

Introduction

Cluster  
Expansions

Results

Conclusion

# Cluster Expansions of Thermal States using Tensor Networks

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## Introduction

Overview  
Simulation

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# Introduction

# Introduction

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Conclusion

- Overview condensed matter physics
  - Macroscopic and microscopic physical properties of matter
    - Metals
    - semiconductors
    - Liquids
    - Bose-Einstein Condensates
    - Magnets
  - Different disciplines
    - Experimental
    - Theoretical
    - Engineering

# Introduction

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- Overview condensed matter physics
- Strongly correlated materials [1]
  - Superconductors
  - Quantum spin liquids
  - Strange metals
  - Correlated topological matter

# Introduction

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- Overview condensed matter physics
- Strongly correlated materials
- How to proceed
  - Material synthesis and discovery
  - Analytical methods
  - Numerical methods

# Simulating Quantum Many-body Systems

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Conclusion

- Equations are known
- Curse of dimensionality
- Numerical methods

# Tensor Networks

## Introduction

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$$|\Psi\rangle = \sum_{i_1 i_2 \dots i_n} C^{i_1 i_2 \dots i_n} |i_1\rangle \otimes |i_2\rangle \otimes \dots \otimes |i_n\rangle. \quad (1)$$

$$\begin{aligned} C^{i_1 i_2 \dots i_n} &= w_l C^{i_1} C^{i_2} \dots C^{i_n} w_r \\ &= \text{---} \bigcirc \text{---} \chi \text{---} \bigcirc \text{---} \dots \text{---} \bigcirc \text{---} \end{aligned} \quad (2)$$

- MPS
- Relevant corner Hilbert space

# Operator Exponential

- (Real) Time evolution:

$$\hat{O} = e^{-i\hat{H}t} \quad (3)$$

- Statistical ensembles:

$$\hat{O} = \frac{e^{-\beta\hat{H}}}{\text{Tr}(e^{-\beta\hat{H}})} \quad (4)$$

Imaginary time ( $\beta = it$ )

$$\hat{O} = \begin{array}{c} \dots & \dots & \dots \\ \dots - \text{[circle with slash]} - \text{[circle with slash]} - \text{[circle with slash]} - \dots \\ | & | & | \\ \dots - \text{[circle with slash]} - \text{[circle with slash]} - \text{[circle with slash]} - \dots \\ | & | & | \\ \dots - \text{[circle with slash]} - \text{[circle with slash]} - \text{[circle with slash]} - \dots \\ \dots & \dots & \dots \end{array} \quad (5)$$

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# Cluster Expansions

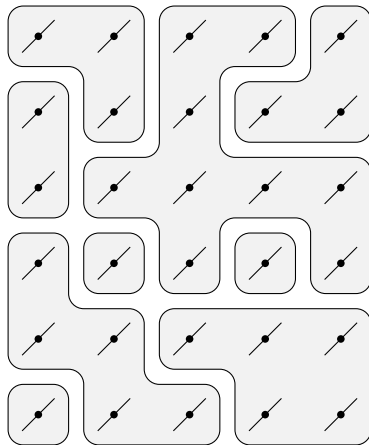
# Cluster Expansions

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$$\blacksquare e^{\hat{H}} = \sum_{\{B\}} \bigotimes_i B_i$$

$$e^{H(1)} = \boxed{\text{diagonal line}} \quad (6)$$

$$e^{H(2)} = \boxed{\text{diagonal line} \quad \text{diagonal line}} + \boxed{\text{diagonal line}} \quad \boxed{\text{diagonal line}} \quad (7)$$

