

Cluster Expansion of Thermal States using Tensor Networks

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Problem Statement

Tensor Networks

Overview Thesis

Cluster Expansion

Solvers

Results

Conclusion and
Outlook

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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_α	
M	$M_{\alpha\beta}$	
$\vec{x} \cdot \vec{y}$	$x_\alpha y_\alpha$	

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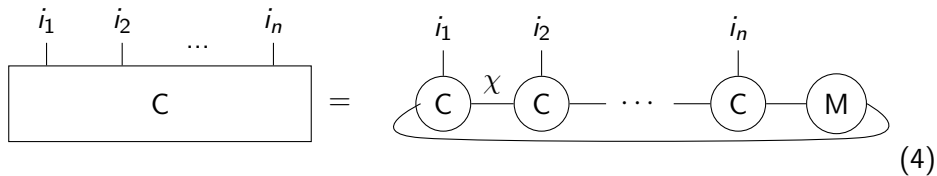
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$$C^{i_1 i_2 \dots i_n} = \text{Tr}(C^{i_1} C^{i_2} \dots C^{i_n} M) \quad (3)$$


$$\text{Diagram illustrating the trace operation in tensor networks. On the left, a rectangular block labeled } C \text{ has indices } i_1, i_2, \dots, i_n \text{ on its top edge. This is set equal to a chain of circular nodes. The first node is labeled } C \text{ with index } i_1, \text{ followed by a node labeled } C \text{ with index } i_2, \text{ then an ellipsis, then a node labeled } C \text{ with index } i_n, \text{ and finally a node labeled } M. \text{ A curved line connects the bottom of the first } C \text{ node to the bottom of the } M \text{ node, representing the trace. The entire expression is labeled (4).}$$

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

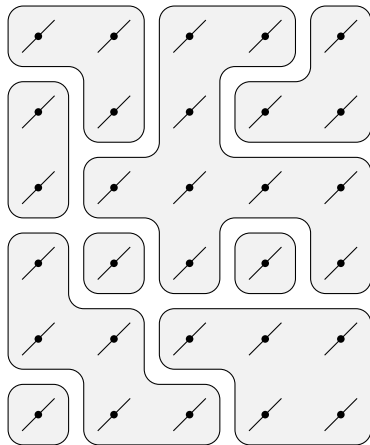
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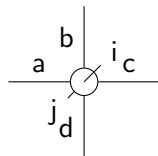
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- $e^{-\beta \hat{H}} = \sum_{\{B_i\}} \bigotimes_i B_i$
- Solves local patch exactly
- Increase size patches
- Encoded by 1 tensor



(7)

Cluster Expansion

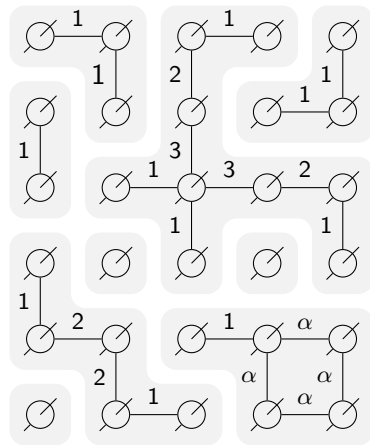
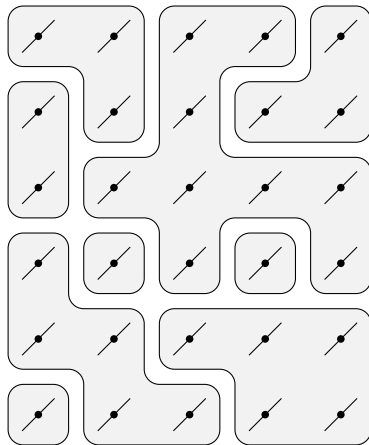
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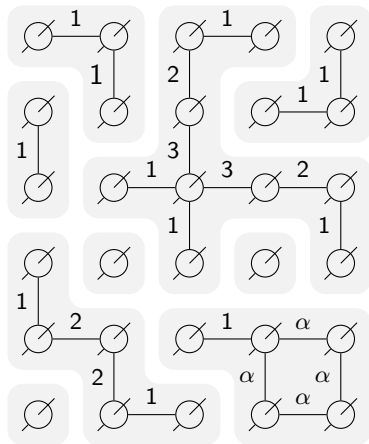
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- Multiple choices for encoding
- Spurious blocks
- Doesn't break symmetry
- Thermodynamic limit
- Tensor Network toolbox



