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

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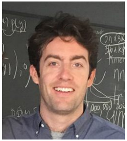

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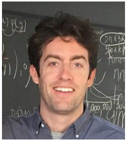

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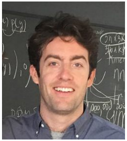

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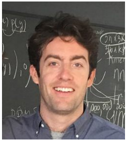

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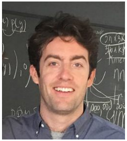

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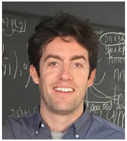

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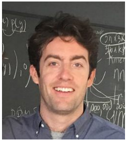

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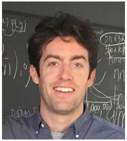

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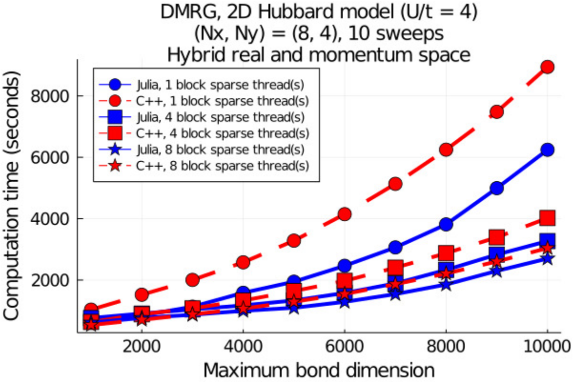

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  - Find out more: github.com/GTorlai/PastaQ.jl

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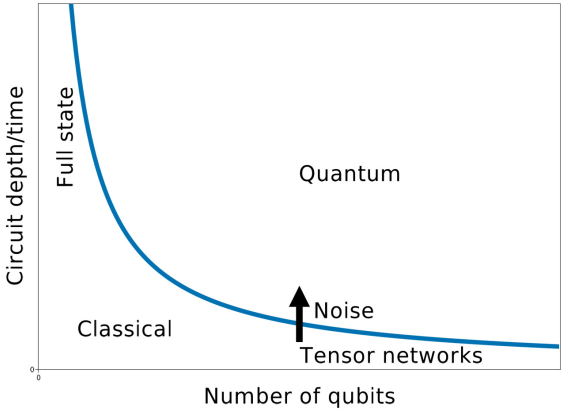
- Tensor networks are a common, general language for reasoning about quantum many-body systems (for example, quantum circuits).

When should I use tensor networks?

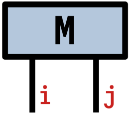
- In my opinion, tensor networks are the best general purpose tool we have right now for studying quantum many-body systems (while we wait for a general purpose quantum computer).



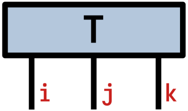
What are tensor networks?

Vector V_i
Order-1 tensor

Matrix M_{ij}
Order-2 tensor



Tensor T_{ijk}
Order-3 tensor



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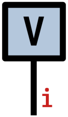

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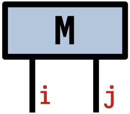

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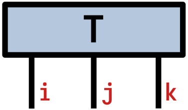
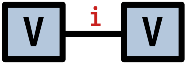
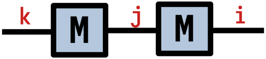


Vector inner product



Matrix-vector multiplication

Matrix-matrix multiplication



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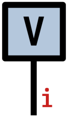

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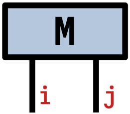

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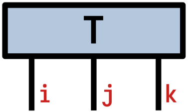

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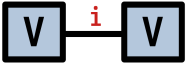

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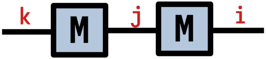
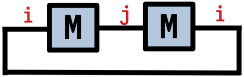
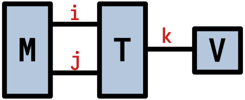


Trace of matrix-matrix multiplication



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> using ITensors

julia> i = Index(2);

julia> A = ITensor(i);

julia> using PastaQ

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

julia>   = 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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using ITensors

i = Index(2)


