

Analyzing Quantum Many-Body Systems with ITensor and PastaQ

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<https://mtfishman.github.io/>

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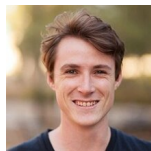
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- ▶ We are hiring postdocs, full-time scientists, part-time and full-time software developers, interns, etc.

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- ▶ Paper: arxiv.org/abs/2007.14822.

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[TODO: Add ITensor C++ vs. Julia benchmark plot]

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

When should I use tensor networks?

- ▶ 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).

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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.
- ▶ 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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2. Add ITensors.jl.

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How do I install ITensor/PastaQ?

1. Download Julia.
2. Add ITensors.jl.
3. Add PastaQ.jl.

[TODO: Add links, show code]

Tutorial: One-site state basics

```
1 using ITensors
2
3 i = Index(2)
4
5
```

```
# Load ITensor

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


Tutorial: One-site state basics

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2
3 i = Index(2)
4
5
```

```
# Load ITensor
# 2-dimensional labeled
# Hilbert space
# (dim=2|id=510)
```

```
1 Zp = ITensor(i)
2 Zp[i=>1] = 1
3
4 Zp = ITensor([1 0], i)
```

```
#  $Z|Z+\rangle = |Z+\rangle$ 
# Construct from a Vector
```

Tutorial: One-site state basics

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

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

Tutorial: One-site state basics

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

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

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

Tutorial: One-site state basics

```
1 using ITensorVisualizationBase: set_backend!
```

Tutorial: One-site state basics

```
1 using ITensorVisualizationBase: set_backend!
```

```
1 back = "UnicodePlots"  
2 set_backend!(back)  
3  
4 @visualize dag(Zp) * Xp
```

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

Tutorial: One-site state basics

```
1 using ITensorVisualizationBase: set_backend!
```

```
1 back = "UnicodePlots"  
2 set_backend!(back)  
3  
4 @visualize dag(Zp) * Xp
```

```
1 back = "Makie"  
2 set_backend!(back)  
3  
4 @visualize dag(Zp) * Xp
```

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

[TODO: Add GLMakie
visualization.]

Tutorial: One-site state basics

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

```
2
```

```
3
```

```
4
```

```
5
```

```
6
```

```
# "S=1/2" defines an  
# operator basis
```

```
#
```

```
# Additionally:
```

```
# "Qubit", "Qudit",
```

```
# "Electron", ...
```

Tutorial: One-site state basics

```
1 i = Index(2, "S=1/2")
2
3
4
5
6
```

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

```
1 Zp = state("Z+", i)
2 Zm = state("Z-", i)
3 Xp = state("X+", i)
4 Xm = state("X-", i)
```

```
# ITensor([1 0], i)
# ITensor([0 1], i)
# (Zp + Zm)/√2
# (Zp - Zm)/√2
```


Tutorial: Custom one-site states

```
1 import ITensors: state
2
3
4 function state(
5     ::StateName "iX-",
6     ::SiteType "S=1/2"
7 )
8     return [im -im]/√2
9 end
```

```
# Overload ITensors.jl
# behavior

# Define a state with the
# name "iX-"
```

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```

```
# Overload ITensors.jl
# behavior

# Define a state with the
# name "iX-"
```

```
1 iXm = state("iX-", i)
2
3 inner(Zp, iXm)
4 inner(Zm, iXm)
```

```
#  $\approx \text{im} * X_m$ 

#  $\approx \text{im}/\sqrt{2}$ 
#  $\approx -\text{im}/\sqrt{2}$ 
```

Tutorial: Priming

```
1 i = Index(2)
2 j = Index(2)
3
4 i == j
```

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

# false
```

Tutorial: Priming

```
1 i = Index(2)
2 j = Index(2)
3
4 i == j
```

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

# false
```

```
1 i
2
3 prime(i)
4 i'
5 i == i'
6 noprime(i')
```

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

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

Tutorial: One-site operators

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

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

Tutorial: One-site operators

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

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

```
1 z = [
2     1 0
3     0 -1
4 ]
5
6 Z = ITensor(z, i', dag(i))
7
8 Z = op("Z", i)
```

```
# Matrix representation
# of Z
```

```
# Convert to ITensor
```

```
# Use predefined definition
```

Tutorial: One-site operators

```
1  Z = op("Z", i)
2  X = op("X", i)
3
4  Zp = state("Z+", i)
5  Zm = state("Z-", i)
```

```
# Z
# X

# |Z+⟩
# |Z-⟩
```