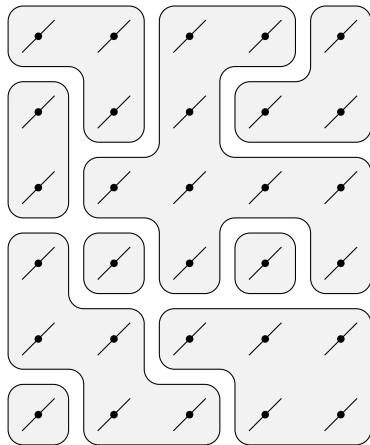
# Cluster Expansions

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- $e^{\hat{H}} = \sum_{\{B\}} \bigotimes_i B_i$
- Finite number of blocks
- Encoded by 1 tensor

$$O^{abcd} = \begin{array}{c} \begin{array}{c} b \\ a \end{array} \begin{array}{c} i \\ c \end{array} \\ \bigcirc \\ \begin{array}{c} j \\ d \end{array} \end{array} \quad (6)$$

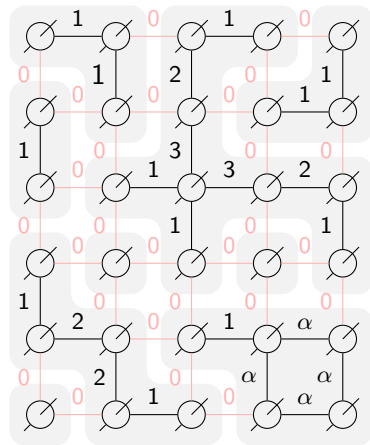
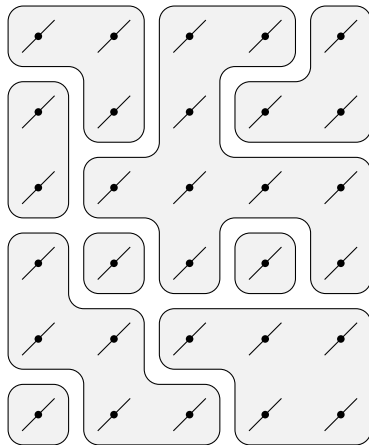
# Cluster Expansions

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# Cluster Expansions

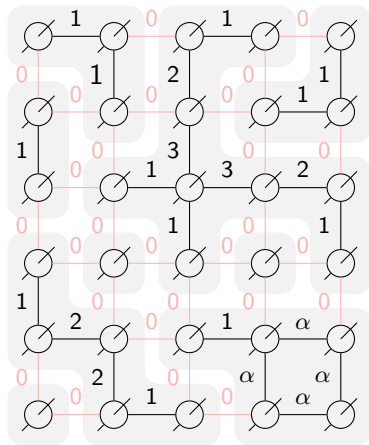
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- Multiple choices for encoding
- Size extensive
- Preserves global and internal symmetries
- Tensor Network toolbox



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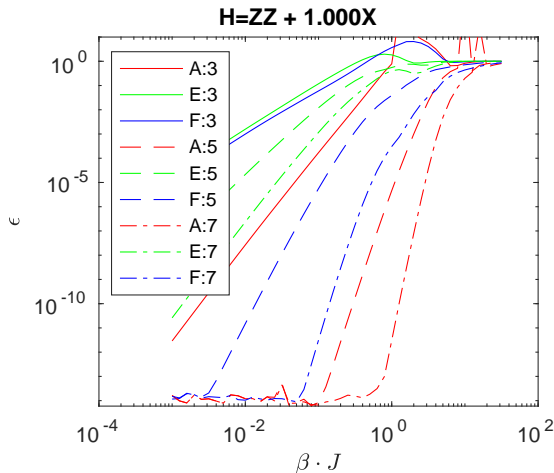
**Results**

1D Exact  
TFI Phase Diagram

Conclusion

# Results

# 1D: Transverse Field Ising (TFI)



- Relative error  $\epsilon$
- Different encodings:
  - A: Small
  - E: Strict
  - F: well-conditioned
- bond dimension

		Encoding	
		A	E/F
Order	3	5	10
	5	21	42
	7	85	170

# Conclusion

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- 2D: similar results
- Real time evolution
- Encoding



