

# Cluster Expansion of Thermal States using Tensor Networks

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## Introduction

Problem Statement

Tensor Networks

Overview Thesis

Cluster Expansion

Solvers

Results

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# Introduction

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- Overview condensed matter physics

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

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

# Simulating Quantum Many-body Systems

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- Equations are known
- Curse of dimensionality
- Tensor networks

# Tensor Networks: Introduction

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

$$C^{i_1 i_2 \dots i_n} = \text{Tr}(C^{i_1} C^{i_2} \dots C^{i_n} M). \quad (2)$$

# Tensor Networks: Graphical Notation

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

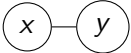
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conventional	Einstein	tensor notation
$\vec{x}$	$x_\alpha$	
$M$	$M_{\alpha\beta}$	
$\vec{x} \cdot \vec{y}$	$x_\alpha y_\alpha$	



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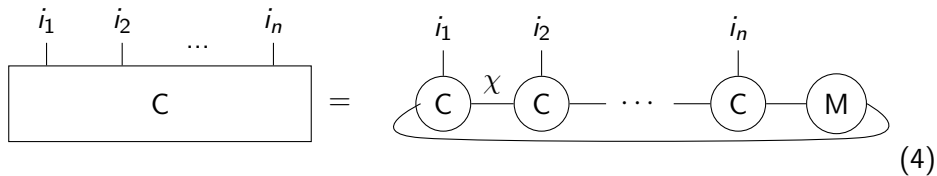
## Cluster Expansion

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$$C^{i_1 i_2 \dots i_n} = \text{Tr}(C^{i_1} C^{i_2} \dots C^{i_n} M) \quad (3)$$


$$\text{Diagram illustrating the trace operation in tensor network notation. A rectangular block labeled } C \text{ with indices } i_1, i_2, \dots, i_n \text{ is equal to a chain of circular blocks labeled } C \text{ and } M \text{ connected by lines, with a trace loop around the first } C \text{ and } M \text{ blocks.} \quad (4)$$

# Tensor Networks: Operators

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$$\hat{O} = \dots \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \dots \quad (5)$$

$$\hat{O} |\psi\rangle = \dots \text{---} \begin{array}{c} \bigcirc \chi \\ | \\ \bigcirc \chi \end{array} \text{---} \begin{array}{c} \bigcirc \\ | \\ \bigcirc \end{array} \text{---} \begin{array}{c} \bigcirc \\ | \\ \bigcirc \end{array} \text{---} \dots = \dots \text{---} \bigcirc \chi^2 \text{---} \bigcirc \text{---} \bigcirc \text{---} \dots \quad (6)$$

# Operator exponential

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- (Real) Time evolution:  $\hat{O} = e^{-i\hat{H}t}$
- Statistical ensembles:  $\hat{O} = e^{-\beta\hat{H}}$

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# Cluster Expansion

# General idea

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$$\bigcirc = \exp(-\beta H(\bigcirc)) \quad (7)$$

$$\overset{1}{\bigcirc - \bigcirc} = \exp -\beta H(\overset{0}{\bigcirc - \bigcirc}) \quad (8)$$

# General idea

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$$\begin{array}{c} \text{1} \quad \text{1} \\ \bigcirc - \bigcirc - \bigcirc \end{array} = \exp -\beta H(\begin{array}{c} \bigcirc - \bigcirc - \bigcirc \\ - \begin{array}{c} \text{0} \quad \text{0} \\ \bigcirc - \bigcirc - \bigcirc \\ \text{1} \quad \text{0} \\ \bigcirc - \bigcirc - \bigcirc \\ \text{0} \quad \text{1} \\ \bigcirc - \bigcirc - \bigcirc \end{array} \end{array}) \quad (9)$$

# General idea

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Cluster Expansion

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$$\begin{array}{c} 1 \quad 1 \\ \bigcirc - \bigcirc - \bigcirc \end{array} = \exp -\beta H(\begin{array}{c} \bigcirc - \bigcirc - \bigcirc \\ - \bigcirc - \bigcirc - \bigcirc \end{array}) \quad (9)$$

# General idea

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Cluster Expansion

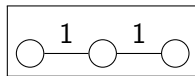
1D

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# 1D: Variant A

Introduction

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1D

2D

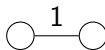
Solvers

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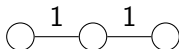
Conclusion