Tutorial: One-site operators

```
1 Z = op("Z", i)
2 X = op("X", i)
3
4 Zp = state("Z+", i)
5 Zm = state("Z-", i)
```

```
# Z
# X

# |Z+⟩
# |Z-⟩
```

```
1 XZp = X * Zp
2 XZp == Zm
3 XZp == Zm'
4 noprime(XZp) == Zm
```

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


Tutorial: One-site operators

[TODO: Add visualization of inner product]

```
1 XZp = X * Zp
2
3 inner(Zm, XZp)
4
5 inner(Zm', XZp)
6 inner(Zp', XZp)
```

$X|Z+\rangle = |Z-\rangle$

error: not a scalar value

≈ 1

≈ 0

Tutorial: One-site operators

[TODO: Add visualization of inner product]

```
1 XZp = X * Zp
2
3 inner(Zm, XZp)
4
5 inner(Zm', XZp)
6 inner(Zp', XZp)
```

```
# X|Z+⟩ = |Z-⟩
# error: not a scalar value
# ≈ 1
# ≈ 0
```

```
1 apply(X, Zp) == Zm
2
3 (dag(Zm)' * X * Zp)[]
4 inner(Zm', X, Zp)
```

```
# false
# ≈ 1
# ≈ 1
```

Tutorial: Custom one-site operators

```
1  import ITensors: op
2
3  function op(
4      ::OpName"iX",
5      ::SiteType"S=1/2"
6  )
7      return [
8          0 im
9          im 0
10     ]
11  end
```

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

Tutorial: Custom one-site operators

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9         im 0
10    ]
11 end
```

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

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

```
# im * X
```

Tutorial: Two-site states

```
1 i1 = Index(2, "S=1/2")
2 i2 = Index(2, "S=1/2")
3
4 i1 == i2
5
6 ZpZm = ITensor(i1, i2)
7 ZpZm[i1=>1, i2=>2] = 1
```

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

# false

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

Tutorial: Two-site states

```
1 i1 = Index(2, "S=1/2")
2 i2 = Index(2, "S=1/2")
3
4 i1 == i2
5
6 ZpZm = ITensor(i1, i2)
7 ZpZm[i1=>1, i2=>2] = 1
```

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

# false

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

```
1 Zp1 = state("Z+", i1)
2 Zp2 = state("Z+", i2)
3
4 Zm1 = state("Z-", i1)
5 Zm2 = state("Z-", i2)
6
7 ZpZm = Zp1 * Zm2
8 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]

```
1 Cat = ITensor(i1, i2)
2 Cat[i1=>1, i2=>2] = 1/√2
3 Cat[i1=>2, i2=>1] = 1/√2
4
5 Cat = (Zp1 * Zm2 +
6        Zm1 * Zp2)/√2
```

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

From single-site states

Tutorial: Two-site states

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

```
1 Cat = ITensor(i1, i2)
2 Cat[i1=>1, i2=>2] = 1/√2
3 Cat[i1=>2, i2=>1] = 1/√2
4
5 Cat = (Zp1 * Zm2 +
6       Zm1 * Zp2)/√2
```

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

From single-site states

```
1 inner(Cat, Cat)
2 inner(ZpZm, Cat)
3
4 U, S, V = svd(ZmZp, i1)
5 s = diag(S)
6
7 U, S, V = svd(Cat, i1)
8 s = diag(S)
```

≈ 1

$\approx 1/\sqrt{2}$

$\approx [1 \ 0]$

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

Tutorial: Two-site operators

[TODO: Add visualization of H]

```
1 H = ITensor(i1', i2', i1, i2)
2 H[i1'=>2, i2'=>1,
3   i1=>2, i2=>1] = -1
4 # ...
```

```
# Make a Hamiltonian:
# Transverse field Ising
# n=2 sites
#  $H = -\sum_j^{n-1} X_j X_{j+1} + h \sum_j^n Z_j$ 
```

Tutorial: Two-site operators

[TODO: Add visualization of H]

```
1 H = ITensor(i1', i2', i1, i2)
2 H[i1'=>2, i2'=>1,
3   i1=>2, i2=>1] = -1
4 # ...
```

Make a Hamiltonian:

Transverse field Ising

n=2 sites

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

```
1 Id1 = op("Id", i1)
2 X1 = op("X", i1)
3 Z1 = op("Z", i1)
4 # ...
```

Alternative:

Build from single-site

operators.

