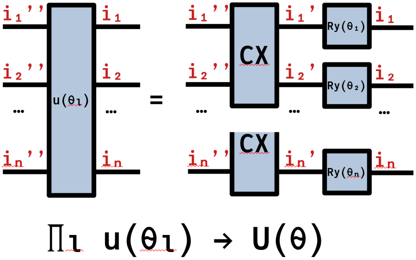
    Uθ = [Uθ; Ry_layer(θl, i)]
  end
  return Uθ
end
```



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)
```

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

Minimize over θ:

$|\theta\rangle = \mathrm{U}(\theta)|0\rangle$

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

Tutorial: n-site states with MPS

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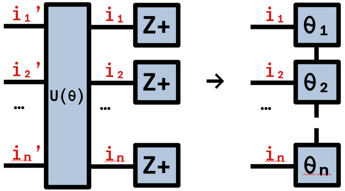

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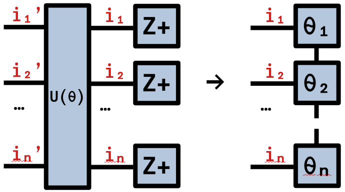


```
maxlinkdim(ψ₀)
maxlinkdim(ψθ)
E(θ₀), norm(∂E(θ₀))
E(θ), norm(∂E(θ))
```

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

Tutorial: n-site states with MPS

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maxlinkdim(ψ₀)
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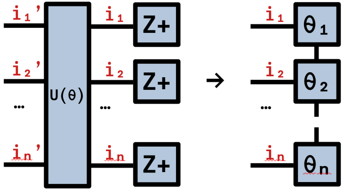

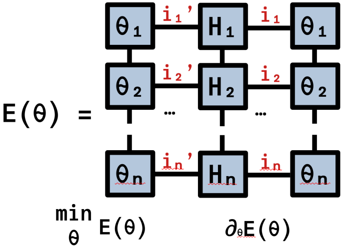

Tutorial: n-site states with MPS

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

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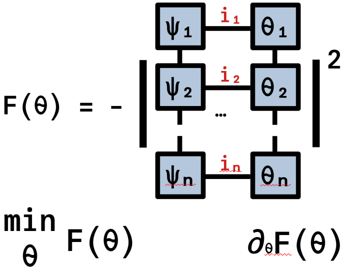

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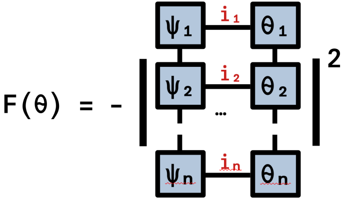

$\min_{\theta} F(\theta)$ $\partial_\theta F(\theta)$

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

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

Other features not mentioned

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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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- 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!