# 2D TFI: Introduction

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Results

1D Exact

TFI Phase Diagram

Conclusion

- Phase Transition
- $\Gamma = 2.5$
- VUMPS
- Order 5

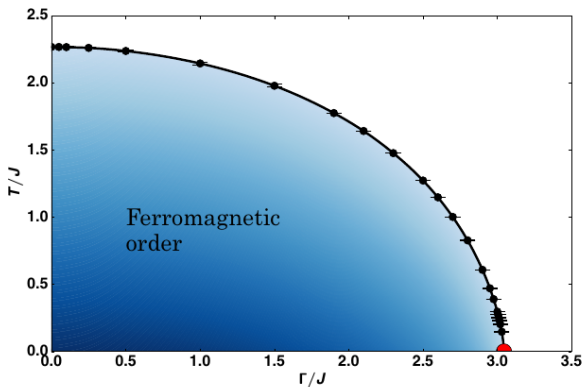


Figure taken from [2]

# TFI Phase Diagram: $\Gamma = 2.5$

Introduction

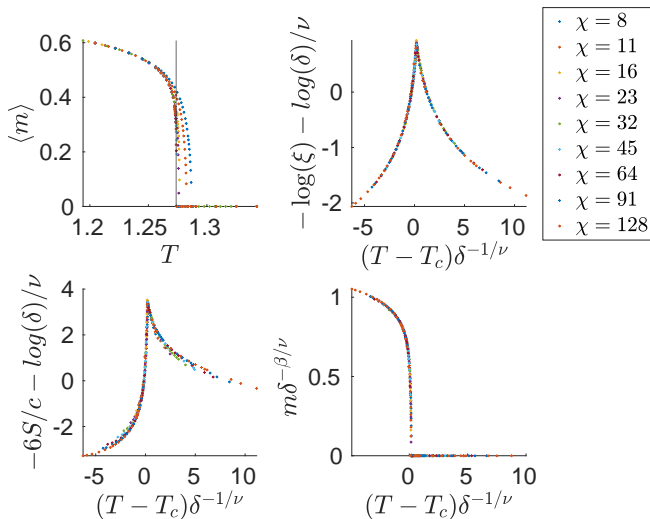
Cluster  
Expansions

Results

1D Exact

TFI Phase Diagram

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	$T_c$
Fit	1.2736(6)
QMC	1.2737(6)
TN	1.2737(2)

Data from [3]

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# Conclusion

# References I



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# References II

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P. Czarnik, P. Corboz, Finite correlation length scaling with infinite projected entangled pair states at finite temperature, Physical Review B 99 (2019) 245107.

doi:10.1103/PhysRevB.99.245107.

Tensor Networks

Linear Solver

Construction

TFI Collapses

Direct Results

Solvers

# Tensor Networks

# Tensor Networks: Introduction

Tensor Networks

Linear Solver

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Direct Results

Solvers

$$|\Psi\rangle = \sum_{i_1 i_2 \dots i_n} C^{i_1 i_2 \dots i_n} |i_1\rangle \otimes |i_2\rangle \otimes \dots \otimes |i_n\rangle. \quad (6)$$

$$C^{i_1 i_2 \dots i_n} = \text{Tr}(C^{i_1} C^{i_2} \dots C^{i_n} M). \quad (7)$$

# Tensor Networks: Graphical Notation

## Tensor Networks



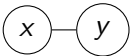
Linear Solver

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conventional	Einstein	tensor notation
$\vec{x}$	$x_\alpha$	
$M$	$M_{\alpha\beta}$	
$\vec{x} \cdot \vec{y}$	$x_\alpha y_\alpha$	



# Tensor Networks: MPS

Tensor Networks

Linear Solver

Construction

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Solvers

$$C^{i_1 i_2 \dots i_n} = \text{Tr}(C^{i_1} C^{i_2} \dots C^{i_n} M) \quad (8)$$

Diagram illustrating the contraction of a tensor  $C$  with indices  $i_1, i_2, \dots, i_n$  and a tensor  $M$  to form a trace. The left side shows a box labeled  $C$  with indices  $i_1, i_2, \dots, i_n$  above it. The right side shows a chain of circles labeled  $C, C, \dots, C, M$  with indices  $i_1, i_2, \dots, i_n$  above the first  $n$  circles. A line connects the last  $C$  to  $M$ , and a line connects  $M$  back to the first  $C$ , forming a trace. The equation is labeled (9).

