

Introduction

Cluster  
Expansions

Results

Conclusion

# Cluster Expansions of Thermal States using Tensor Networks

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Introduction

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Conclusion

- Introduction
- Cluster Expansions
- Results

## Introduction

Overview  
Simulation

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# Introduction

# Introduction

Introduction

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- 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
  - High  $T_c$  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

Introduction

Overview

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Conclusion

- Equations are known
- Curse of dimensionality
- Numerical methods

# Tensor Networks

## Introduction

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

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

- Matrix Product State
- Relevant corner Hilbert space



# Operator Exponential

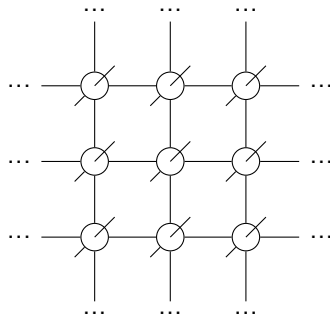
## ■ Time evolution:

$$\hat{H} |\Psi(t)\rangle = i \frac{d}{dt} |\Psi(t)\rangle \quad (3)$$

$$|\Psi(t)\rangle = e^{-i\hat{H}t} |\Psi(0)\rangle \quad (4)$$

## ■ Statistical ensembles:

$$\hat{\rho} = \frac{e^{-\beta\hat{H}}}{\text{Tr}(e^{-\beta\hat{H}})} \quad (5)$$



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# Cluster Expansions

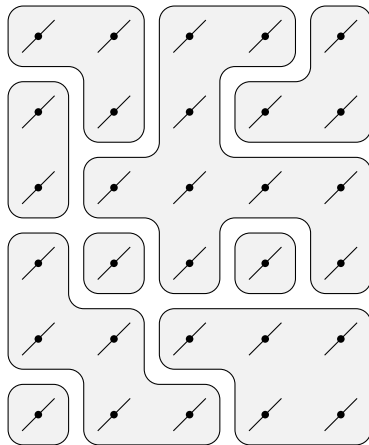
# Cluster Expansions

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

$$e^{-\beta H(1)} = \boxed{\diagup}$$

$$e^{-\beta H(2)} = \boxed{\diagup \quad \diagup} + \boxed{\diagup} \boxed{\diagup}$$

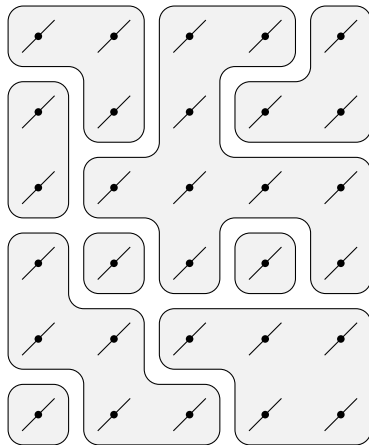
# Cluster Expansions

Introduction

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

$$e^{-\beta H(3)} =$$

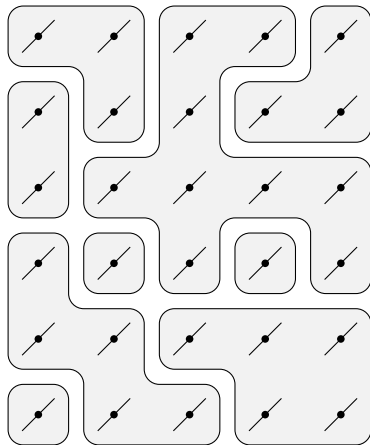
# Cluster Expansions

Introduction

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

$$O^{abcd} = \begin{array}{c} \begin{array}{ccccc} & & b & & \\ & a & \circ & i & c \\ & j & d & & \end{array} \end{array}$$

