

Introduction

Cluster  
Expansions

Results

Conclusion and  
Outlook

# Cluster Expansions of Thermal States using Tensor Networks

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## Introduction

Overview

Simulation

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# Introduction

# Introduction

Introduction

Overview

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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 [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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- Equations are known
- Curse of dimensionality
- Numerical methods
  - Exact diagonalisation
  - (post-) Hartree Fock methods, DFT methods
  - Monte Carlo methods
  - Tensor Networks

# Tensor Networks

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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

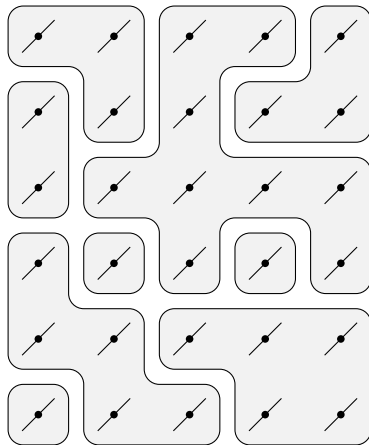
# Cluster Expansions

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

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

$$e^{H(2)} = \boxed{\text{two diagonal lines through dots}} + \boxed{\text{diagonal line through a dot}} \boxed{\text{diagonal line through a dot}} \quad (7)$$

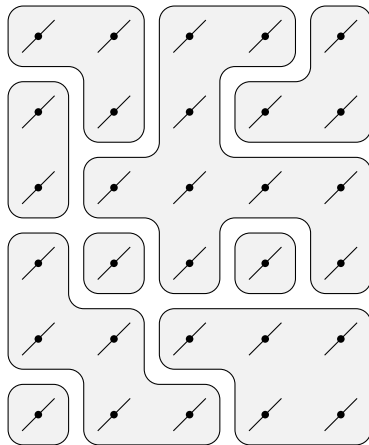
# Cluster Expansions

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

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

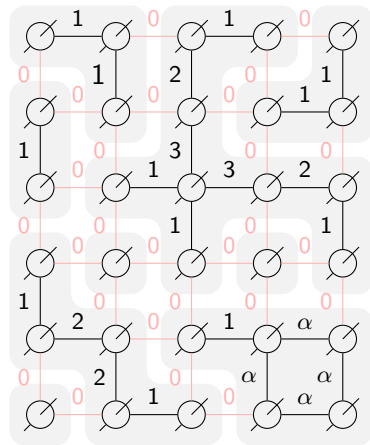
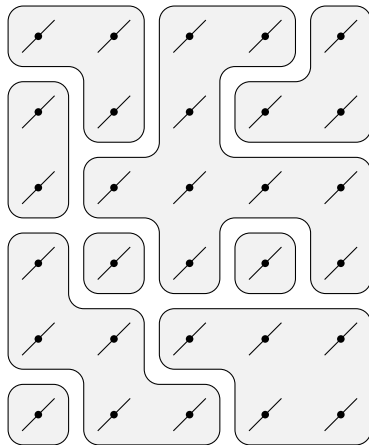
# Cluster Expansions

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# Cluster Expansions

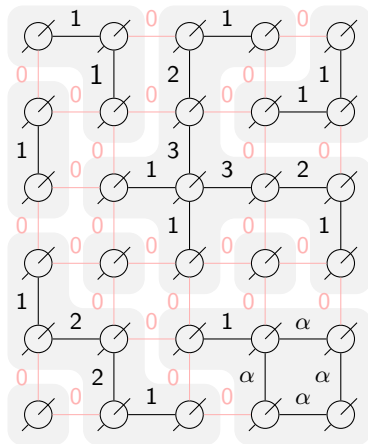
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- Multiple choices for encoding
- Solvers
  - Linear
  - Nonlinear



# Advantages

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- Doesn't break symmetry
- Thermodynamic limit
- Tensor Network toolbox

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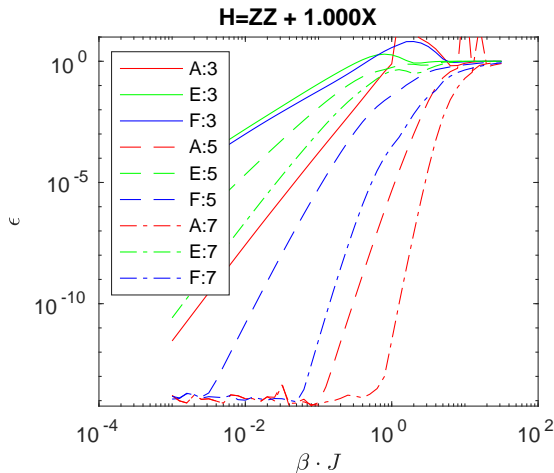
**Results**