# Tensor Networks: Operators

Tensor Networks

Linear Solver

Construction

TFI Collapses

Direct Results

Solvers

$$\hat{O} = \dots \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \dots \quad (10)$$

$$\hat{O} |\psi\rangle = \dots \text{---} \begin{array}{c} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \dots \\ | \quad | \quad | \\ \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \dots \\ | \quad | \quad | \end{array} \dots = \dots \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \dots \quad (11)$$

Tensor Networks

Linear Solver

Construction

TFI Collapses

Direct Results

Solvers

# Linear Solver

# Linear Solver: Inversion Scheme

Tensor Networks

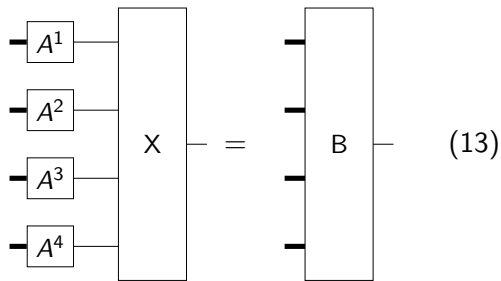
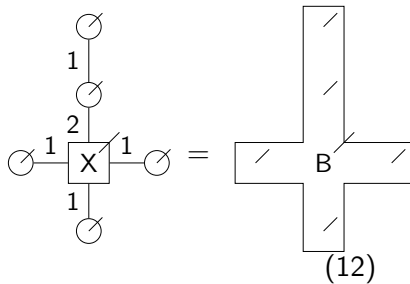
Linear Solver

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# Linear Solver: Inversion Scheme

Tensor Networks

Linear Solver

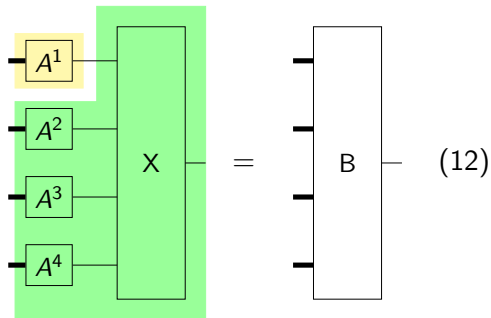
Construction

TFI Collapses

Direct Results

Solvers

- Invert  $A^i$  separately
  - Fast
  - Numerically unstable



# Linear Solver: Inversion Scheme

Tensor Networks

Linear Solver

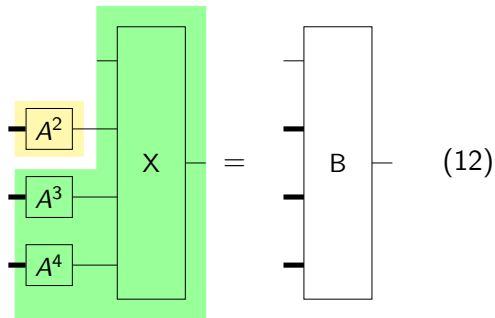
Construction

TFI Collapses

Direct Results

Solvers

- Invert  $A^i$  separately
  - Fast
  - Numerically unstable



# Linear Solver: Inversion Scheme

Tensor Networks

Linear Solver

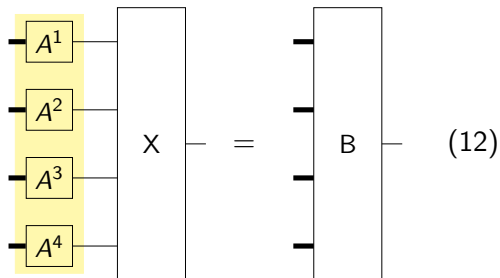
Construction

TFI Collapses

Direct Results

Solvers

- Invert  $A^i$  separately
- Full inversion
  - Slow
  - Stable for pseudoinverse



