

Cluster Expansion of Thermal States using Tensor Networks

David Devoogdt

Faculty of Engineering and Architecture
Ghent University

June 16, 2021

Introduction

Problem Statement

Tensor Networks

Cluster Expansion

Solvers

Results

Conclusion

Introduction

Introduction

Problem Statement

Tensor Networks

Cluster Expansion

Solvers

Results

Conclusion



Introduction

Problem Statement

Tensor Networks

Cluster Expansion

Solvers

Results

Conclusion

Variant A

Introduction

Problem Statement

Tensor Networks

Cluster Expansion

Solvers

Results

Conclusion

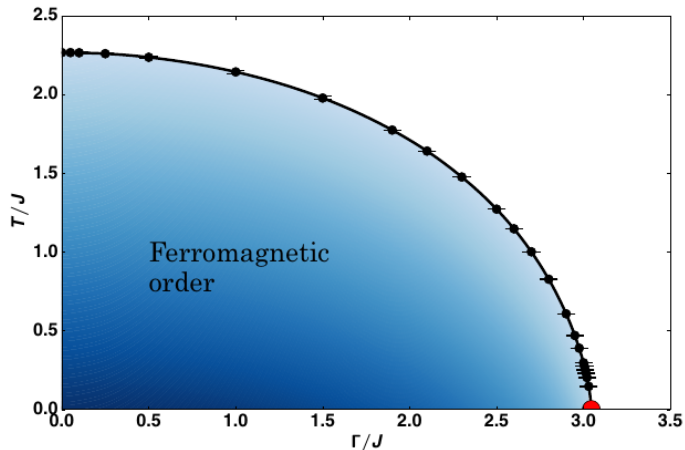


Figure: Figure taken from [1]

Introduction

Cluster Expansion

1D

2D

Solvers

Results

Conclusion

Cluster Expansion

General idea

Introduction

Cluster Expansion

1D

2D

Solvers

Results

Conclusion

$$\bigcirc = \exp(-\beta H(\bigcirc)) \quad (1)$$

$$\overset{1}{\bigcirc - \bigcirc} = \exp -\beta H(\overset{0}{\bigcirc - \bigcirc}) \quad (2)$$

General idea

Introduction

Cluster Expansion

1D

2D

Solvers

Results

Conclusion

$$\begin{array}{c} \text{1} \quad \text{1} \\ \bigcirc - \bigcirc - \bigcirc \end{array} = \exp -\beta H(\begin{array}{c} \bigcirc - \bigcirc - \bigcirc \\ - \begin{array}{c} \text{0} \quad \text{0} \\ \bigcirc - \bigcirc - \bigcirc \\ \text{1} \quad \text{0} \\ \bigcirc - \bigcirc - \bigcirc \\ \text{0} \quad \text{1} \\ \bigcirc - \bigcirc - \bigcirc \end{array} \end{array}) \quad (3)$$

General idea

Introduction

Cluster Expansion

1D

2D

Solvers

Results

Conclusion

$$\begin{array}{c} 1 \quad 1 \\ \bigcirc - \bigcirc - \bigcirc = \exp -\beta H(\bigcirc - \bigcirc - \bigcirc) \\ - \bigcirc - \bigcirc - \bigcirc \end{array} \quad (3)$$

General idea

Introduction

Cluster Expansion

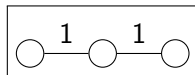
1D

2D

Solvers

Results

Conclusion



(3)

1D: Variant A

Introduction

Cluster Expansion

1D

2D

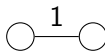
Solvers

Results

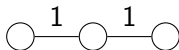
Conclusion



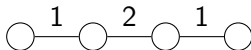
(4a)



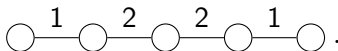
(4b)



(4c)



(4d)



(4e)

1D: Variant E

Introduction

Cluster Expansion

1D

2D

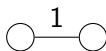
Solvers

Results

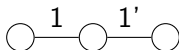
Conclusion



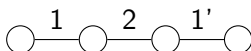
(5a)



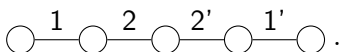
(5b)



(5c)



(5d)



(5e)

1D: Variant F

Introduction

Cluster Expansion

1D

2D

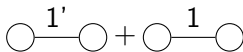
Solvers

Results

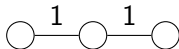
Conclusion



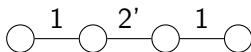
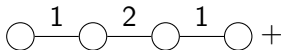
(6a)



(6b)



(6c)



(6d)



(6e)

2D: Linear Blocks

Introduction

Cluster Expansion

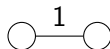
1D

2D

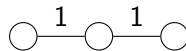
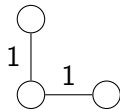
Solvers

Results

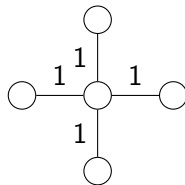
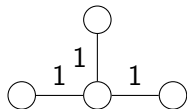
Conclusion



(7a)



(7b)



(7c)