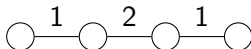
(10a)



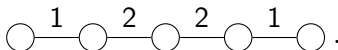
(10b)



(10c)



(10d)



(10e)

# 1D: Variant E

Introduction

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1D

2D

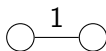
Solvers

Results

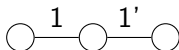
Conclusion



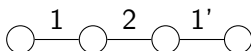
(11a)



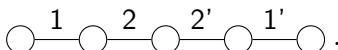
(11b)



(11c)



(11d)



(11e)

# 1D: Variant F

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1D

2D

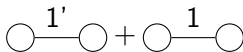
Solvers

Results

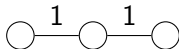
Conclusion



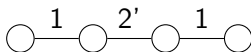
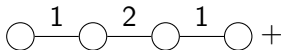
(12a)



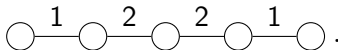
(12b)



(12c)



(12d)



(12e)

## 2D: Linear Blocks

Introduction

Cluster Expansion

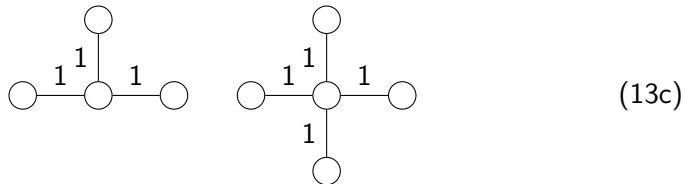
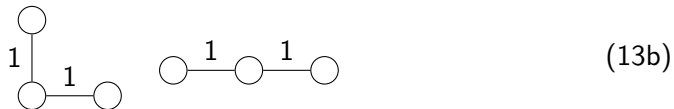
1D

2D

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## 2D: Nonlinear Blocks

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Cluster Expansion

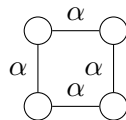
1D

2D

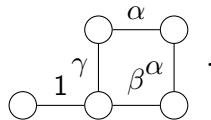
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Nonlinear Solver

Sequential Linear Solver

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# Solvers

# Linear Solver: Standard Form

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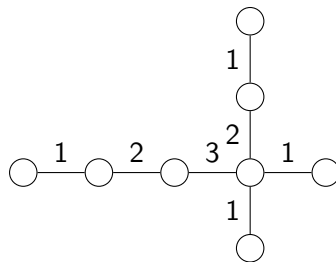
Linear Solver

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# Linear Solver: Standard Form

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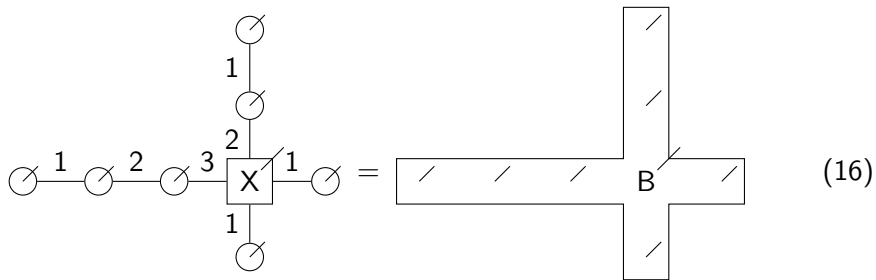
Linear Solver

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# Linear Solver: Standard Form

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$$\begin{array}{c} \boxed{\diagup} \\ | \\ \boxed{\diagup} - \boxed{X} - \boxed{\diagup} \\ | \\ \boxed{\diagup} \end{array} = \begin{array}{c} \boxed{\diagup} \\ | \\ \boxed{\diagup} - \boxed{B} - \boxed{\diagup} \\ | \\ \boxed{\diagup} \end{array} \quad (16)$$

# Linear Solver: Standard Form

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$$\begin{array}{c} l^1 \\ l^2 \\ l^3 \\ l^4 \end{array} \begin{array}{c} \boxed{A^1} \\ \boxed{A^2} \\ \boxed{A^3} \\ \boxed{A^4} \end{array} \begin{array}{c} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{array} \begin{array}{c} \boxed{X} \\ \boxed{X} \\ \boxed{X} \\ \boxed{X} \end{array} \begin{array}{c} j \\ j \\ j \\ j \end{array} = \begin{array}{c} l^1 \\ l^2 \\ l^3 \\ l^4 \end{array} \begin{array}{c} \boxed{B} \\ \boxed{B} \\ \boxed{B} \\ \boxed{B} \end{array} \begin{array}{c} j \\ j \\ j \\ j \end{array} \quad (16)$$