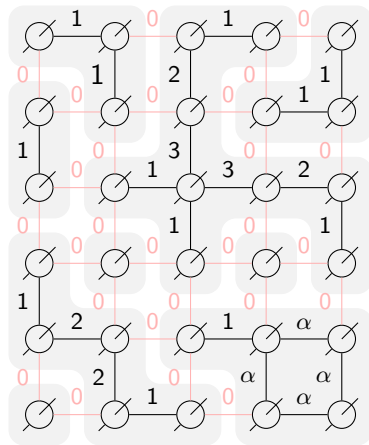
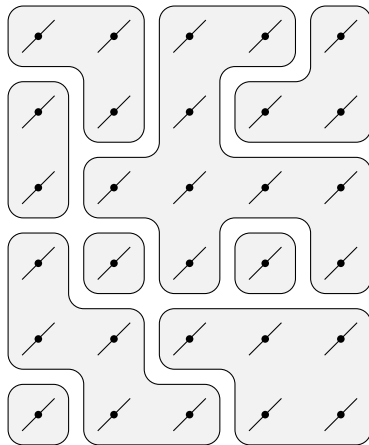
# Cluster Expansions

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# Cluster Expansions

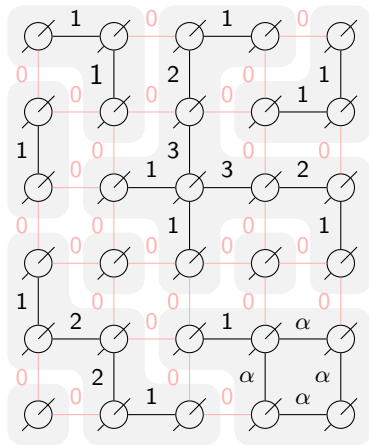
Introduction

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



Introduction

Cluster  
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**Results**

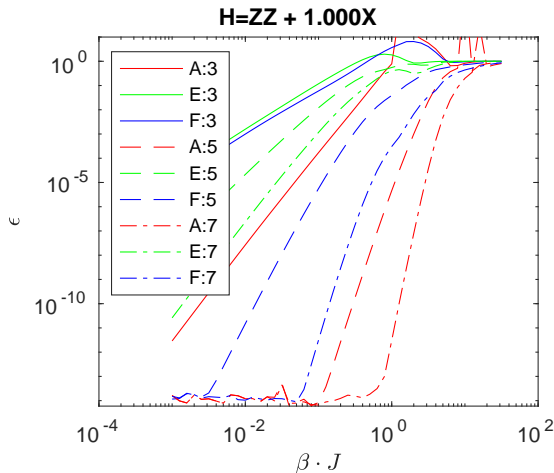
1D Exact  
TFI Phase Diagram

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

Introduction

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1D Exact  
TFI Phase Diagram

Conclusion

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

# 2D TFI: Introduction

Introduction

Cluster  
Expansions

Results

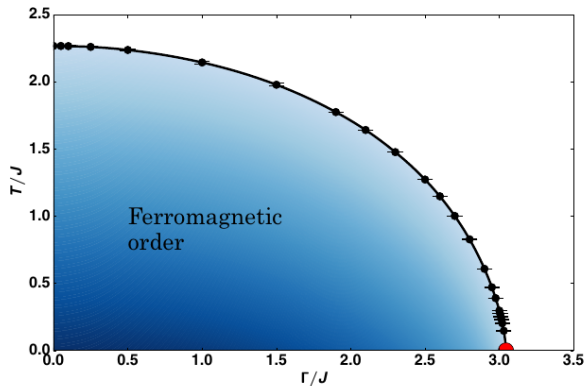
1D Exact

TFI Phase Diagram

Conclusion

- Different phases
- $\Gamma = 2.5$
- VUMPS
- Order 5

$$\hat{H} = -J \sum_{\langle ij \rangle} Z_i Z_j + \Gamma \sum_i X_i \quad (6)$$



# Criticality

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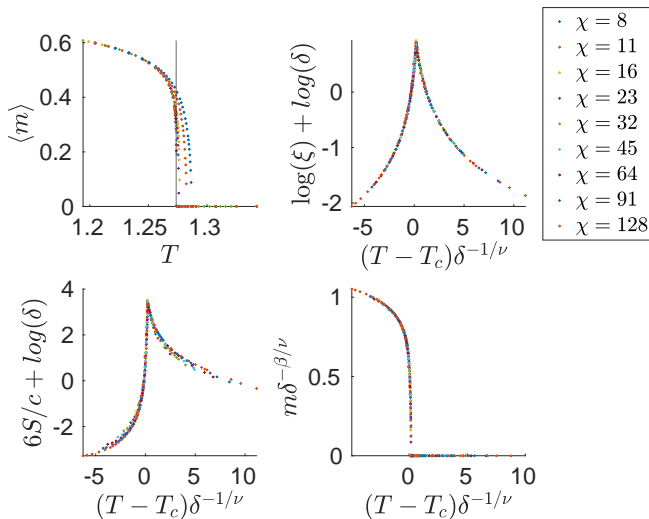
1D Exact