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Linear Solver

Nonlinear Solver

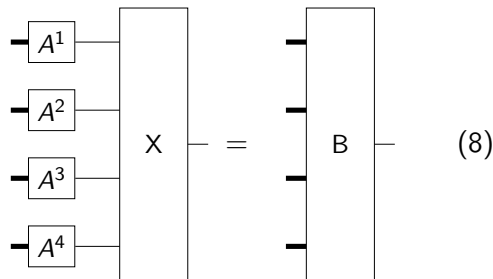
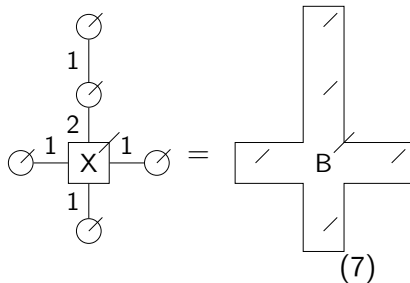
Sequential Linear Solver

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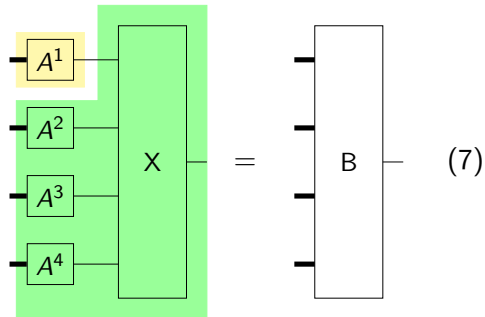
Solvers

Linear Solver: Inversion Scheme



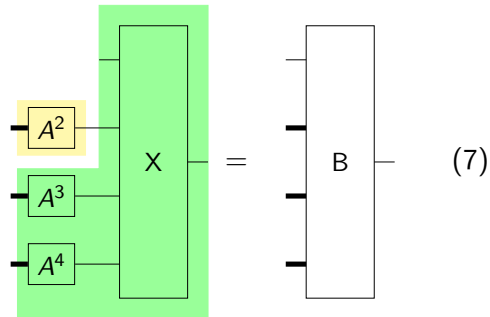
Linear Solver: Inversion Scheme

- Invert A^i separately
 - Fast
 - Numerically unstable



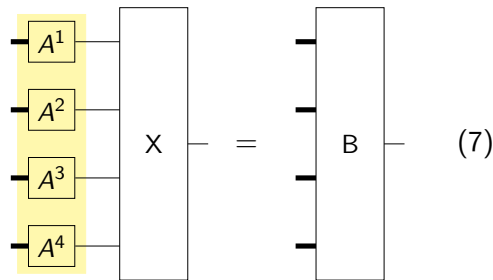
Linear Solver: Inversion Scheme

- Invert A^i separately
 - Fast
 - Numerically unstable



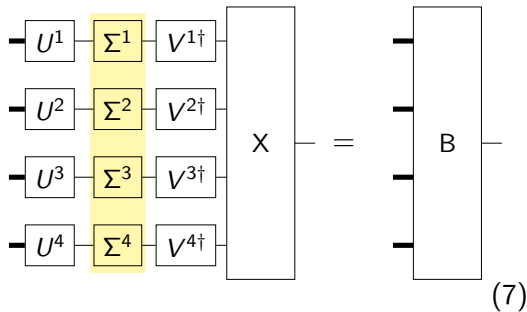
Linear Solver: Inversion Scheme

- 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

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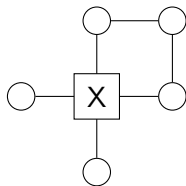
Linear Solver