Less error-prone.

```
5
6 XX = X1 * X2
7 ZI = Z1 * Id2
8 IZ = Id1 * Z2
9
10 h = 1.0
11 H = -XX + h * (ZI + IZ)
```

Tutorial: Two-site operators

[TODO: Add visualization of $\langle H \rangle$]

```
1 ZpZp = Zp1 * Zp2
2
3
4
5 (dag(ZpZp)' * H * ZpZp)[]
6 inner(ZpZp', H, ZpZp)
7 inner(ZpZp, apply(H, ZpZp))
```

```
# Expectation value:
#  $\langle H \rangle = \langle Z+Z+ | H | Z+Z+ \rangle$ 
```

```
#  $\approx 2$ 
```

Tutorial: Two-site operators

[TODO: Add visualization of $\langle H \rangle$]

```
1 ZpZp = Zp1 * Zp2
2
3
4
5 (dag(ZpZp)' * H * ZpZp)[]
6 inner(ZpZp', H, ZpZp)
7 inner(ZpZp, apply(H, ZpZp))
```

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

≈ 2

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

$\approx [-\sqrt{5} \ -1 \ 1 \ \sqrt{5}]$

Tutorial: Custom two-site operators

```
1 import ITensors: op
2
3 function op(
4     ::OpName"CRy",
5     ::SiteType"S=1/2";
6      $\theta$ 
7 )
8     c = cos( $\theta/2$ )
9     s = sin( $\theta/2$ )
10    return [
11        1 0 0 0
12        0 1 0 0
13        0 0 c -s
14        0 0 s  c
15    ]
16 end
```

```
# Controlled-Ry (CRy)
# rotation gate

# CRy( $\theta$ )
```

Tutorial: Custom two-site operators

[TODO: Add visualization of CH|ZpZm>]

```
1 CH = op("CRy", i1, i2;  
2        $\theta=\pi/2$ )
```

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

Tutorial: Custom two-site operators

[TODO: Add visualization of $\text{CH}|Z_p Z_m\rangle$]

```
1 CH = op("CRy", i1, i2;  
2          $\theta=\pi/2$ )
```

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

```
1 ZpZm = Zp1 * Zm2  
2  
3 CH_Xm = apply(CH, ZpZm)  
4  
5 CH_Xm  $\approx$  Zp1 * Xm2
```

```
#  $|Z+Z-\rangle = |Z+\rangle_1 |Z-\rangle_2$   
#  $\text{CH}|Z+Z-\rangle = |Z+X-\rangle$   
# true
```

Tutorial: Two-site state optimization

[TODO: Add visualization of minimizing $\langle \psi | H | \psi \rangle$]

```
1 function E( $\psi$ )
2    $\psi H \psi = \text{inner}(\psi', H, \psi)$ 
3    $\psi \psi = \text{inner}(\psi, \psi)$ 
4   return  $\psi H \psi / \psi \psi$ 
5 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

[TODO: Add visualization of minimizing $\langle \psi | H | \psi \rangle$]

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1 function E( $\psi$ )
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```
# Function to minimize:
# Expectation value of the
# energy.
#
#  $E(\psi) = \langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle$ 
```

```
1 function minimize(f, f, x;
2   nsteps,  $\gamma$ )
3   for n in 1:nsteps
4      $x = x - \gamma * f(x)$ 
5   end
6   return x
7 end
```

```
# Simple gradient descent.
# Must provide function  $f(x)$ 
# to minimize and  $\partial f(x)$ ,
# the gradient of  $f$  at  $x$ .

#  $\gamma$  is the gradient
# descent step size.
```

Tutorial: Two-site state optimization

[TODO: Add visualization of minimizing $\langle \mathbf{v} | \mathbf{H} | \mathbf{v} \rangle$]

```
1 using Zygote
2
3  $\partial \mathbf{E}(\psi) = \text{gradient}(\mathbf{E}, \psi)[1]$ 
4
5  $\psi_0 = (\mathbf{Z}_{p1} * \mathbf{Z}_{m2} +$ 
6          $\mathbf{Z}_{m1} * \mathbf{Z}_{p2}) / \sqrt{2}$ 
7
```

```
# Using Zygote for automatic
# differentiation of the energy.
#
# Starting state:
#
#  $|\psi_0\rangle = (|Z+Z+\rangle +$ 
#              $|Z-Z-\rangle) / \sqrt{2}$ 
```