TFI Phase Diagram

Conclusion

- Phase transition
- Power law
- Finite size scaling ( $\chi, \delta^{-1}$ )
- Data collapse
  - Observables:  $m$ ,  $S$  and  $\xi$
  - Parameters:  $T_c$

# TFI Phase Diagram: $\Gamma = 2.5$



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

Data from [1]

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# Conclusion

# Conclusion

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- Cluster expansions work extremely well for some encodings
- Stable and fast framework

# References I

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P. Czarnik and P. Corboz.

Finite correlation length scaling with infinite projected entangled pair states at finite temperature.

*Physical Review B*, 99:245107, 2019.



S. Hesselmann and S. Wessel.

Thermal Ising transitions in the vicinity of two-dimensional quantum critical points.

*PHYSICAL REVIEW B*, 93:155157, 2016.



Tensor Networks

Linear Solver

Construction

TFI Collapses

Direct Results

Solvers

# Tensor Networks

# Tensor Networks: Introduction

Tensor Networks

Linear Solver

Construction

TFI Collapses

Direct Results

Solvers

$$|\Psi\rangle = \sum_{i_1 i_2 \dots i_n} C^{i_1 i_2 \dots i_n} |i_1\rangle \otimes |i_2\rangle \otimes \dots \otimes |i_n\rangle. \quad (7)$$

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

# Tensor Networks: Graphical Notation

## Tensor Networks



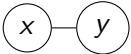
Linear Solver

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Solvers

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

TFI Collapses

Direct Results

Solvers

$$C^{i_1 i_2 \dots i_n} = \text{Tr}(C^{i_1} C^{i_2} \dots C^{i_n} M) \quad (9)$$

The diagram shows the trace of a product of tensors  $C$  and  $M$ . On the left, a large rectangle labeled  $C$  has indices  $i_1, i_2, \dots, i_n$  above it. This is equated to a tensor network on the right. The network consists of a sequence of circles: the first  $n-1$  are labeled  $C$  and the last is labeled  $M$ . Each  $C$  circle has an index  $i_1, i_2, \dots, i_n$  above it. The circles are connected in a chain, with an additional connection from the first  $C$  circle back to the  $M$  circle, forming a closed loop. The label  $\chi$  is placed between the first two  $C$  circles. The entire expression is labeled (10) on the right.

# Tensor Networks: Operators

Tensor Networks

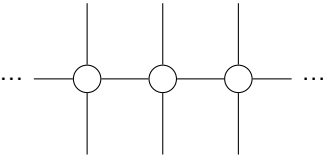
Linear Solver

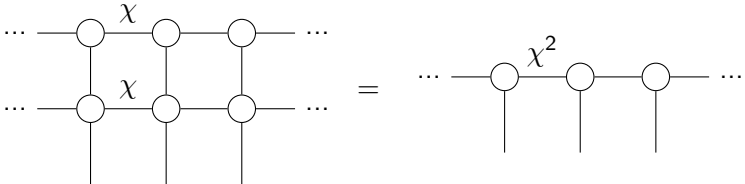
Construction

TFI Collapses

Direct Results

Solvers

$$\hat{O} = \dots \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \dots \quad (11)$$


$$\hat{O} |\psi\rangle = \dots \text{---} \begin{array}{c} \bigcirc \chi \\ | \\ \bigcirc \chi \end{array} \text{---} \begin{array}{c} \bigcirc \\ | \\ \bigcirc \end{array} \text{---} \begin{array}{c} \bigcirc \\ | \\ \bigcirc \end{array} \text{---} \dots = \dots \text{---} \bigcirc \chi^2 \text{---} \bigcirc \text{---} \bigcirc \text{---} \dots \quad (12)$$


