

# Cluster Expansion of Thermal States using Tensor Networks

David Devoogdt

Faculty of Engineering and Architecture  
Ghent University

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## Introduction

Problem Statement

Tensor Networks

Overview Thesis

Cluster Expansion

Solvers

Results

Conclusion

# Introduction

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Introduction

Problem Statement

Tensor Networks

Overview Thesis

Cluster Expansion

Solvers

Results

Conclusion

- Overview condensed matter physics

# Introduction

Introduction

Problem Statement

Tensor Networks

Overview Thesis

Cluster Expansion

Solvers

Results

Conclusion

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

# Introduction

Introduction

Problem Statement

Tensor Networks

Overview Thesis

Cluster Expansion

Solvers

Results

Conclusion

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

# Simulating Quantum Many-body Systems

Introduction

Problem Statement

Tensor Networks

Overview Thesis

Cluster Expansion

Solvers

Results

Conclusion

- Equations are known
- Curse of dimensionality
- Tensor networks

# Tensor Networks: Introduction

Introduction

Problem Statement

Tensor Networks

Overview Thesis

Cluster Expansion

Solvers

Results

Conclusion

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

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

# Tensor Networks: Graphical Notation

## Introduction

Problem Statement

Tensor Networks



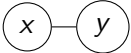
Overview Thesis

## Cluster Expansion

Solvers

Results

Conclusion

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



## Introduction

Problem Statement

Tensor Networks

Overview Thesis

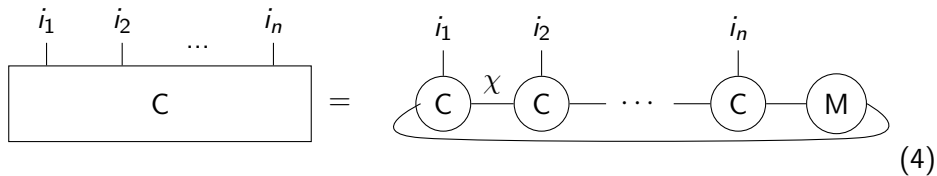
## Cluster Expansion

Solvers

Results

Conclusion

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


$$\text{Diagram illustrating the trace operation in tensor networks. On the left, a rectangular tensor } C \text{ with indices } i_1, i_2, \dots, i_n \text{ is shown. This is equal to a trace of a product of tensors. On the right, a chain of tensors } C^{i_1}, C^{i_2}, \dots, C^{i_n} \text{ is connected by horizontal lines. The first tensor } C^{i_1} \text{ is also connected to a tensor } M \text{ by a curved line, representing the trace operation. The entire expression is labeled (4).}$$

# Tensor Networks: Operators

Introduction

Problem Statement

Tensor Networks

Overview Thesis

Cluster Expansion

Solvers

Results

Conclusion

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

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

# Operator exponential

Introduction

Problem Statement

Tensor Networks

Overview Thesis

Cluster Expansion

Solvers

Results

Conclusion

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

Introduction

Cluster Expansion

Solvers

Results

Conclusion

# Cluster Expansion

# Cluster Expansion

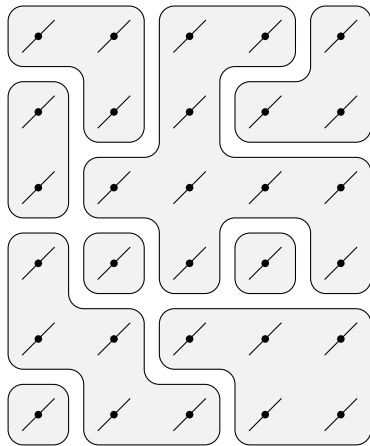
Introduction

Cluster Expansion

Solvers

Results

Conclusion



- $\sum_{\{B_i\}} \bigotimes_i B_i = e^{-\beta \hat{H}}$
- Increase size patches
- Thermodynamic limit
- Patches encoded by 1 tensor:

$$(7)$$

# Cluster Expansion

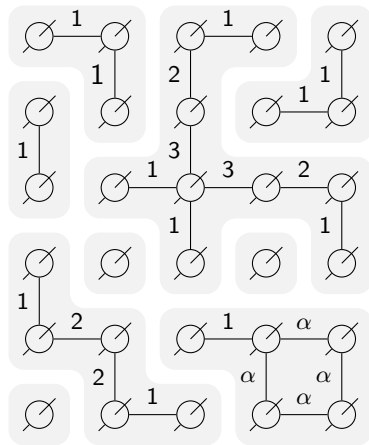
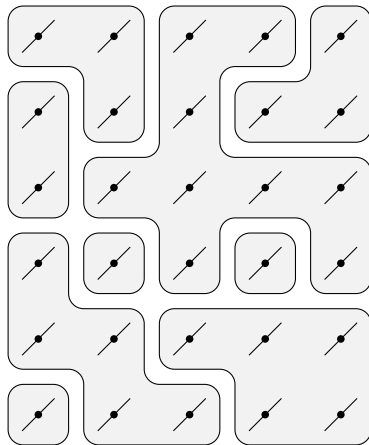
Introduction

Cluster Expansion

Solvers

Results

Conclusion



Introduction

Cluster Expansion

**Solvers**

Linear Solver

Nonlinear Solver

Sequential Linear Solver

Results

Conclusion

# Solvers

# Linear Solver: Standard Form

Introduction

Cluster Expansion

Solvers

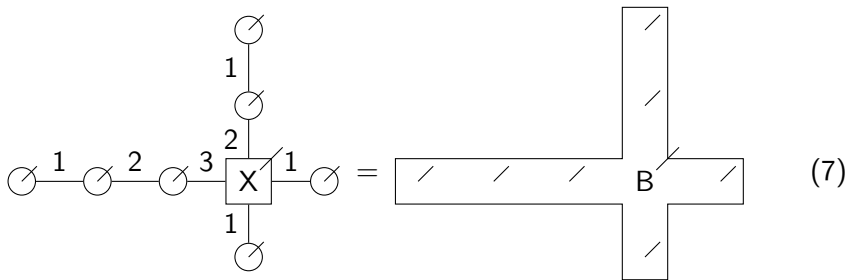
Linear Solver

Nonlinear Solver

Sequential Linear Solver

Results

Conclusion





# Linear Solver: Standard Form

Introduction

Cluster Expansion

Solvers

Linear Solver

Nonlinear Solver

Sequential Linear Solver

Results

Conclusion

The diagram illustrates the transformation of a node  $X$  into a node  $B$  in a linear solver's standard form. On the left, node  $X$  is a central square with a diagonal slash and the letter 'X'. It is connected to four smaller squares, each containing a diagonal slash, representing its initial cluster. An equals sign follows. On the right, node  $B$  is a larger central square with a diagonal slash and the letter 'B'. It is connected to four larger rectangular shapes, each containing a diagonal slash, representing its expanded cluster. The equation is labeled (7) on the far right.

$$\text{Node } X \text{ with 4 children} = \text{Node } B \text{ with 4 children} \quad (7)$$

# Linear Solver: Standard Form

Introduction

Cluster Expansion

Solvers

Linear Solver

Nonlinear Solver

Sequential Linear Solver

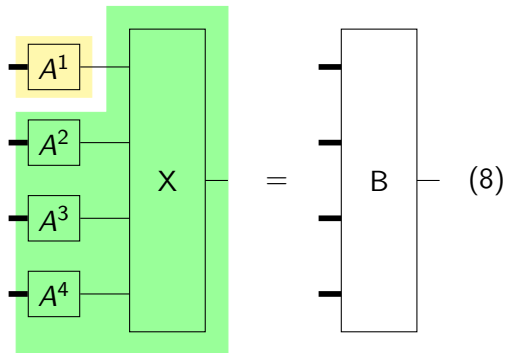
Results

Conclusion

$$\begin{matrix} A^1 \\ A^2 \\ A^3 \\ A^4 \end{matrix} \rightarrow X = B \quad (7)$$