1D Exact  
TFI Phase Diagram

Conclusion and  
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# 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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Results

1D Exact

TFI Phase Diagram

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- Large  $\beta$ -steps
- Real time evolution
- Encoding
- Truncation  $\chi$

# 2D TFI: Introduction

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1D Exact

TFI Phase Diagram

Conclusion and  
Outlook

- Phase Transition
- Criticality
- Finite size scaling
  - Observables:  
 $m$ ,  $S$  and  $\xi$
  - Parameters:  
 $T_c$ , exponents
- $\Gamma = 2.5$
- VUMPS ( $\chi, \delta^{-1}$ )

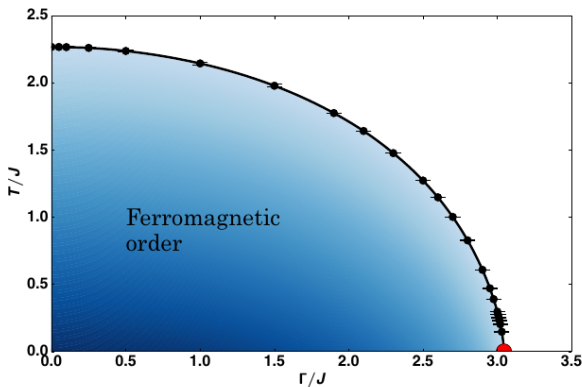


Figure taken from [2]

# TFI Phase Diagram: $\Gamma = 2.5$

Introduction

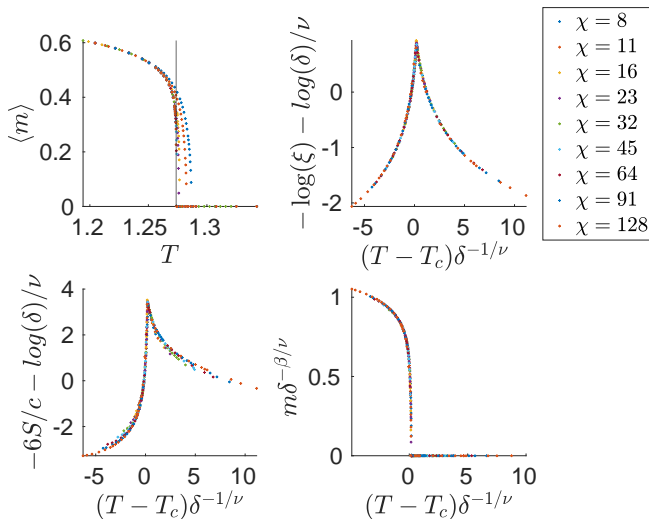
Cluster  
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1D Exact

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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 and Outlook

# Conclusion

Introduction

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- Construction fast and stable
- Cluster expansions work well in 1D and 2D
- Real time evolution

# Outlook

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- 3D
- Incorporating internal symmetries
- Lattices

# 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

Construction

TFI Collapses

Direct Results

Solvers

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

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

# Tensor Networks: Graphical Notation

## Tensor Networks



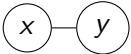
Linear Solver

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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

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Direct Results

Solvers

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

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 rectangular 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 curved line connects the bottom of the first circle to the bottom of the last circle, representing a trace. The label  $\chi$  is placed between the first two circles.

(9)

# Tensor Networks: Operators

Tensor Networks

Linear Solver

Construction

TFI Collapses

Direct Results

Solvers

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

$$\hat{O} |\psi\rangle = \dots \text{---} \begin{array}{c} \bigcirc \chi \\ | \\ \bigcirc \chi \end{array} \text{---} \begin{array}{c} \bigcirc \\ | \\ \bigcirc \end{array} \text{---} \begin{array}{c} \bigcirc \\ | \\ \bigcirc \end{array} \text{---} \dots = \dots \text{---} \bigcirc \chi^2 \text{---} \bigcirc \text{---} \bigcirc \text{---} \dots \quad (11)$$