Tensor Networks

Linear Solver

Construction

TFI Collapses

Direct Results

Solvers

# Linear Solver

# Linear Solver: Inversion Scheme

Tensor Networks

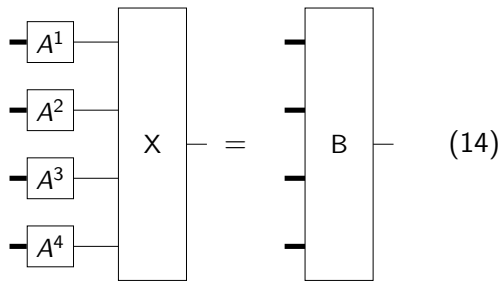
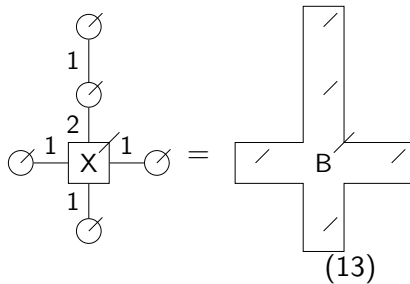
Linear Solver

Construction

TFI Collapses

Direct Results

Solvers



# Linear Solver: Inversion Scheme

Tensor Networks

Linear Solver

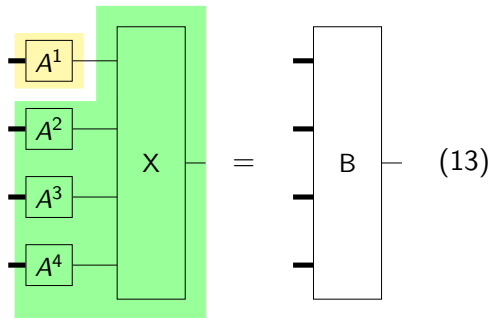
Construction

TFI Collapses

Direct Results

Solvers

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





# Linear Solver: Inversion Scheme

Tensor Networks

Linear Solver

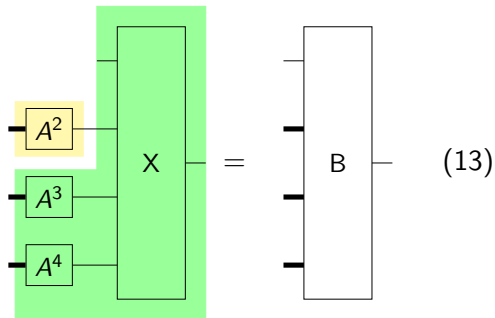
Construction

TFI Collapses

Direct Results

Solvers

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


$$\begin{matrix} A^2 \\ A^3 \\ A^4 \end{matrix} \rightarrow X = B \quad (13)$$

# Linear Solver: Inversion Scheme

Tensor Networks

Linear Solver

Construction

TFI Collapses

Direct Results

Solvers

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

The diagram illustrates the full inversion scheme for a linear solver. On the left, a vertical stack of four yellow boxes labeled  $A^1$ ,  $A^2$ ,  $A^3$ , and  $A^4$  is shown. Each box has a horizontal line extending to the right, connecting to a large vertical rectangle labeled  $X$ . To the right of  $X$  is an equals sign, followed by another large vertical rectangle labeled  $B$ . The rectangle  $B$  has four horizontal lines extending from its left side, corresponding to the inputs from the  $A^i$  boxes. The entire equation is labeled (13) on the far right.

$$\begin{matrix} A^1 \\ A^2 \\ A^3 \\ A^4 \end{matrix} \rightarrow X = B \quad (13)$$

# Linear Solver: Inversion Scheme

Tensor Networks

Linear Solver

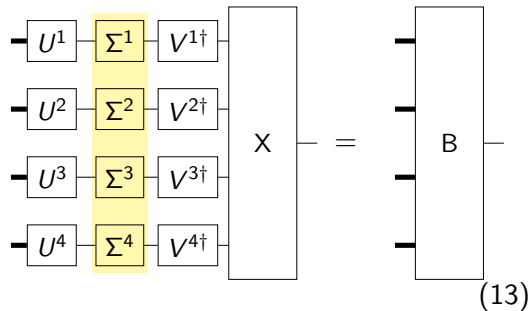
Construction

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

$$O^{00} = \begin{array}{c} i \\ | \\ 0 \text{ --- } \bigcirc \text{ --- } 0 \\ | \\ j \end{array} = \bigcirc \quad (14)$$

$$O^{01} O^{10} = \bigcirc \text{ --- } 1 \text{ --- } \bigcirc \quad (15)$$

# General idea

Tensor Networks

Linear Solver

Construction

1D

2D

TFI Collapses

Direct Results

Solvers

$$\bigcirc = \exp(-\beta H(\bigcirc)) \quad (16)$$

$$\overset{1}{\bigcirc} - \bigcirc = \exp -\beta H(\bigcirc - \bigcirc) \quad (17)$$