# Linear Solver: Inversion Scheme

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



# Linear Solver: Inversion Scheme

Introduction

Cluster Expansion

Solvers

Linear Solver

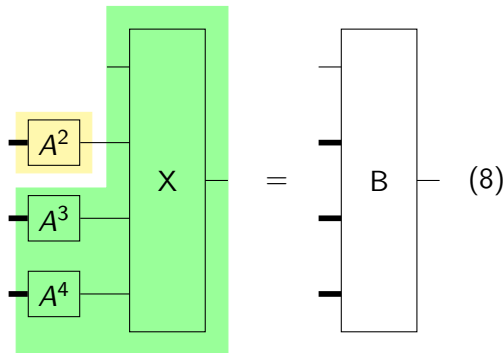
Nonlinear Solver

Sequential Linear Solver

Results

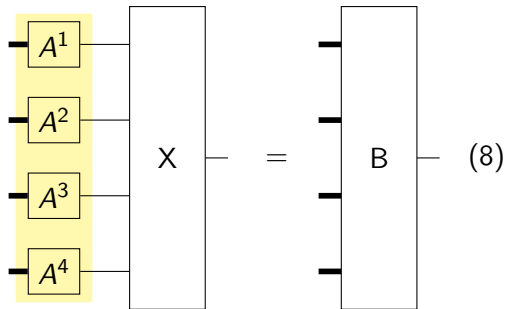
Conclusion

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



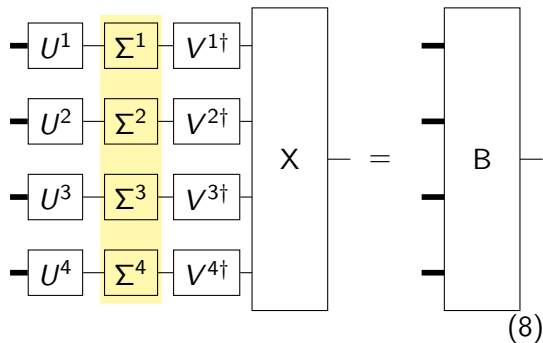
# Linear Solver: Inversion Scheme

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



# Linear Solver: Inversion Scheme

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



# Linear Solver: Applicability

Introduction

Cluster Expansion

Solvers

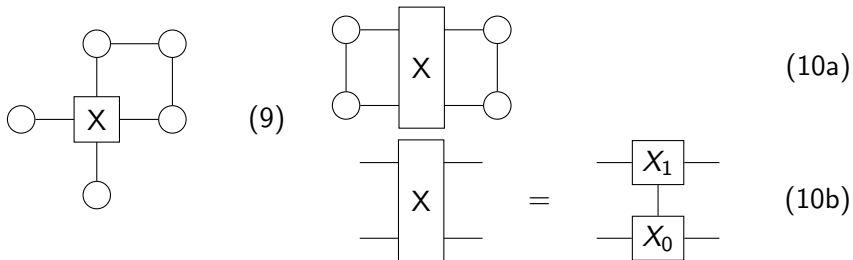
Linear Solver

Nonlinear Solver

Sequential Linear Solver

Results

Conclusion



# Nonlinear Solver

Introduction

Cluster Expansion

Solvers

Linear Solver

**Nonlinear Solver**

Sequential Linear Solver

Results

Conclusion

- Nonlinear least squares
- Jacobian
- Permutations



# Sequential Linear Solver

Introduction

Cluster Expansion

Solvers

Linear Solver

Nonlinear Solver

Sequential Linear Solver

Results

Conclusion

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

Introduction

Cluster Expansion

Solvers

**Results**

1D exact

2D exact

2D Transverse Ising  
model

Conclusion

# Results

# 1D: Transverse Field Ising

Introduction  
Cluster Expansion  
Solvers  
Results  
1D exact  
2D exact  
2D Transverse Ising  
model  
Conclusion