2D: Nonlinear Blocks

Introduction

Cluster Expansion

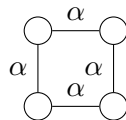
1D

2D

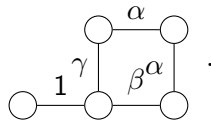
Solvers

Results

Conclusion



(8)



(9)

Introduction

Cluster Expansion

Solvers

Linear Solver

Nonlinear Solver

Sequential Linear Solver

Results

Conclusion

Solvers

Linear Solver: Standard Form

Introduction

Cluster Expansion

Solvers

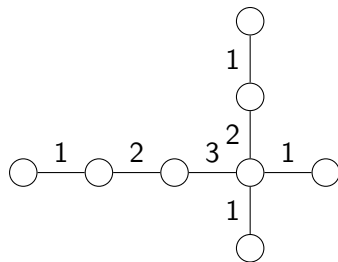
Linear Solver

Nonlinear Solver

Sequential Linear Solver

Results

Conclusion



(10)

Linear Solver: Standard Form

Introduction

Cluster Expansion

Solvers

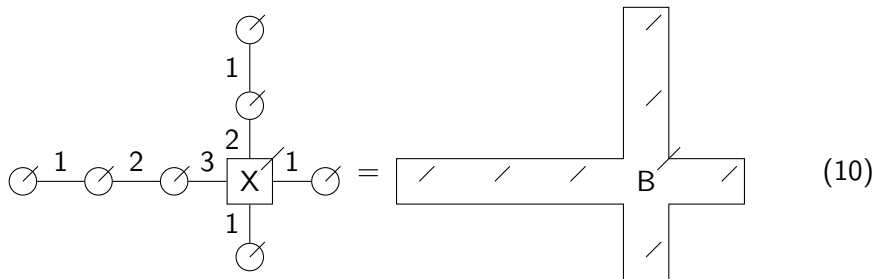
Linear Solver

Nonlinear Solver

Sequential Linear Solver

Results

Conclusion



Linear Solver: Standard Form

Introduction

Cluster Expansion

Solvers

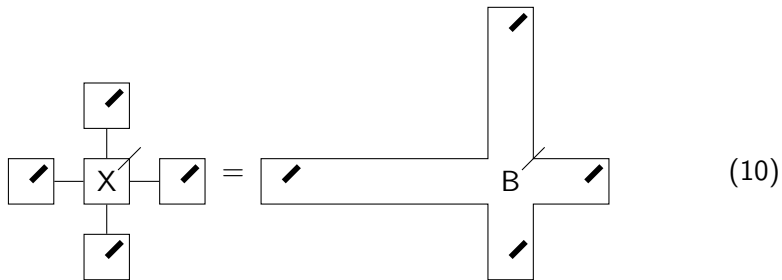
Linear Solver

Nonlinear Solver

Sequential Linear Solver

Results

Conclusion


$$\begin{array}{c} \boxed{\diagup} \\ | \\ \boxed{\diagup} \text{---} \boxed{X} \text{---} \boxed{\diagup} \\ | \\ \boxed{\diagup} \end{array} = \begin{array}{c} \boxed{\diagup} \\ | \\ \boxed{\diagup} \text{---} \boxed{B} \text{---} \boxed{\diagup} \\ | \\ \boxed{\diagup} \end{array} \quad (10)$$

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

Introduction

Cluster Expansion

Solvers

Linear Solver

Nonlinear Solver

Sequential Linear Solver

Results

Conclusion

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

Linear Solver: Inversion Scheme

Introduction

Cluster Expansion

Solvers

Linear Solver

Nonlinear Solver

Sequential Linear Solver

Results

Conclusion

- 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

Introduction

Cluster Expansion

Solvers

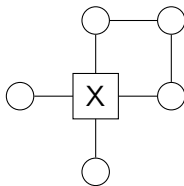
Linear Solver

Nonlinear Solver

Sequential Linear Solver

Results

Conclusion



(11)

Linear Solver: Applicability

Introduction

Cluster Expansion

Solvers

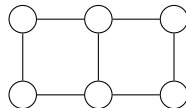
Linear Solver

Nonlinear Solver

Sequential Linear Solver

Results

Conclusion



(12)

Linear Solver: Applicability

Introduction

Cluster Expansion

Solvers

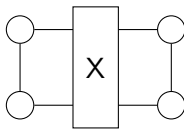
Linear Solver

Nonlinear Solver

Sequential Linear Solver

Results

Conclusion



(12)

Linear Solver: Applicability

Introduction

Cluster Expansion

Solvers

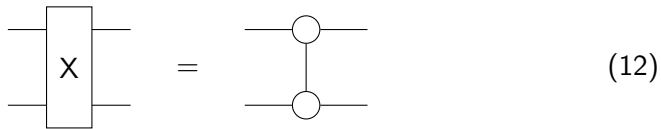
Linear Solver

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

Introduction

Cluster Expansion

Solvers

Results

Conclusion

Conclusion

References I

Introduction

Cluster Expansion

Solvers

Results

Conclusion



S. Hesselmann, S. Wessel, Thermal Ising transitions in the vicinity of two-dimensional quantum critical points, PHYSICAL REVIEW B 93 (2016) 155157.

doi:10.1103/PhysRevB.93.155157.