$\overset{0}{- \bigcirc} - \bigcirc$

# General idea

Tensor Networks

Linear Solver

Construction

1D

2D

TFI Collapses

Direct Results

Solvers

$$\begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{c} 1 \quad 1 \\ 0 \quad 0 \\ 1 \quad 0 \\ 0 \quad 1 \end{array} = \exp -\beta H(\text{---} \text{---} \text{---}) \quad (18)$$

# General idea

Tensor Networks

Linear Solver

Construction

1D

2D

TFI Collapses

Direct Results

Solvers

$$\begin{array}{c} \text{1} \quad \text{1} \\ \bigcirc - \bigcirc - \bigcirc = \exp -\beta H(\bigcirc - \bigcirc - \bigcirc) \\ \\ - \bigcirc - \bigcirc - \bigcirc \end{array} \quad (18)$$



# General idea

Tensor Networks

Linear Solver

**Construction**

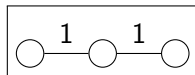
1D

2D

TFI Collapses

Direct Results

Solvers



(18)

# 1D: Variant A

Tensor Networks

Linear Solver

Construction

1D

2D

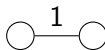
TFI Collapses

Direct Results

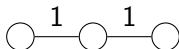
Solvers



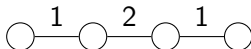
(19a)



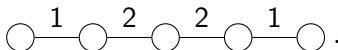
(19b)



(19c)



(19d)



(19e)

# 1D: Variant E

Tensor Networks

Linear Solver

Construction

1D

2D

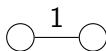
TFI Collapses

Direct Results

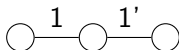
Solvers



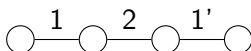
(20a)



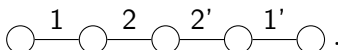
(20b)



(20c)



(20d)



(20e)

# 1D: Variant F

Tensor Networks

Linear Solver

Construction

1D

2D

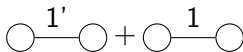
TFI Collapses

Direct Results

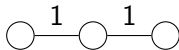
Solvers



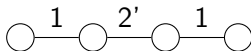
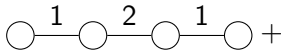
(21a)



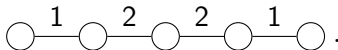
(21b)



(21c)



(21d)



(21e)

Tensor Networks

Linear Solver

Construction

1D

2D

TFI Collapses

Direct Results

Solvers

$$O^{0000} = \begin{array}{c} \begin{array}{c} 0 \\ \diagup \\ \text{---} \end{array} \begin{array}{c} 0 \\ \diagdown \\ \text{---} \end{array} \\ \begin{array}{c} \text{---} \\ \diagdown \\ j_0 \end{array} \end{array} = \bigcirc \quad (22)$$

## 2D: Linear Blocks

Tensor Networks

Linear Solver

Construction

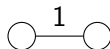
1D

2D

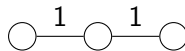
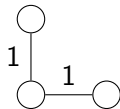
TFI Collapses

Direct Results

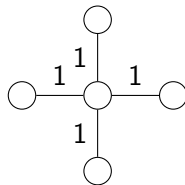
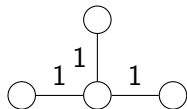
Solvers



(23a)



(23b)



(23c)

## 2D: Nonlinear Blocks

Tensor Networks

Linear Solver

Construction

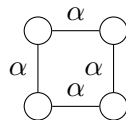
1D

2D

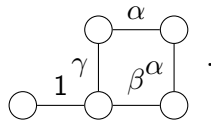
TFI Collapses

Direct Results

Solvers



(24)



(25)