# Linear Solver: Inversion Scheme

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

# Linear Solver: Inversion Scheme

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- Invert  $A^i$  separately
- Full inversion  $A = A^1 \otimes A^2 \dots \otimes A^m$ 
  - Slow
  - Stable for pseudoinverse

# Linear Solver: Inversion Scheme

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- Invert  $A^i$  separately
- Full inversion  $A = A^1 \otimes A^2 \dots \otimes A^m$
- Sparse full inversion
  - $A^i = U \Sigma V^\dagger$
  - $S = S^1 \otimes S^2 \dots \otimes S^m$

# Linear Solver: Applicability

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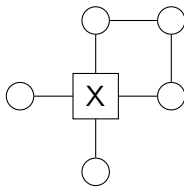
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# Linear Solver: Applicability

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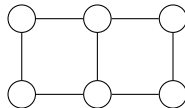
Linear Solver

Nonlinear Solver

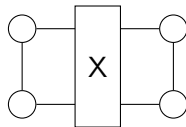
Sequential Linear Solver

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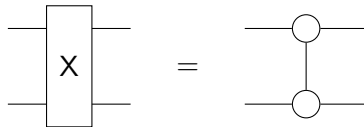
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(19a)



(19b)

# Nonlinear Solver

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**Nonlinear Solver**

Sequential Linear Solver

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- Nonlinear least squares
- Jacobian
- Permutations



# Sequential Linear Solver

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

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**Results**

1D exact

2D exact

2D Transverse Ising  
model

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# Results

# 1D: Transverse Field Ising

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1D exact

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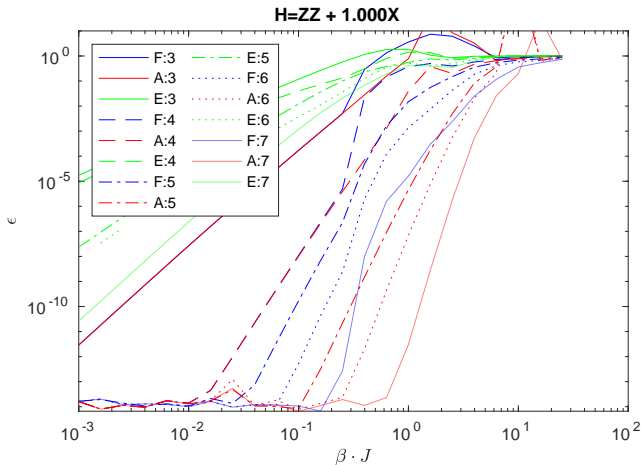


Table:  $\chi$

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

# 1D: Heisenberg XXX

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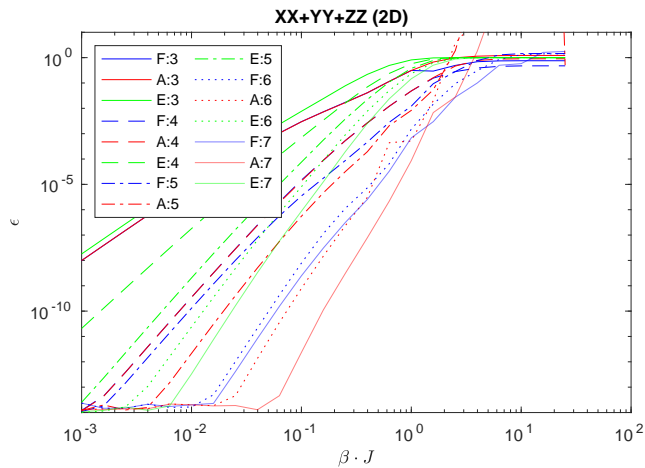
Results