Tutorial: Two-site state optimization

[TODO: Add visualization of minimizing $\langle \mathbf{v} | \mathbf{H} | \mathbf{v} \rangle$]

```
1 using Zygote
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3  $\partial \mathbf{E}(\psi) = \text{gradient}(\mathbf{E}, \psi)[1]$ 
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```
# Using Zygote for automatic
# differentiation of the energy.
#
# Starting state:
#
#  $|\psi_0\rangle = (|Z+Z+\rangle +$ 
#              $|Z-Z-\rangle) / \sqrt{2}$ 
```

```
1  $\psi = \text{minimize}(\mathbf{E}, \partial \mathbf{E}, \psi_0;$ 
2          $\text{nsteps}=10, \gamma=0.1)$ 
3
4
5  $\mathbf{E}(\psi_0), \text{norm}(\partial \mathbf{E}(\psi_0))$ 
6  $\mathbf{E}(\psi), \text{norm}(\partial \mathbf{E}(\psi))$ 
7
```

```
# Minimize:
#
#  $\mathbf{E}(\psi) = \langle \psi | \mathbf{H} | \psi \rangle / \langle \psi | \psi \rangle$ 
#
# (-1, 4)
# (-2.236068, 4.2766287e-6)
#  $\approx (-\sqrt{5}, 0)$ 
```

Tutorial: Two-site circuit optimization

```
1  function op(  
2      ::OpName"U",  
3      ::SiteType"S=1/2";  
4       $\theta_1, \theta_2$   
5  )  
6      c1 = cos( $\theta_1/2$ )  
7      s1 = sin( $\theta_1/2$ )  
8      c2 = cos( $\theta_2/2$ )  
9      s2 = sin( $\theta_2/2$ )  
10     return [  
11         c1 0 0 -s1  
12         0 c2 -s2 0  
13         0 s2 c2 0  
14         s1 0 0 c1  
15     ]  
16 end
```

```
# Circuit optimization.  
#  
# Note: This is a Matchgate.  
# We could do this  
# with free fermions.
```

Tutorial: Two-site circuit optimization

[TODO: Add visualization of minimizing $\langle 0|UHU|0\rangle$]

```
1   $\psi_0 = Z_{p1} * Z_{p2}$ 
2
3  function E( $\theta$ )
4       $\theta_1, \theta_2 = \theta$ 
5       $U_\theta = \text{op}(\text{"U"}, i1, i2;$ 
6                   $\theta_1=\theta_1, \theta_2=\theta_2)$ 
7       $\psi_\theta = \text{apply}(U_\theta, \psi_0)$ 
8      return inner( $\psi_\theta'$ , H,  $\psi_\theta$ )
9  end
```

```
# References state:
#  $|0\rangle = |Z+Z+\rangle$ 

# Find  $U(\theta)$  that minimizes
#
#  $E(\theta) = \langle 0|U(\theta)^\dagger H U(\theta)|0\rangle$ 
#      =  $\langle \theta|H|\theta\rangle$ 
```

Tutorial: Two-site circuit optimization

[TODO: Add visualization of minimizing $\langle 0 | U H U | 0 \rangle$]

```
1  $\psi_0 = Z_{p1} * Z_{p2}$ 
2
3 function E( $\theta$ )
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6                  $\theta_1=\theta_1, \theta_2=\theta_2)$ 
7      $\psi_\theta = \text{apply}(U_\theta, \psi_0)$ 
8     return inner( $\psi_\theta', H, \psi_\theta$ )
9 end
```

```
# References state:
#  $|0\rangle = |Z+Z+\rangle$ 

# Find  $U(\theta)$  that minimizes
#
#  $E(\theta) = \langle 0 | U(\theta)^\dagger H U(\theta) | 0 \rangle$ 
#            $= \langle \theta | H | \theta \rangle$ 
```

```
1  $\theta_0 = [\pi/2, 0]$ 
2  $\theta = \text{minimize}(E, \partial E, \theta_0;$ 
3                  $\text{nsteps}=30, \gamma=0.1)$ 
4
5  $E(\theta_0), \text{norm}(\partial E(\theta_0))$ 
6  $E(\theta), \text{norm}(\partial E(\theta))$ 
```

```
#  $E(\theta_0), \text{norm}(\partial E(\theta_0)) =$ 
#    $(-1, 2)$ 

#  $E(\theta), \text{norm}(\partial E(\theta)) =$ 
#    $(-2.2360675, 0.0014603)$ 
```

Tutorial: Two-site fidelity optimization

[TODO: Add visualization of minimizing $\langle v|U|v_0\rangle$]

```
1   $\psi_0 = Z_{p1} * Z_{p2}$ 
2   $\psi = (Z_p Z_p + Z_m Z_m) / \sqrt{2}$ 
3
4  function F( $\theta$ )
5       $\theta_1, \theta_2 = \theta$ 
6       $U_\theta = \text{op}(\text{"U"}, i_1, i_2;$ 
7                   $\theta_1=\theta_1, \theta_2=\theta_2)$ 
8       $\psi_\theta = \text{apply}(U_\theta, \psi_0)$ 
9      return -abs(inner( $\psi, \psi_\theta$ ))
10 end
```

```
# Reference state:
#  $|0\rangle = |Z+Z+\rangle$ 

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

# Find  $U(\theta)$  that minimizes
#
#  $F(\theta) = -|\langle\psi|U(\theta)|0\rangle|$ 
```