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

Linear Solver

Construction

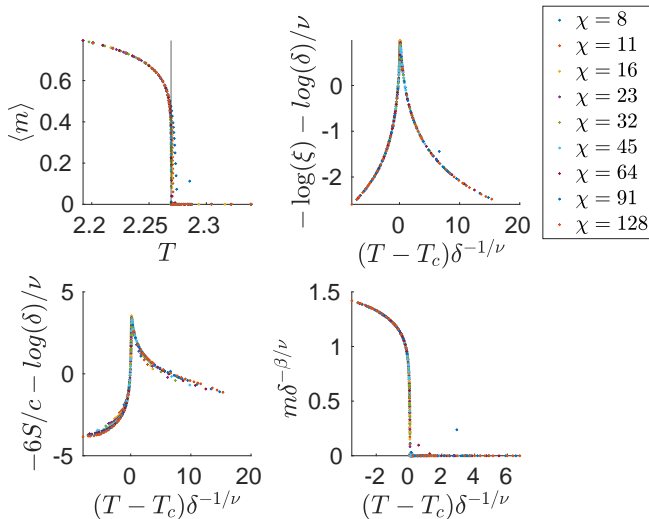
TFI Collapses

$g = 0.0$

$g = 2.9$

Direct Results

Solvers



	$T_c$
Fit	2.691(9)
Exact	2.691853

Tensor Networks

Linear Solver

Construction

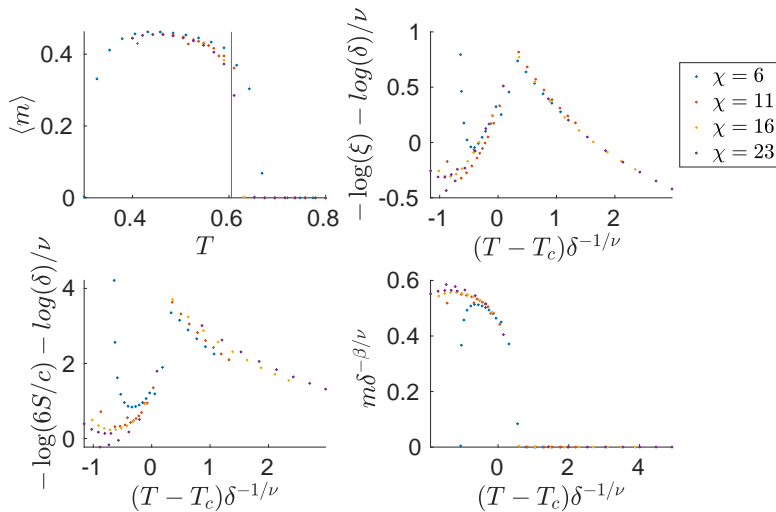
TFI Collapses

$g = 0.0$

$g = 2.9$

Direct Results

Solvers



Tensor Networks

Linear Solver

Construction

TFI Collapses

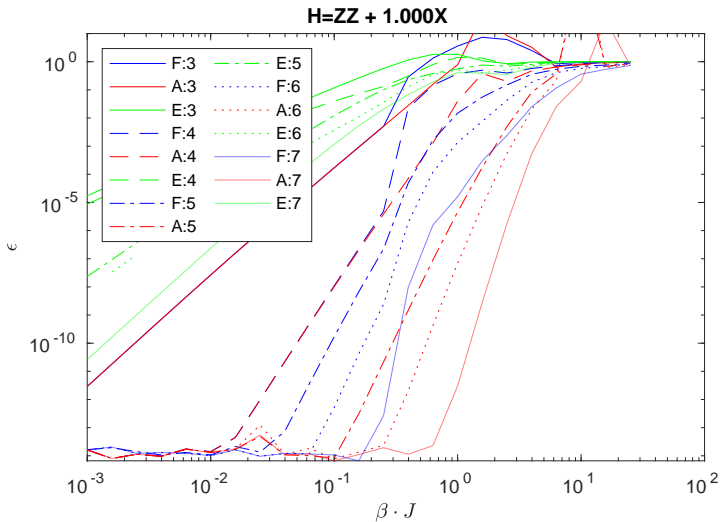
**Direct Results**

2D Exact

Solvers

## Direct Results

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



Tensor Networks

Linear Solver

Construction

TFI Collapses

Direct Results

2D Exact

Solvers

# 1D: Heisenberg XXX

Tensor Networks

Linear Solver

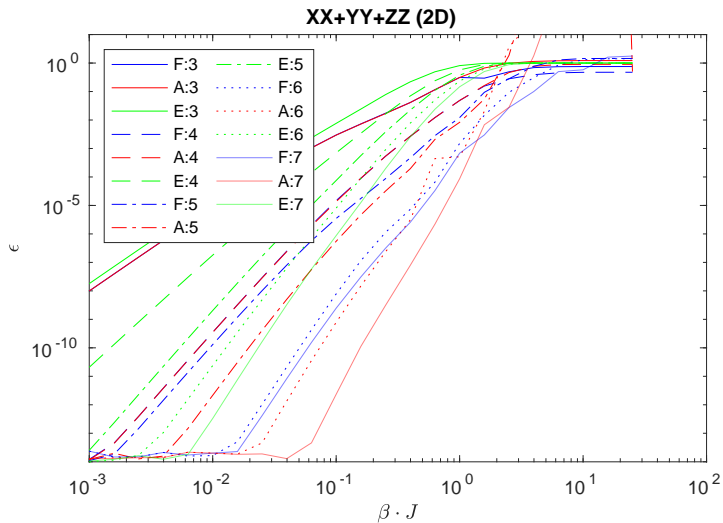
Construction

TFI Collapses

Direct Results

2D Exact

Solvers



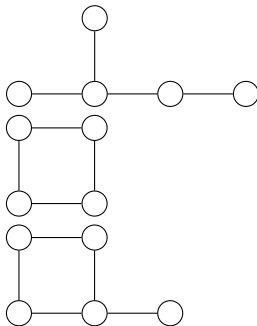
## 2D: Encodings + Error Measure

- Relative error  $\epsilon$  more challenging
- Encodings based on A (order 5)

- No loops

- +Plaquette

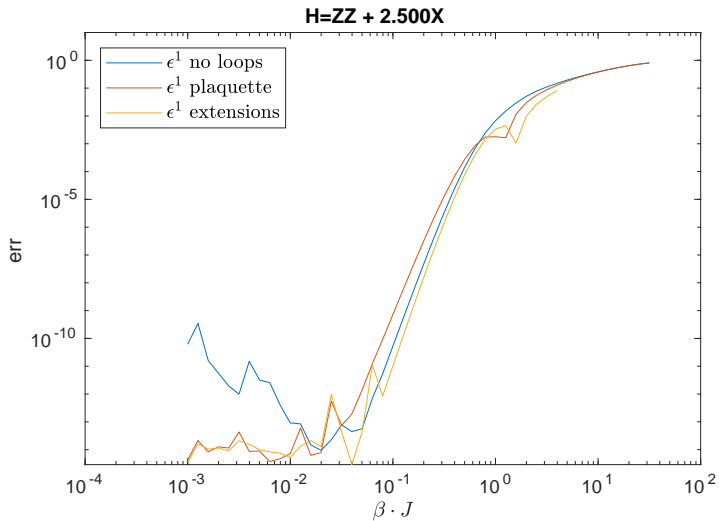
- +Extensions



	$\chi$
no loops	21
plaquette	27