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Tutorial: One-site state basics

```julia
using ITensors

i = Index(2)


```

```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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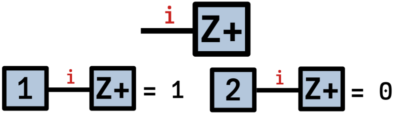

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```
Zp = ITensor([1, 0], i)
Zm = ITensor([0, 1], i)
Xp = ITensor([1, 1]/√2, i)
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$$|Z+\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \ |Z-\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

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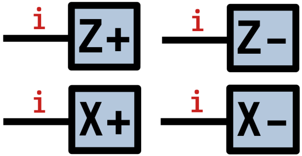

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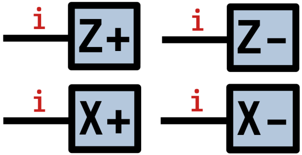


```
(Zp + Zm)/√2
dag(Zp) * Xp
(dag(Zp) * Xp)[]
inner(Zp, Xp)
norm(Xp)
```

$\approx$ Xp

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

$\approx 1/\sqrt{2}$

$\approx 1/\sqrt{2}$

≈ 1

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norm(Xp)
```
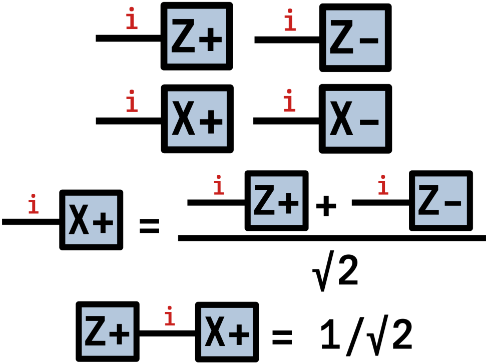
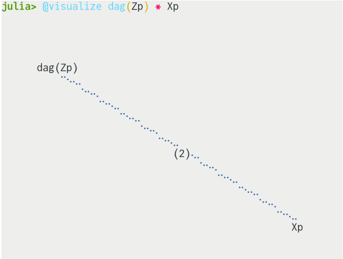



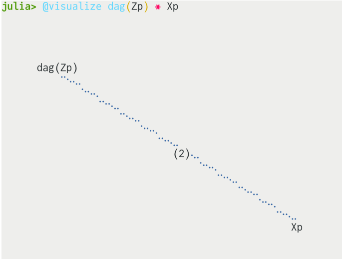
Tutorial: One-site state basics

```
using ITensorUnicodePlots

@visualize dag(Zp) * Xp
```

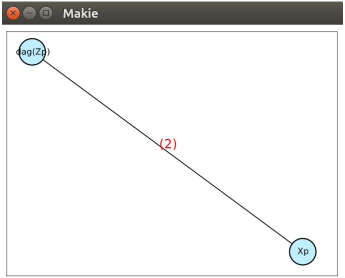


Tutorial: One-site state basics

```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/$\sqrt{2}$

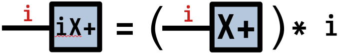
Tutorial: Custom one-site states

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



Tutorial: Priming

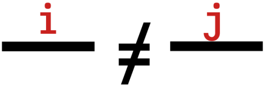
```
i = Index(2)
j = Index(2)

i == j
```

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

false

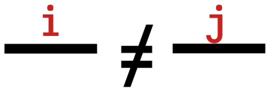
Tutorial: Priming

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

i == j
```



Tutorial: Priming

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

i == j
```




```
i

prime(i)
i'
i == i'
noprime(i')
```

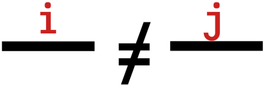
(dim=2|id=837)

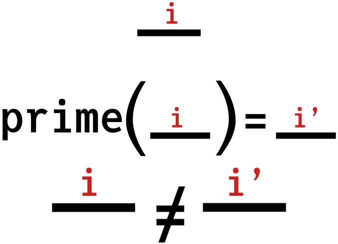
(dim=2|id=837)'
(dim=2|id=837)'
false
(dim=2|id=837)

Tutorial: Priming

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

i == j
```

```
i

prime(i)
i'
i == i'
noprime(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)
```

```
# Z
# X

# |Z+⟩
# |Z−⟩
```