# Linear Solver: Inversion Scheme

Tensor Networks

Linear Solver

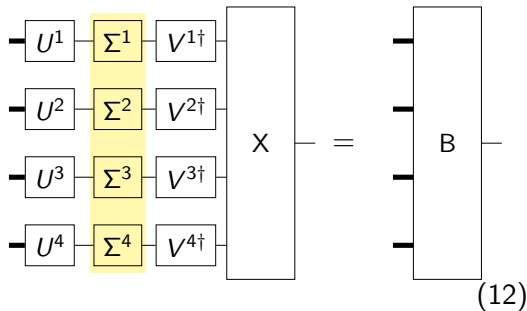
Construction

TFI Collapses

Direct Results

Solvers

- Invert  $A^i$  separately
- Full inversion
- Sparse full inversion
  - $A^i = U^i \Sigma^i V^{i\dagger}$





Tensor Networks

Linear Solver

**Construction**

1D

2D

TFI Collapses

Direct Results

Solvers

# Construction

# Notation

Tensor Networks

Linear Solver

Construction

1D

2D

TFI Collapses

Direct Results

Solvers

$$O^{00} = \begin{array}{c} i \\ | \\ 0 \text{ --- } \bigcirc \text{ --- } 0 \\ | \\ j \end{array} = \bigcirc \quad (13)$$

$$O^{01} O^{10} = \bigcirc \text{ --- } 1 \text{ --- } \bigcirc \quad (14)$$

# General idea

Tensor Networks

Linear Solver

Construction

1D

2D

TFI Collapses

Direct Results

Solvers

$$\bigcirc = \exp(-\beta H(\bigcirc)) \quad (15)$$

$$\overset{1}{\bigcirc} - \bigcirc = \exp -\beta H(\overset{1}{\bigcirc} - \bigcirc) \quad (16)$$
$$-\bigcirc \overset{0}{-} \bigcirc$$

# General idea

Tensor Networks

Linear Solver

Construction

1D

2D

TFI Collapses

Direct Results

Solvers

$$\begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \end{array} \begin{array}{cc} 1 & 1 \\ 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{array} \text{---} = \exp -\beta H(\text{---} \text{---} \text{---}) \quad (17)$$

# General idea

Tensor Networks

Linear Solver

Construction

1D

2D

TFI Collapses

Direct Results

Solvers

$$\begin{array}{c} \text{1} \quad \text{1} \\ \bigcirc - \bigcirc - \bigcirc = \exp -\beta H(\bigcirc - \bigcirc - \bigcirc) \\ \\ - \bigcirc - \bigcirc - \bigcirc \end{array} \quad (17)$$

# General idea

Tensor Networks

Linear Solver

**Construction**

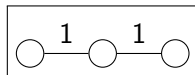
1D

2D

TFI Collapses

Direct Results

Solvers



(17)

# 1D: Variant A

Tensor Networks

Linear Solver

Construction

1D

2D

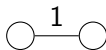
TFI Collapses

Direct Results

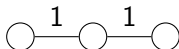
Solvers



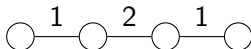
(18a)



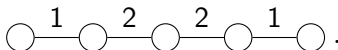
(18b)



(18c)



(18d)



(18e)

# 1D: Variant E

Tensor Networks

Linear Solver

Construction

1D

2D

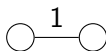
TFI Collapses

Direct Results

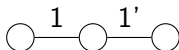
Solvers



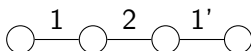
(19a)