Tensor Networks

Linear Solver

Construction

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# Linear Solver

# Linear Solver: Inversion Scheme

Tensor Networks

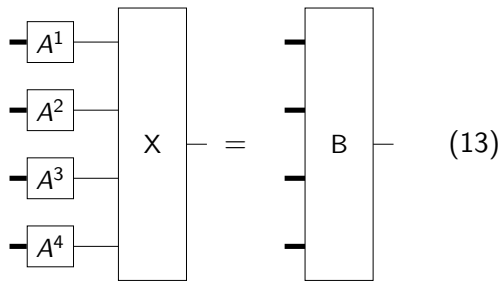
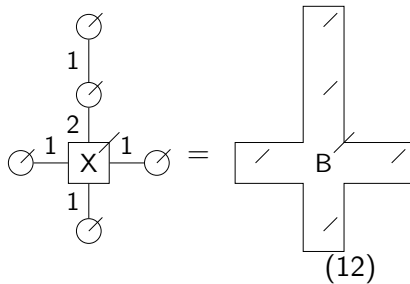
Linear Solver

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# Linear Solver: Inversion Scheme

Tensor Networks

Linear Solver

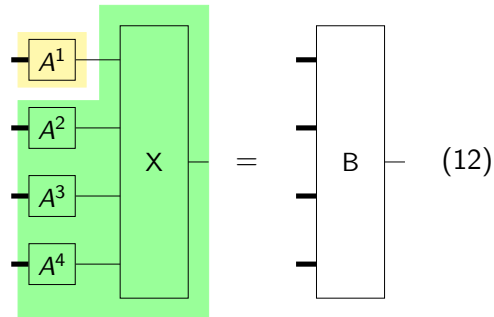
Construction

TFI Collapses

Direct Results

Solvers

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





# Linear Solver: Inversion Scheme

Tensor Networks

Linear Solver

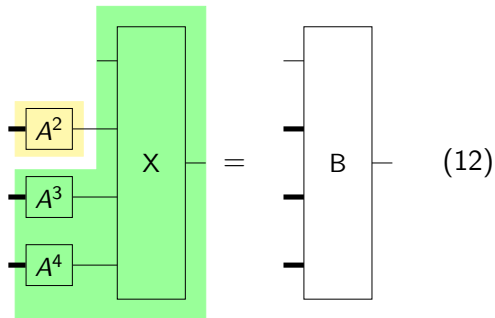
Construction

TFI Collapses

Direct Results

Solvers

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



# Linear Solver: Inversion Scheme

Tensor Networks

Linear Solver

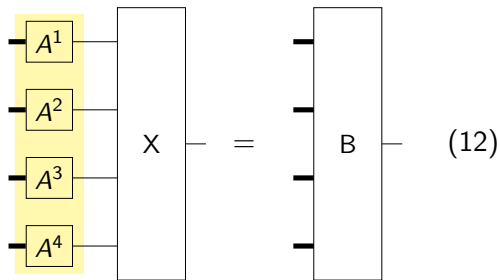
Construction

TFI Collapses

Direct Results

Solvers

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



# Linear Solver: Inversion Scheme

Tensor Networks

Linear Solver

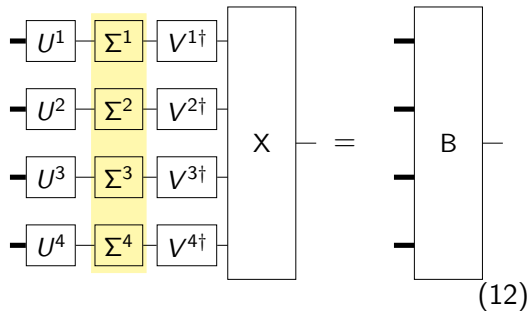
Construction

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

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1D

2D

TFI Collapses

Direct Results

Solvers

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

(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**

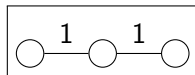
1D

2D

TFI Collapses

Direct Results

Solvers



(17)

# 1D: Variant A

Tensor Networks

Linear Solver

Construction

1D

2D

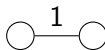
TFI Collapses

Direct Results

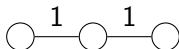
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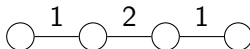
(18a)



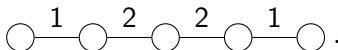
(18b)



(18c)



(18d)



(18e)

# 1D: Variant E

Tensor Networks

Linear Solver

Construction

1D

2D

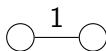
TFI Collapses

Direct Results

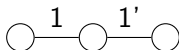
Solvers



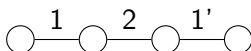
(19a)



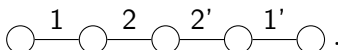
(19b)



(19c)



(19d)



(19e)

# 1D: Variant F

Tensor Networks

Linear Solver

Construction

1D

2D

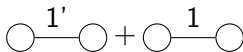
TFI Collapses

Direct Results

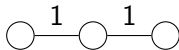
Solvers



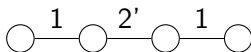
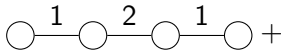
(20a)