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

```
# X|Z+⟩ = |Z−⟩
# false
# true
# true
```

Tutorial: One-site operators

[TODO: Add visualization of inner product]

```
XZp = X * Zp

inner(Zm, XZp)

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

```
# X|Z+⟩ = |Z−⟩

# error: not a scalar value

# ≈ 1
# ≈ 0
```

Tutorial: One-site operators

[TODO: Add visualization of inner product]

```
XZp = X * Zp

inner(Zm, XZp)

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

```
# X|Z+⟩ = |Z−⟩

# error: not a scalar value

# ≈ 1
# ≈ 0
```

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

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

```
# ≈ 1
# ≈ 1

# = noprime(X * Zp)
# ≈ 1
```

Tutorial: Custom one-site operators

```julia
import ITensors: op

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

```julia
# 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
```

```
# Overload ITensors.jl
# behavior
```

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

```
# im * X
```

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+⟩1|Z−⟩2 = |Z+Z−⟩
```

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

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

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

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

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

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

$|Z-\rangle_1$
$|Z-\rangle_2$

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

Tutorial: Two-site states

[TODO: Add visualization of inner(Cat, Cat), SVD]

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

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

```
# (|Z+⟩|Z−⟩ + |Z−⟩|Z+⟩)/√2




# From single−site states
```

Tutorial: Two-site states

[TODO: Add visualization of inner(Cat, Cat), SVD]

```
Cat = ITensor(i1, i2)                # (|Z+⟩|Z−⟩ + |Z−⟩|Z+⟩)/√2
Cat[i1=>1, i2=>2] = 1/√2
Cat[i1=>2, i2=>1] = 1/√2

Cat = (Zp1 * Zm2 +                   # From single−site states
          Zm1 * Zp2)/√2
```

```
inner(Cat, Cat)                      # ≈ 1
inner(ZpZm, Cat)                     # ≈ 1/√2

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

U, S, V = svd(Cat, i1)
s = diag(S)                          # ≈ [1/√2, 1/√2]
```

Tutorial: Two-site operators

[TODO: Add visualization of H]

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

```
# Make a Hamiltonian:
# Transverse field Ising
# n=2 sites
# H = -∑_j^{n-1} Z_j Z_{j+1} + h ∑_j^n X_j
```

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

Tutorial: Two-site operators

[TODO: Add visualization of H]

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

```
# Make a Hamiltonian:
# Transverse field Ising
# n=2 sites
```

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

```
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

[TODO: Add visualization of <H>]

```
ZpZp = Zp1 * Zp2



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

```
# Expectation value:
# ⟨H⟩ = ⟨Z+Z+|H|Z+Z+⟩



# ≈ −1
```

Tutorial: Two-site operators

[TODO: Add visualization of <H>]

```
ZpZp = Zp1 * Zp2



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

```
# Expectation value:
# ⟨H⟩ = ⟨Z+Z+|H|Z+Z+⟩



# ≈ −1
```

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

```
# ≈ [−√2, −1, 1, √2]
```

Tutorial: Custom two-site operators

```julia
import ITensors: op

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

```julia
# Controlled−Ry (CRy)
# rotation gate

# CRy(θ)
```

Tutorial: Custom two-site operators

[TODO: Add visualization of CH|ZpZm>]

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

```
# Controlled−Hadamard gate
# CH = CRy(θ=π/2)
```

Tutorial: Custom two-site operators

[TODO: Add visualization of CH|ZpZm>]