1D exact

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## 2D: TFI

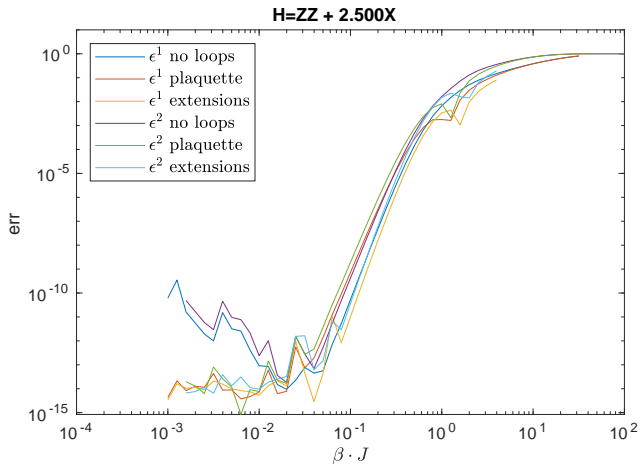


Table:  $\chi$

no loops	21
loops	27
extensions	43

## 2D: TFI

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1D exact

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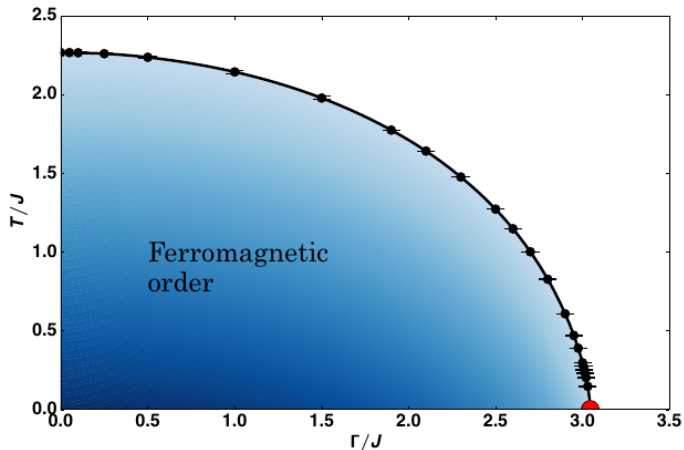


Figure: Figure taken from [2]

# 2D: Classical Ising

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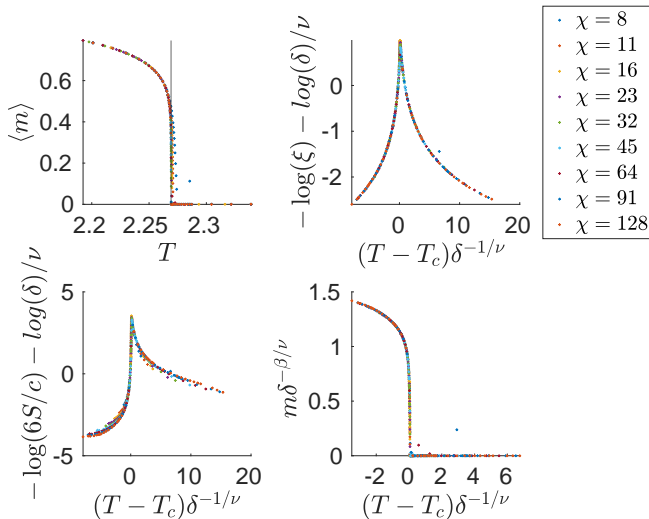
Results

1D exact

2D exact

2D Transverse Ising  
model

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	$T_c$
Fit	2.691(9)
Exact	2.691853

# 2D: TFI $g = 2.5$

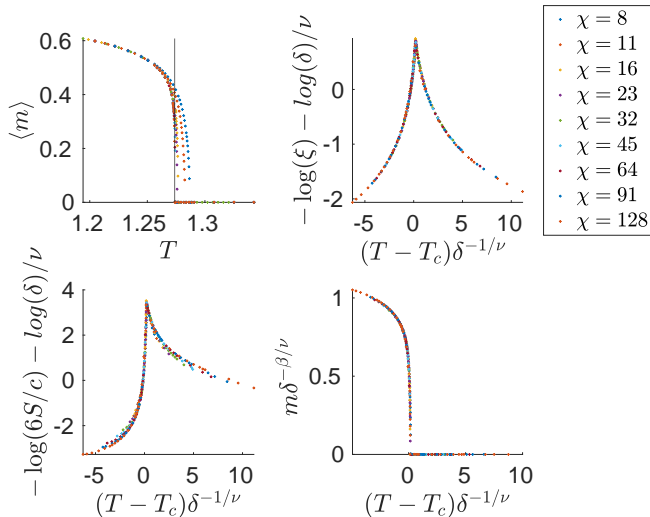


Table: Data from [3]

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



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# References I



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# References II

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