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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Who am I?

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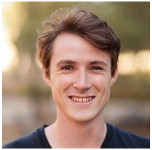

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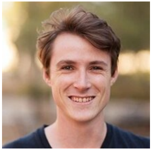

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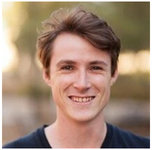

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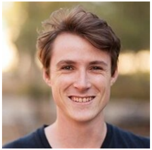

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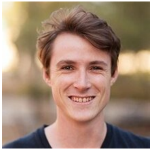

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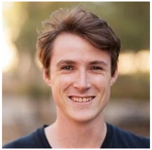

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- We are hiring postdocs, full-time scientists, part-time and full-time software developers, interns, etc.

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

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- Many sites or qubits in your system: linear or log scaling in the system size.

[TODO: “Quantum volume” schematic plot.]

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

[TODO: "Quantum volume" schematic plot.]

What are tensor networks?

[TODO: Show drawings of tensor networks.]

How do I install ITensor/PastaQ?

1. Download Julia.

[TODO: Add links, show code]

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3. Add PastaQ.jl.

[TODO: Add links, show code]

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

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

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

```julia
# Z|Z+⟩ = |Z+⟩


# 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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# 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

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

Tutorial: One-site state basics

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using ITensorVisualizationBase: set_backend!
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```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

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```

```
# "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–"
```

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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
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```
# (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

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

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

Tutorial: One-site operators

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

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

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

```
# 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)

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inner(Zp', XZp)
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# 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

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function op(
  ::OpName"iX",
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end
```

```
# Overload ITensors.jl
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```

```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−⟩
```

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ZpZm[i1=>1, i2=>2] = 1
```

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# (dim=2|id=505|"S=1/2")
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```julia
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 = −∑_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]

```
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```

```
# 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)[]
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```

```
# 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>]

```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)
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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
# differentation of the energy.

# ≈ 2
```

Tutorial: Two-site state optimization

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

```
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
```

```
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]

```julia
# Circuit as a vector of gates:
U(θ, i1, i2) = [
  op("Ry", i1; θ=θ[1]),
  op("Ry", i2; θ=θ[2]),
  op("CNOT", i1, i2),
  op("Ry", i1; θ=θ[3]),
  op("Ry", i2; θ=θ[4]),
]
```

```julia
# PastaQ notation:
u(θ, j1, j2) = [
  ("Ry", j1, (; θ=θ[1])),
  ("Ry", j2, (; θ=θ[2])),
  ("CNOT", j1, j2),
  ("Ry", j1, (; θ=θ[3])),
  ("Ry", j2, (; θ=θ[4])),
]
U(θ, i1, i2) =
  buildcircuit(u(θ, 1, 2), [i1, i2])
```

Tutorial: Two-site circuit optimization

[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)
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end
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# 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>]

```
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

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```
# 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))
```

```
# 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                    # 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>]

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n = 30                                  # n−site state
i = [Index(2, "S=1/2")
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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>]

```
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>]

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j = n ÷ 2
X_j = op("X", i[j])

X_jZp = apply(X_j, Zp)


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```

```
# j = n ÷ 2
# X_j

# X_j|Z+Z+...Z+⟩ =
#     |Z+Z+...Z−...Z+⟩

# |Z+Z+...Z−...Z+⟩
```

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

```
# 1
# ≈ 0
# ≈ 1
```

Tutorial: n-site states with MPS

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

```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 minimizing <psi|H|psi>]

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    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

\# ⟨Z+Z+...Z+|H|Z+Z+...Z+⟩ ≈

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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- More general built-in tensor networks beyond MPS/MPO
- More HPC with multithreaded and multiprocessor parallelism and GPUs
- 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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