Analyzing Quantum Many-Body Systems with ITensor and PastaQ

Matthew Fishman
Center for Computational Quantum Physics (CCQ)
Flatiron Institute, NY
https://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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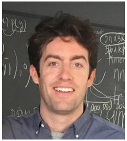
What is ITensor?

- Stands for “Intelligent Tensor”.



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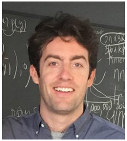

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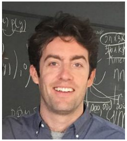

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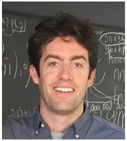

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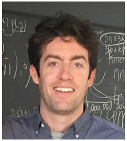

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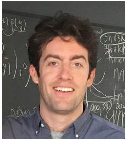

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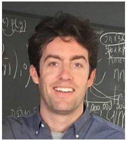

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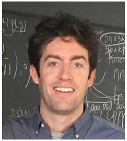

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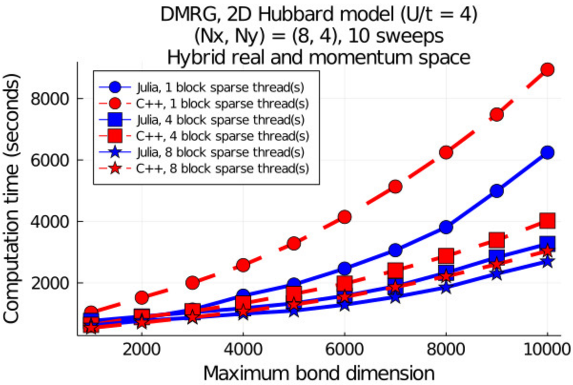
- Porting the full ITensor library took about $1\frac{1}{2}$ years.



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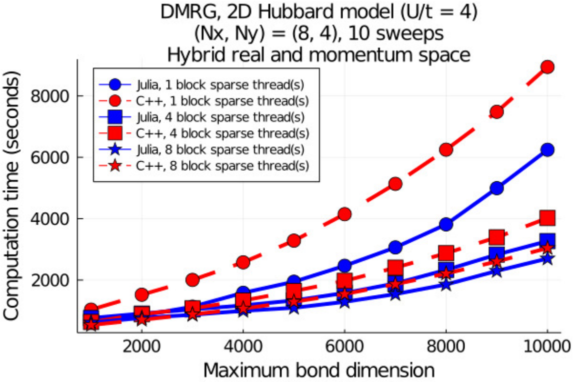

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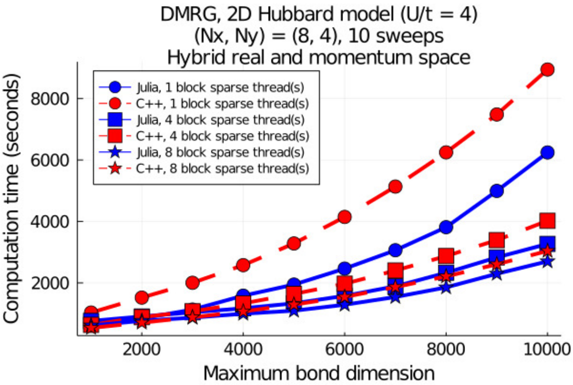

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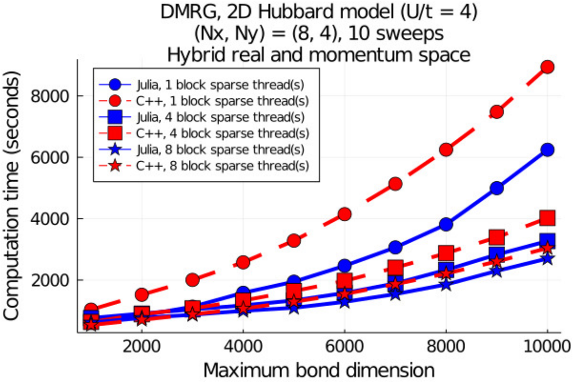

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  - Find out more: github.com/GTorlai/PastaQ.jl

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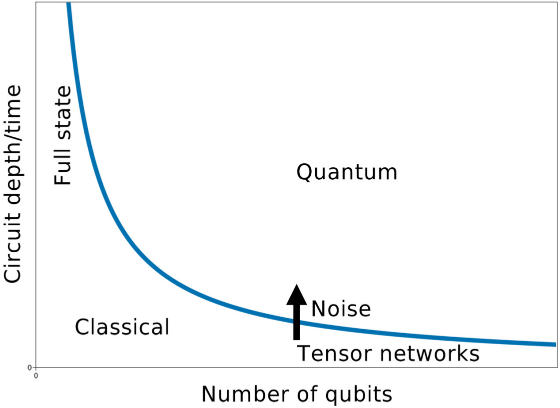
  - This is not the focus of ITensor and PastaQ at the moment, specialized libraries like Yao.jl may be faster.
- Tensor networks are a common, general language for reasoning about quantum many-body systems (for example, quantum circuits).

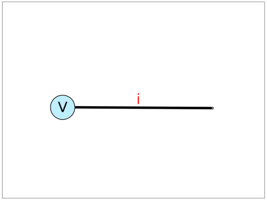
When should I use tensor networks?

- 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).

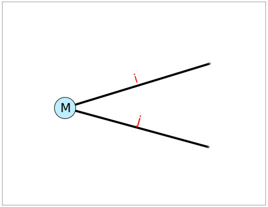


What are tensor networks?