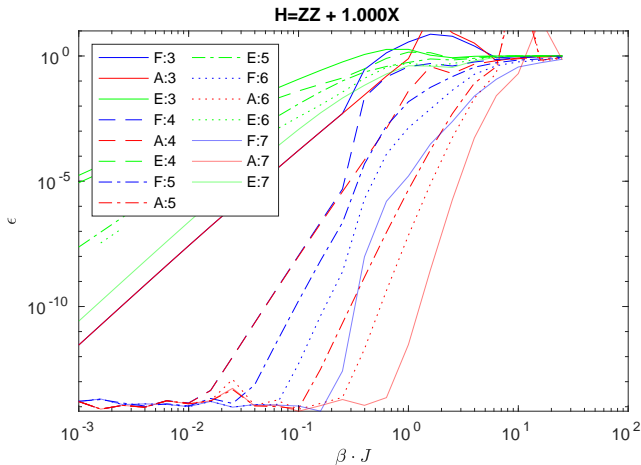


Table:  $\chi$

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

# 1D: Heisenberg XXX

Introduction

Cluster Expansion

Solvers

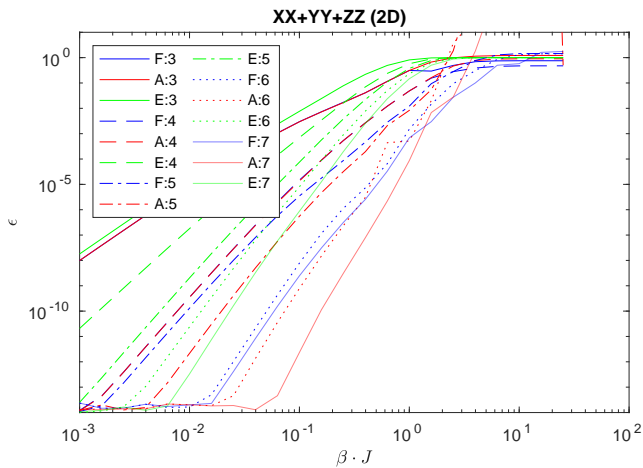
Results

1D exact

2D exact

2D Transverse Ising  
model

Conclusion



# 2D: TFI

- Introduction
- Cluster Expansion
- Solvers
- Results
  - 1D exact
  - 2D exact
  - 2D Transverse Ising model
- Conclusion