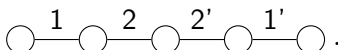
(19b)



(19c)



(19d)



(19e)



# 1D: Variant F

Tensor Networks

Linear Solver

Construction

1D

2D

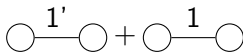
TFI Collapses

Direct Results

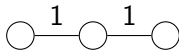
Solvers



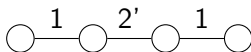
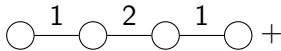
(20a)



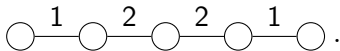
(20b)



(20c)



(20d)



(20e)

Tensor Networks

Linear Solver

Construction

1D

2D

TFI Collapses

Direct Results

Solvers

$$O^{0000} = \begin{array}{c} \begin{array}{c} 0 \\ \diagup \\ \text{---} \end{array} \begin{array}{c} 0 \\ \diagdown \\ \text{---} \end{array} \\ \begin{array}{c} \text{---} \\ \diagdown \\ j_0 \end{array} \end{array} = \bigcirc \quad (21)$$

## 2D: Linear Blocks

Tensor Networks

Linear Solver

Construction

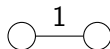
1D

2D

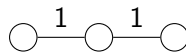
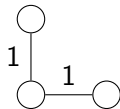
TFI Collapses

Direct Results

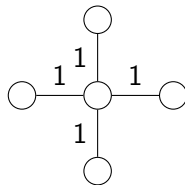
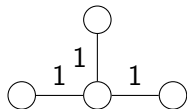
Solvers



(22a)



(22b)



(22c)

## 2D: Nonlinear Blocks

Tensor Networks

Linear Solver

Construction

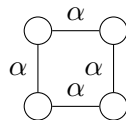
1D

2D

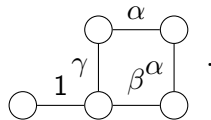
TFI Collapses

Direct Results

Solvers



(23)



(24)

Tensor Networks

Linear Solver

Construction

**TFI Collapses**

$g = 0.0$

$g = 2.9$

Direct Results

Solvers

## TFI Collapses

# TFI Phase Diagram: Classical Ising

Tensor Networks

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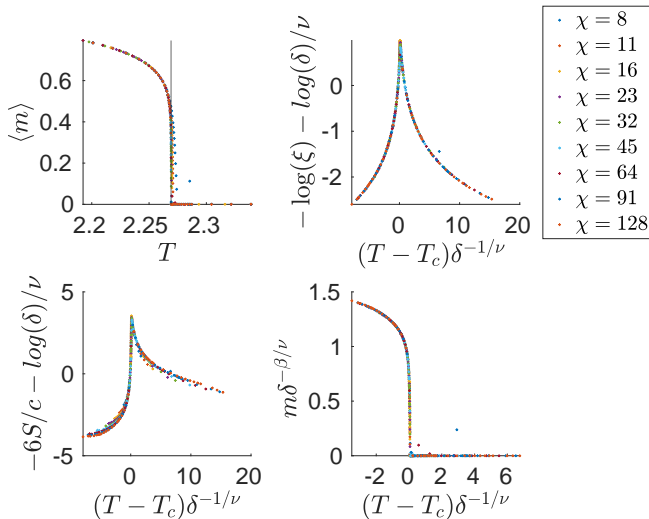
TFI Collapses