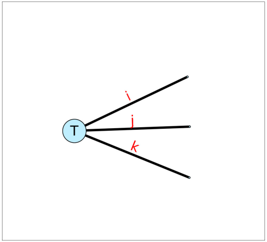
Vector V_i
Order-1 tensor



Matrix M_{ij}
Order-2 tensor



Tensor T_{ijk}
Order-3 tensor



[TODO: Add examples of matvec, matmul, trace]

How do I install ITensor/PastaQ?

1. Download Julia: julialang.org/downloads
2. Launch Julia:

```
$ julia
```

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

```
using ITensors

i = Index(2)


```

```
# Load ITensor

# 2−dimensional labeled
# Hilbert space
# (dim=2|id=510)
```

Tutorial: One-site state basics

```julia
using ITensors          # Load ITensor

i = Index(2)            # 2-dimensional labeled
                        # Hilbert space
                        # (dim=2|id=510)
```

```julia
Zp = ITensor(i)         # Z|Z+⟩ = |Z+⟩
Zp[i=>1] = 1

Zp = ITensor([1, 0], i) # Construct from a Vector
```

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

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

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

```
# ≈ Xp
# ≈ ITensor(1/√2)
# ≈ 1/√2
# ≈ 1/√2
# ≈ 1
```

Tutorial: One-site state basics

```
using ITensorVisualizationBase: set_backend!
```

Tutorial: One-site state basics

```julia
using ITensorVisualizationBase: set_backend!
```

```julia
back = "UnicodePlots"
set_backend!(back)

@visualize dag(Zp) * Xp
```

```
# TODO: Add
    UnicodePlots
    visualization.
```

Tutorial: One-site state basics

```
using ITensorVisualizationBase: set_backend!
```

```
back = "UnicodePlots"
set_backend!(back)

@visualize dag(Zp) * Xp
```

```
back = "Makie"
set_backend!(back)

@visualize dag(Zp) * Xp
```

```
# TODO: Add
    UnicodePlots
    visualization.
```

[TODO: Add GLMakie visualization.]

Tutorial: One-site state basics

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

```
# "S=1/2" defines an
# operator basis
#
# Additionally:
# "Qubit", "Qudit",
# "Electron", ...
```

Tutorial: One-site state basics

```
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

```
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-",
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  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)
```

```
# ≈ im ∗ Xm

# ≈ im/√2
# ≈ −im/√2
```

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
```

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

# false
```

```
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: One-site operators

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

```julia
# TODO: Diagram
# Set elements
```

Tutorial: One-site operators

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Z[i'=>1, i=>1] = 1
Z[i'=>2, i=>2] = -1
```

```
# TODO: Diagram
# Set elements
```

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

Z = ITensor(z, i', dag(i))

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

```
# Matrix representation
# of 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
```

```
# 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
```

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

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

```
# im * X
```

Tutorial: Two-site states

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

i1 == i2

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

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

# 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+⟩₁|Z−⟩₂ = |Z+Z−⟩
```

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

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

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

```
# |Z+⟩₁
# |Z+⟩₂

# |Z−⟩₁
# |Z−⟩₂

# |Z+Z−⟩ = |Z+⟩₁|Z−⟩₂
# |Z−Z+⟩ = |Z−⟩₁|Z+⟩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 = -\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

```
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

[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>]

```
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>]

```
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
```

Tutorial: Two-site state optimization

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

```julia
ψ0 = (Zp1 * Zm2 +          # |ψ0⟩ = (|Z+Z+⟩ +
      Zm1 * Zp2)/√2        #         |Z−Z−⟩)/√2

E(ψ0)                      # ≈ −1

using Zygote: gradient     # Using Zygote for automatic
∂E(ψ) = gradient(E, ψ)[1]  # differentation of the energy.

norm(∂E(ψ0))               # ≈ 2
```

```julia
ψ = minimize(E, ∂E, ψ0;          # Minimize over ψ:
      nsteps=10, γ=0.1)          # E(ψ) = ⟨ψ|H|ψ⟩/⟨ψ|ψ⟩

E(ψ0), norm(∂E(ψ0))              # (−1, 2)
E(ψ), norm(∂E(ψ))                # (−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>]

```julia
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>]

```
ψ_0 = Zp1 * Zp2


function E(θ)
  ψ_θ = apply(U(θ), ψ_0)
  return inner(ψ_θ', H, ψ_θ)
end
```

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

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

```
θ_0 = [0, 0, 0, 0]
θ = minimize(E, ∂E, θ_0;
        nsteps=40, γ=0.5)

E(θ_0), norm(∂E(θ_0))
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>]

```
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))
F(θ), norm(∂F(θ))
```

```
# ≈ (−0.5, 0.5)
# ≈ (−0.9938992, 0.07786879)
```

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
```

Tutorial: n-site states with MPS

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

```julia
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
```

```julia
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>]

```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+⟩
```

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

[TODO: Add visualization of H]

```
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

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

```
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]

```
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)
```

```
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]

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

```julia
function U(θ, i; nlayers)
  n = length(i)
  Uθ = 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
```

```julia
# U(θ) = Ry₁(θ₁) ... Ryₙ(θₙ)
#        CX₁,₂ ... CXₙ₋₁,ₙ
#        Ry₁(θₙ₊₁) ... Ryₙ(θ₂ₙ)
#        ...
```

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]

```
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⟩
```

```
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
```

Tutorial: n-site states with MPS

[TODO: Add visualization of H]

```
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
```

```
maxlinkdim(ψ_0)
maxlinkdim(ψ_θ)
F(θ_0), norm(∂F(θ_0))
F(θ), norm(∂F(θ))
```

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

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