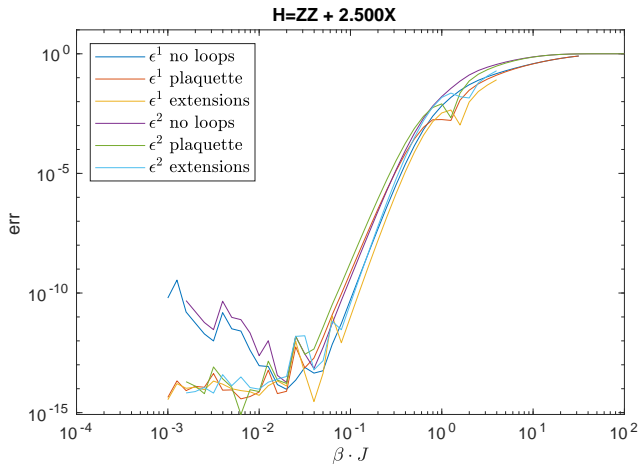


Table:  $\chi$

no loops	21
loops	27
extensions	43

# 2D: TFI

Introduction

Cluster Expansion

Solvers

Results

1D exact

2D exact

2D Transverse Ising  
model

Conclusion

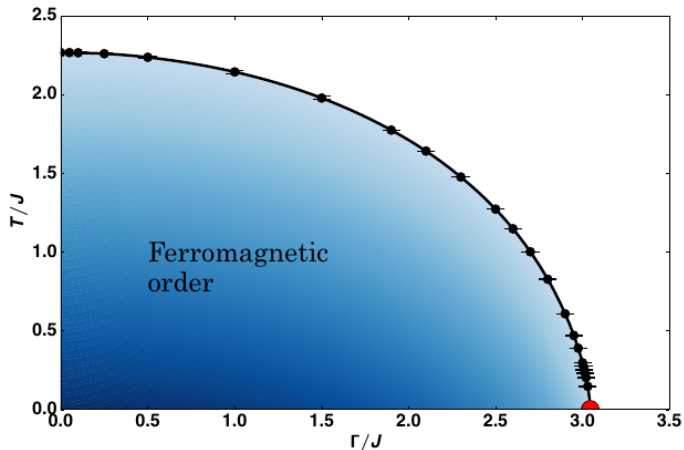
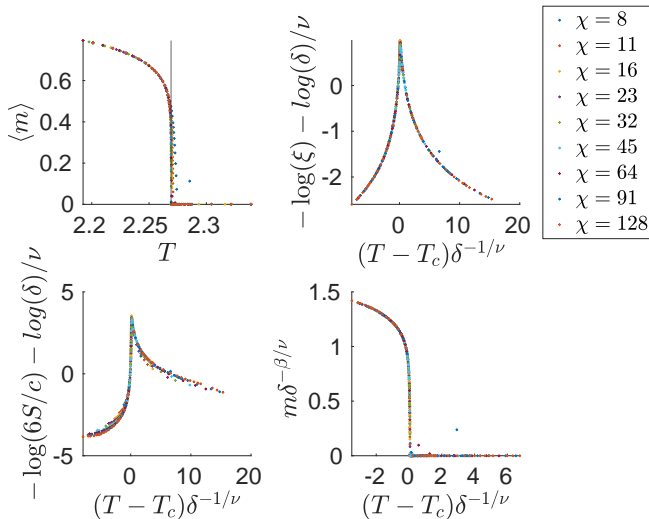


Figure: Figure taken from [2]

# 2D: Classical Ising

Introduction
Cluster Expansion
Solvers
Results
1D exact
2D exact
2D Transverse Ising model
Conclusion



	$T_c$
Fit	2.691(9)
Exact	2.691853

# 2D: TFI $g = 2.5$

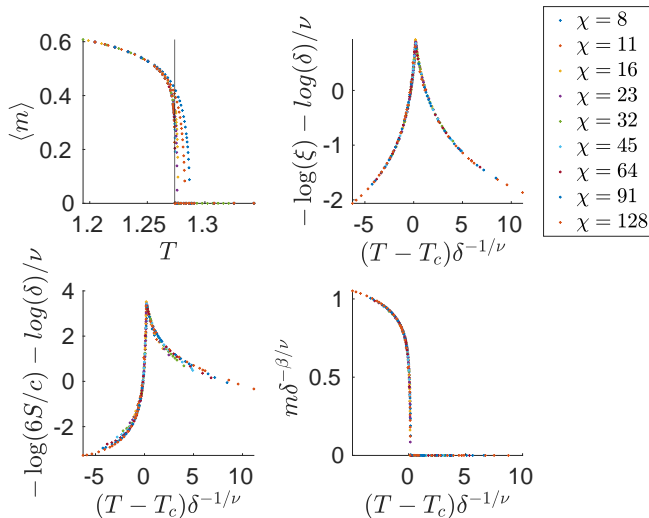


Table: Data from [3]

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



Introduction

Cluster Expansion

Solvers

Results

Conclusion

# Conclusion

# References I



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Introduction

Cluster Expansion

Solvers

Results

Conclusion

# References II

Introduction

Cluster Expansion

Solvers

Results

Conclusion



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