$g = 0.0$

$g = 2.9$

Direct Results

Solvers



	$T_c$
Fit	2.691(9)
Exact	2.691853

Tensor Networks

Linear Solver

Construction

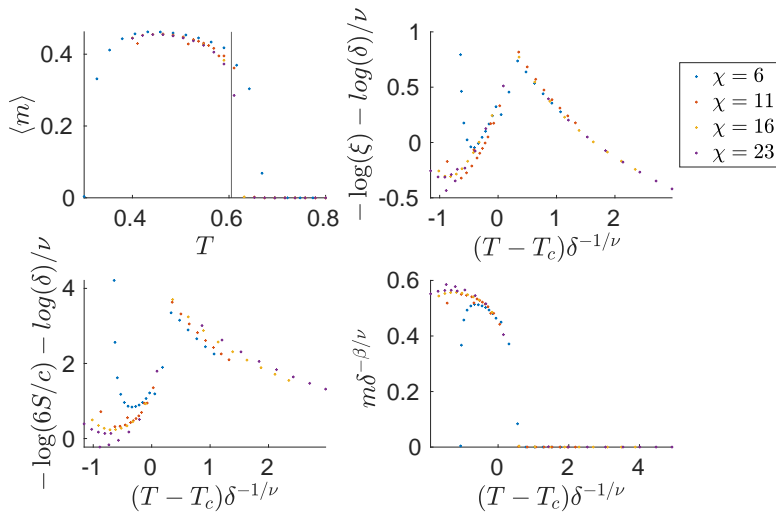
TFI Collapses

$g = 0.0$

$g = 2.9$

Direct Results

Solvers



Tensor Networks

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TFI Collapses

**Direct Results**

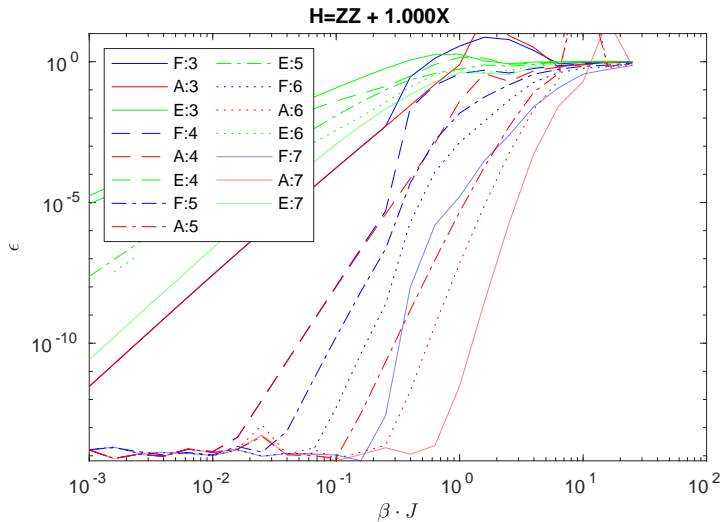
2D Exact

Solvers

## Direct Results



# 1D: Transverse Field Ising (TFI): full



Tensor Networks

Linear Solver

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TFI Collapses

Direct Results

2D Exact

Solvers

# 1D: Heisenberg XXX

Tensor Networks

Linear Solver

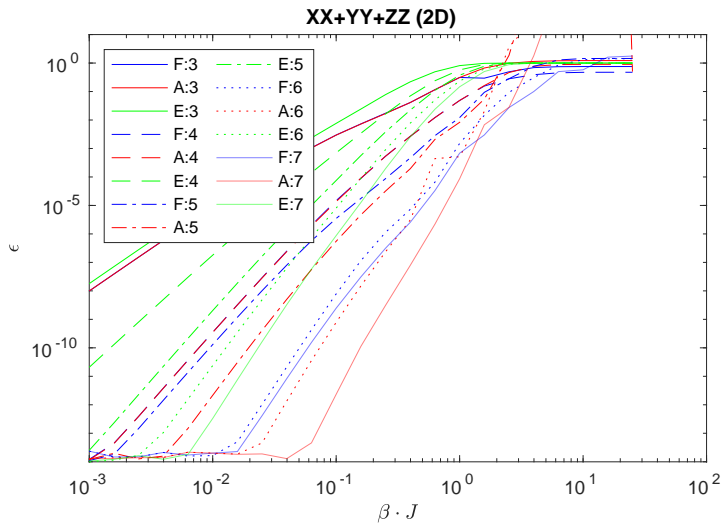
Construction

TFI Collapses

Direct Results

2D Exact

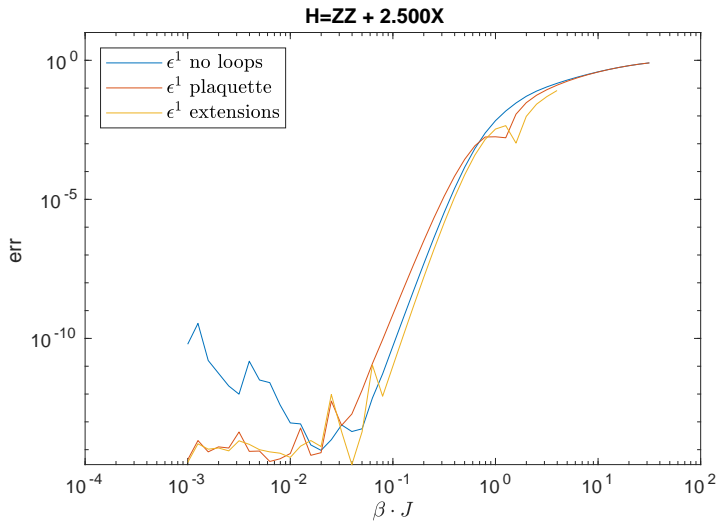
Solvers





## 2D: Transverse Field Ising

Tensor Networks  
Linear Solver  
Construction  
TFI Collapses  
Direct Results  
2D Exact  
Solvers



Tensor Networks

Linear Solver

Construction

TFI Collapses

Direct Results

**Solvers**

Linear Solver

Nonlinear Solver

Sequential Linear Solver

# Solvers

# Linear solver

- $AX = B$
- Invert leg per leg
- Pseudoinverse

The diagram shows a square tensor labeled 'X' with four legs. The top leg has a circle at its end with the number '1' above it. The bottom leg has a circle at its end with the number '1' below it. The left leg has a circle at