extensions	43

## 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 two circles, each labeled '1'. The bottom leg has one circle labeled '1'. The left leg has one circle labeled '1'. The right leg has one circle labeled '1'. 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 has two diagonal lines. To the right of the cross is the label '(26)'.

$$\text{Diagram of } X \text{ with legs } 1, 1, 1, 1 = \text{Diagram of } B \text{ (cross shape)} \quad (26)$$

# Linear Solver: Applicability

Tensor Networks

Linear Solver

Construction

TFI Collapses

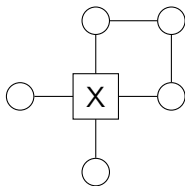
Direct Results

Solvers

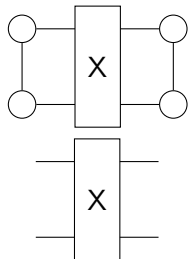
Linear Solver

Nonlinear Solver

Sequential Linear Solver

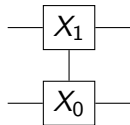


(27)



(28a)

=



(28b)

# Nonlinear Solver

Tensor Networks

Linear Solver

Construction

TFI Collapses

Direct Results

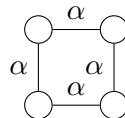
Solvers

Linear Solver

**Nonlinear Solver**

Sequential Linear Solver

- Nonlinear least squares
- Jacobian
- Permutations



(29)

# 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