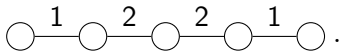
(20b)



(20c)



(20d)



(20e)

Tensor Networks

Linear Solver

Construction

1D

2D

TFI Collapses

Direct Results

Solvers

$$O^{0000} = \begin{array}{c} \begin{array}{c} 0 \\ \diagup \\ \text{---} \end{array} \begin{array}{c} 0 \\ \diagdown \\ \text{---} \end{array} \begin{array}{c} i_0 \\ \diagup \\ \text{---} \end{array} \begin{array}{c} j_0 \\ \diagdown \\ \text{---} \end{array} \end{array} = \bigcirc \quad (21)$$

## 2D: Linear Blocks

Tensor Networks

Linear Solver

Construction

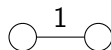
1D

2D

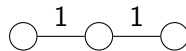
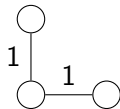
TFI Collapses

Direct Results

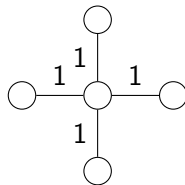
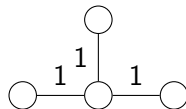
Solvers



(22a)



(22b)



(22c)

## 2D: Nonlinear Blocks

Tensor Networks

Linear Solver

Construction

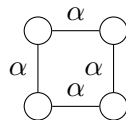
1D

2D

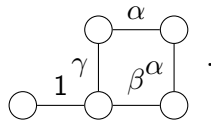
TFI Collapses

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

Linear Solver

Construction

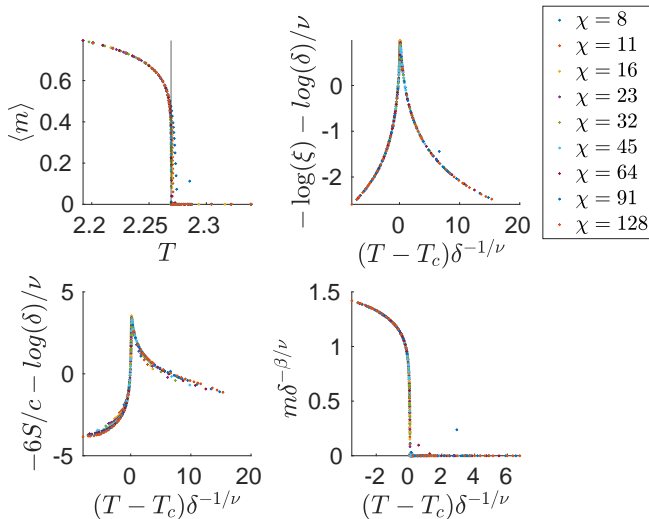
TFI Collapses

$g = 0.0$

$g = 2.9$

Direct Results