its end with the number '1' to its left. The right leg has a circle at its end with the number '1' to its right. The number '2' is placed between the top and bottom legs on the left side. This is followed by an equals sign and a cross-shaped tensor labeled 'B'. The vertical bar of the cross has two diagonal lines, and the horizontal bar also has two diagonal lines. To the right of the cross is the label '(25)'.

$$\text{Diagram of } X \text{ with legs } 1, 1, 1, 1 \text{ and index } 2 = \text{Diagram of } B \text{ (cross shape)} \quad (25)$$

# Linear Solver: Applicability

Tensor Networks

Linear Solver

Construction

TFI Collapses

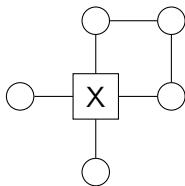
Direct Results

Solvers

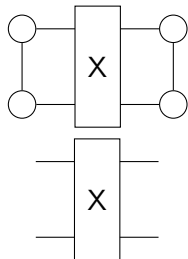
Linear Solver

Nonlinear Solver

Sequential Linear Solver

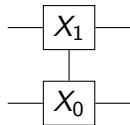


(26)



(27a)

=



(27b)

# Nonlinear Solver

Tensor Networks

Linear Solver

Construction

TFI Collapses

Direct Results

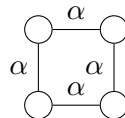
Solvers

Linear Solver

**Nonlinear Solver**

Sequential Linear Solver

- Nonlinear least squares
- Jacobian
- Permutations



(28)



# Sequential Linear Solver

Tensor Networks

Linear Solver

Construction

TFI Collapses

Direct Results

Solvers

Linear Solver

Nonlinear Solver

**Sequential Linear Solver**

- Based on linear solver
- Sweep over unknown tensors
- Permutations