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

```
# Controlled−Hadamard gate
# CH = CRy(θ=π/2)
```

```
ZpZm = Zp1 * Zm2

CH_Xm = apply(CH, ZpZm)

CH_Xm ≈ Zp1 * Xm2
```

```
# |Z+Z−⟩ = |Z+⟩₁|Z−⟩₂

# CH|Z+Z−⟩ = |Z+X−⟩

# true
```

Tutorial: Two-site state optimization

[TODO: Add visualization of minimizing <v|H|v>]

```julia
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(ψ) = ⟨ψ|H|ψ⟩/⟨ψ|ψ⟩
```

Tutorial: Two-site state optimization

[TODO: Add visualization of minimizing <v|H|v>]

```
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(ψ) = ⟨ψ|H|ψ⟩/⟨ψ|ψ⟩
```

```
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

[TODO: Add visualization of minimizing <v|H|v>]

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

E(ψ₀)

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

norm(∂E(ψ₀))
```

```julia
# |ψ₀⟩ = (|Z+Z+⟩ +
#          |Z−Z−⟩)/√2

# ≈ −1

# Using Zygote for automatic
# differentiation of the energy.

# ≈ 2
```

Tutorial: Two-site state optimization

[TODO: Add visualization of minimizing <v|H|v>]

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

E(ψ0)

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

norm(∂E(ψ0))
```

```
# |ψ0⟩ = (|Z+Z+⟩ +
#          |Z−Z−⟩)/√2

# ≈ −1

# Using Zygote for automatic
# differentation of the energy.

# ≈ 2
```

```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(ψ) = ⟨ψ|H|ψ⟩/⟨ψ|ψ⟩

# (−1, 2)
# (−1.4142131, 0.0010865277)
#        ≈ (−√2, 0)
```

Tutorial: Two-site circuit optimization

[TODO: Add visualization of U]

```
# 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

[TODO: Add visualization of minimizing <0|UHU|0>]

```
ψ0 = Zp1 * Zp2


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

```
# References state:
# |0⟩ = |Z+Z+⟩

# Find θ that minimizes:
# E(θ) = ⟨0|U(θ)† H U(θ)|0⟩
#      = ⟨θ|H|θ⟩
```

Tutorial: Two-site circuit optimization

[TODO: Add visualization of minimizing <0|UHU|0>]

```
ψ0 = Zp1 * Zp2


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

```
# References state:
# |0⟩ = |Z+Z+⟩

# Find θ that minimizes:
# E(θ) = ⟨0|U(θ)† H U(θ)|0⟩
#      = ⟨θ|H|θ⟩
```

```
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, √3/2)
# (−1.4142077, 0.0017584116)
#      ≈ (−√2, 0)
```

Tutorial: Two-site fidelity optimization

[TODO: Add visualization of minimizing <v|U|v0>]

```julia
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⟩ = |Z+Z+⟩

# Target state:
# |ψ⟩ = (|Z+Z+⟩ +
#          |Z−Z−⟩)/√2

# Find θ that minimizes:
# F(θ) = −|⟨ψ|U(θ)|0⟩|^2
```

Tutorial: Two-site fidelity optimization

[TODO: Add visualization of minimizing <v|U|v0>]

```
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⟩ = |Z+Z+⟩

# Target state:
# |ψ⟩ = (|Z+Z+⟩ +
#          |Z−Z−⟩)/√2

# Find θ that minimizes:
# F(θ) = −|⟨ψ|U(θ)|0⟩|^2
```

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

F(θ0), norm(∂F(θ0))      # ≈ (−0.5, 0.5)
F(θ), norm(∂F(θ))        # ≈ (−0.9938992, 0.07786879)
```

Tutorial: n-site states with MPS

[TODO: Add visualization of <Zp|Cat>]

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

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

Cat = (Zp + Zm)/√2

```

```
# n−site state



# |Z+Z+...Z+⟩
# |Z−Z−...Z−⟩

# (|Z+Z+...Z+⟩ +
#  |Z−Z−...Z−⟩)/√2
```

Tutorial: n-site states with MPS

[TODO: Add visualization of <Zp|Cat>]