Tutorial: Two-site fidelity optimization

[TODO: Add visualization of minimizing $\langle \psi | U | \psi_0 \rangle$]

```
1   $\psi_0 = Z_{p1} * Z_{p2}$ 
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4  function F( $\theta$ )
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# Reference state:
#  $|0\rangle = |Z+Z+\rangle$ 

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

# Find  $U(\theta)$  that minimizes
#
#  $F(\theta) = -|\langle \psi | U(\theta) | 0 \rangle|$ 
```

```
1   $\theta_0 = [0, 0]$ 
2   $\theta = \text{minimize}(\text{F}, \partial \text{F}, \theta_0;$ 
3                   $\text{nsteps}=50, \gamma=0.1)$ 
4
5   $\text{F}(\theta_0), \text{norm}(\partial \text{F}(\theta_0))$ 
```

```
#  $\text{F}(\theta_0), \text{norm}(\partial \text{F}(\theta_0)) =$ 
#    $(-0.5, 0.5)$ 

#  $\text{F}(\theta), \text{norm}(\partial \text{F}(\theta)) =$ 
#    $(-0.9938992, 0.07786879)$ 
```


Tutorial: n -site states with MPS

[TODO: Add visualization of $\langle Z_p | \text{Cat} \rangle$]

```
1  n = 30
2  i = [Index(2, "S=1/2") for
3      j in 1:n]
4
5  Zp = MPS(i, "Z+")
6  Zm = MPS(i, "Z-")
7
8  Cat = (Zp + Zm)/√2
9
```

n -site state

$|Z+Z+\dots Z+\rangle$

$|Z-Z-\dots Z-\rangle$

$(|Z+Z+\dots Z+\rangle +$

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

Tutorial: n -site states with MPS

[TODO: Add visualization of $\langle Z_p | \text{Cat} \rangle$]

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9
```

n -site state

$|Z+Z+\dots Z+\rangle$

$|Z-Z-\dots Z-\rangle$

$(|Z+Z+\dots Z+\rangle +$

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

```
1  maxlinkdim(Zp)
2  maxlinkdim(Cat)
3  norm(Cat)
4  inner(Zp, Zp)
5  inner(Zm, Zp)
6  inner(Zp, Cat)
```

1

2

≈ 1

≈ 1

≈ 0

$\approx 1/\sqrt{2}$

Tutorial: n -site states with MPS

[TODO: Add visualization of minimizing $\langle \text{psi} | H | \text{psi} \rangle$]

```
1  j = n ÷ 2
2  Xj = op("X", i[j])
3
4  XjZp = apply(Xj, Zp)
5
6
7  state = [k == j ? "Z-" : "Z+"
8           for k in 1:n]
9  XjZp = MPS(i, state)
```

```
# j = n ÷ 2
# Xj

# Xj|Z+Z+...Z+⟩ =
#   |Z+Z+...Z-...Z+⟩

# |Z+Z+...Z-...Z+⟩
```

Tutorial: n -site states with MPS

[TODO: Add visualization of minimizing $\langle \text{psi} | H | \text{psi} \rangle$]

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7  state = [k == j ? "Z-" : "Z+"]
8          for k in 1:n]
9  XjZp = MPS(i, state)
```

```
# j = n ÷ 2
# Xj
# Xj|Z+Z+...Z+⟩ =
#   |Z+Z+...Z-...Z+⟩
# |Z+Z+...Z-...Z+⟩
```

```
1  maxlinkdim(XjZp)
2  inner(Zp, XjZp)
3  inner(XjZp, apply(Xj, Zp))
```

```
# 1
# ≈ 0
# ≈ 1
```

Tutorial: n -site states with MPS

[TODO: Add visualization of minimizing $\langle \text{psi} | H | \text{psi} \rangle$]

```
1 function ising(n; h)
2   H = OpSum()
3   for j in 1:(n - 1)
4     H -= "Z", j, "Z", j + 1
5   end
6   for j in 1:n
7     H += h, "X", j
8   end
9   return H
10 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 $\langle \psi | H | \psi \rangle$]

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1 function ising(n; h)
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5   end
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7     H += h, "X", j
8   end
9   return H
10 end
```

n sites

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

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

= 3

$$\# \langle Z_+ Z_+ \dots Z_+ | H | Z_+ Z_+ \dots Z_+ \rangle \approx$$

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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