Solvers



	$T_c$
Fit	2.691(9)
Exact	2.691853

Tensor Networks

Linear Solver

Construction

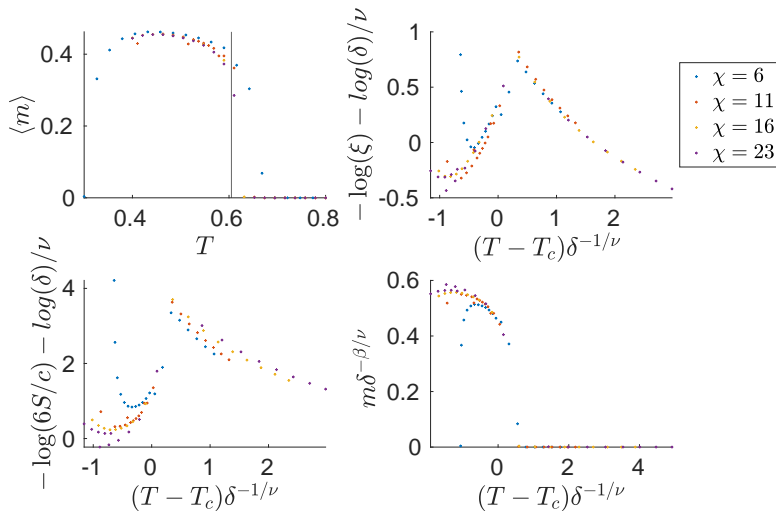
TFI Collapses

$g = 0.0$

$g = 2.9$

Direct Results

Solvers



Tensor Networks

Linear Solver

Construction

TFI Collapses

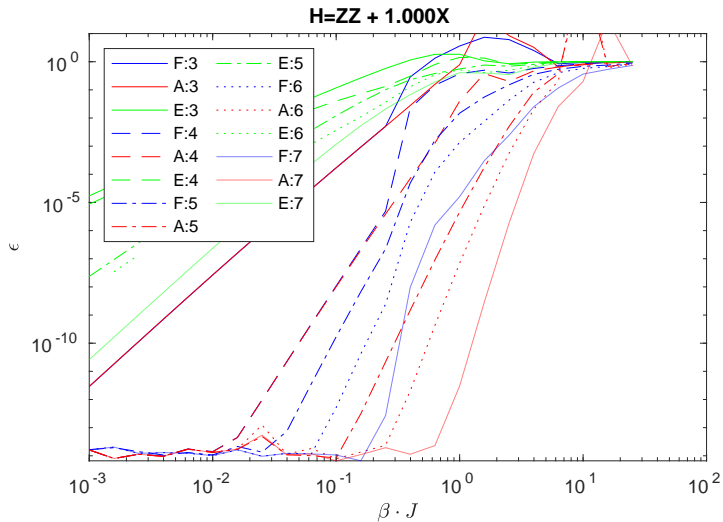
**Direct Results**

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

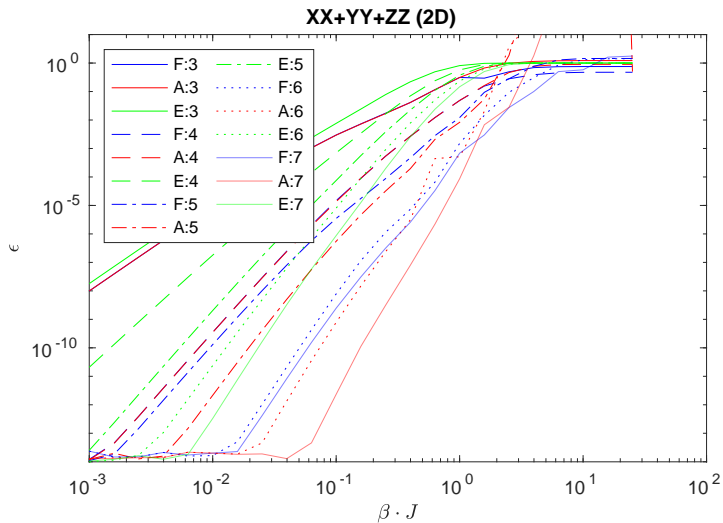
Construction

TFI Collapses

Direct Results

2D Exact

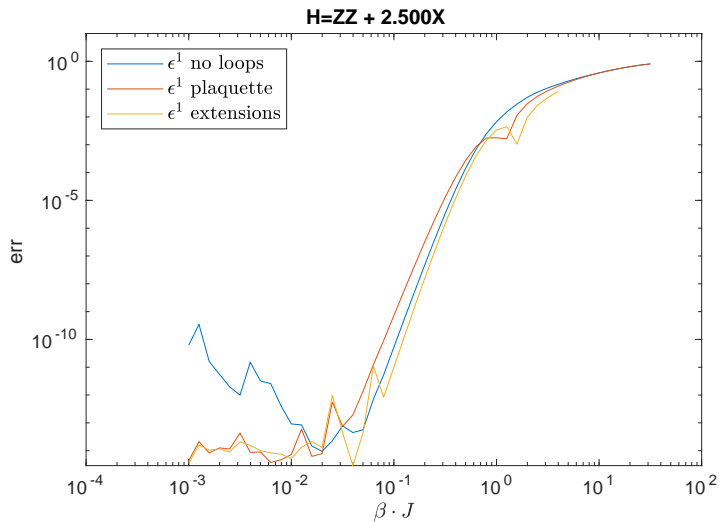
Solvers





## 2D: 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

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

# Linear Solver: Applicability

Tensor Networks

Linear Solver

Construction

TFI Collapses

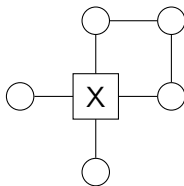
Direct Results

Solvers

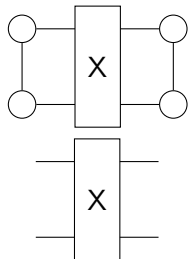
Linear Solver

Nonlinear Solver

Sequential Linear Solver

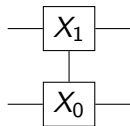


(26)



(27a)

=



(27b)

# Nonlinear Solver

Tensor Networks

Linear Solver

Construction

TFI Collapses

Direct Results

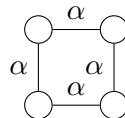
Solvers

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