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

Zp = MPS(i, "Z+")                     # |Z+Z+...Z+⟩
Zm = MPS(i, "Z-")                     # |Z-Z-...Z-⟩

Cat = (Zp + Zm)/√2                    # (|Z+Z+...Z+⟩ +
                                      #  |Z-Z-...Z-⟩)/√2
```

```
maxlinkdim(Zp)                        # 1 (product state)
maxlinkdim(Cat)                       # 2 (entangled state)
inner(Zp, Zp)                         # ⟨Z+|Z+⟩ ≈ 1
inner(Zm, Zp)                         # ⟨Z-|Z+⟩ ≈ 0
norm(Cat)                             # (⟨Z+| + ⟨Z-|)(|Z+⟩ + |Z+⟩)/2
                                      #       ≈ 1
```

Tutorial: n-site states with MPS

[TODO: Add visualization of minimizing <psi|H|psi>]

```
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+⟩ =
#     |Z+Z+...Z−...Z+⟩

# |Z+Z+...Z−...Z+⟩
```

Tutorial: n-site states with MPS

[TODO: Add visualization of minimizing <psi|H|psi>]

```julia
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+⟩ =
#     |Z+Z+...Z−...Z+⟩

# |Z+Z+...Z−...Z+⟩
```

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

```
# 1 (product state)
# ≈ 0
# ≈ 1
```

Tutorial: n-site states with MPS

[TODO: Add visualization of H]

```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 states with MPS

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  end
  return H
end
```

n sites

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

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

= 3 (local Hamiltonian)

⟨Z+Z+...Z+|H|Z+Z+...Z+⟩

Tutorial: n-site states with MPS

[TODO: Add visualization of H]

```
ψ0 = MPS(i, "Z+")                         # |0⟩ = |Z+Z+...Z+⟩

ψ = minimize(E, ∂E, ψ0;                   # Minimize over ψ:
        nsteps=50, γ=0.1,                 # ⟨ψ|H|ψ⟩/⟨ψ|ψ⟩
        maxdim=10, cutoff=1e-5)

E_dmrg, ψ_dmrg = dmrg(H, ψ0;              # DMRG solves:
        nsweeps=10,                       # H|ψ⟩ ≈ |ψ⟩
        maxdim=10, cutoff=1e-5)
```

Tutorial: n-site states with MPS

[TODO: Add visualization of H]

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        maxdim=10, cutoff=1e-5)
```

```
maxlinkdim(ψ0)                             # = 1 (product state)
maxlinkdim(ψ)                              # = 3 (entangled state)
maxlinkdim(ψ_dmrg)                         # = 2 (entangled state)
E(ψ0), norm(∂(ψ0))                         # ≈ (−29, 5.4772256)
E(ψ), norm(∂E(ψ))                          # ≈ (−31.0317917, 0.06673780)
E(ψ_dmrg), norm(∂E(ψ_dmrg))                # ≈ (−31.0356110, 0.02413237)
```

Tutorial: n-site states with MPS

[TODO: Add visualization of H]

```
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 states with MPS

[TODO: Add visualization of H]

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```

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

```julia
# U(θ) = Ry_1(θ_1) ... Ry_n(θ_n)
#        CX_{1,2} ... CX_{n-1,n}
#        Ry_1(θ_{n+1}) ... Ry_n(θ_{2n})
#        ...
```

Tutorial: n-site states with MPS

[TODO: Add visualization of H]

```
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⟩ = |Z+Z+...Z+⟩

# Minimize over θ:
# |θ⟩ = U(θ)|0⟩
# E(θ) = ⟨θ|H|θ⟩
```

Tutorial: n-site states with MPS

[TODO: Add visualization of H]

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```
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# E(θ) = ⟨θ|H|θ⟩
```

```
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

[TODO: Add visualization of H]

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

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

```
# |0⟩ = |Z+Z+...Z+⟩

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

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```
# |0⟩ = |Z+Z+...Z+⟩

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

```
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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