Nonlinear Solver

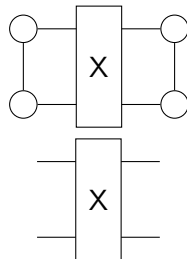
Sequential Linear Solver

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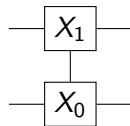


(8)



(9a)

=



(9b)

Nonlinear Solver

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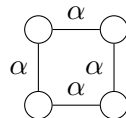
Nonlinear Solver

Sequential Linear Solver

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- Nonlinear least squares
- Jacobian
- Permutations



(10)

Sequential Linear Solver

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

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1D exact

2D exact

2D Transverse Ising
model

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1D: Cluster expansions

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- Relative error ϵ
- Different encodings blocks
 - A: small bond dimension
 - E: no spurious blocks
 - F: well conditioned

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

1D: Transverse Field Ising

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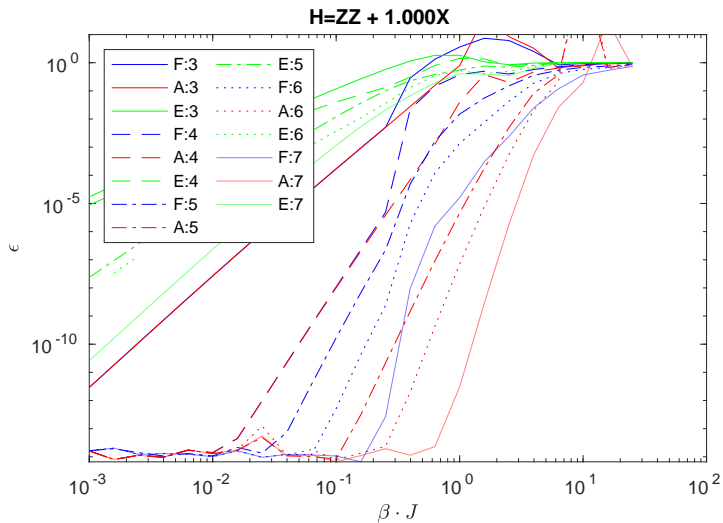
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1D: Heisenberg XXX

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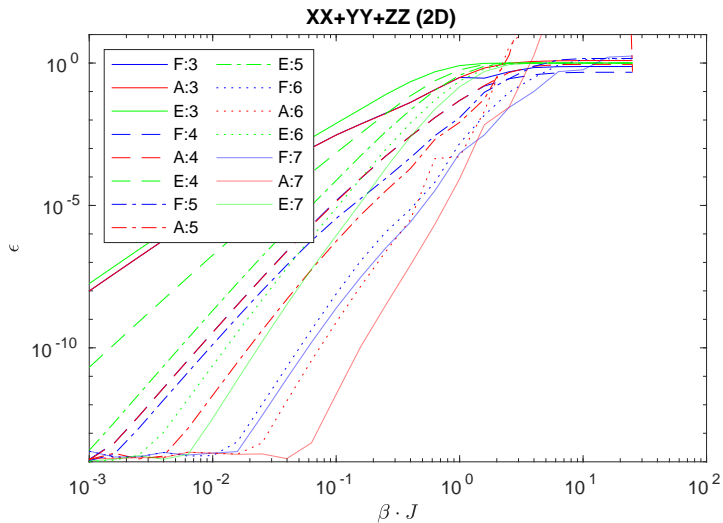
Results

1D exact

2D exact

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model

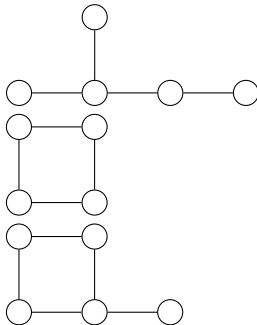
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2D: Cluster expansions

- Relative error ϵ
- Encodings based on A (order 5)

- No loops



- +Plaquette

- +Extensions

	χ
no loops	21
loops	27
extensions	43

2D: TFI

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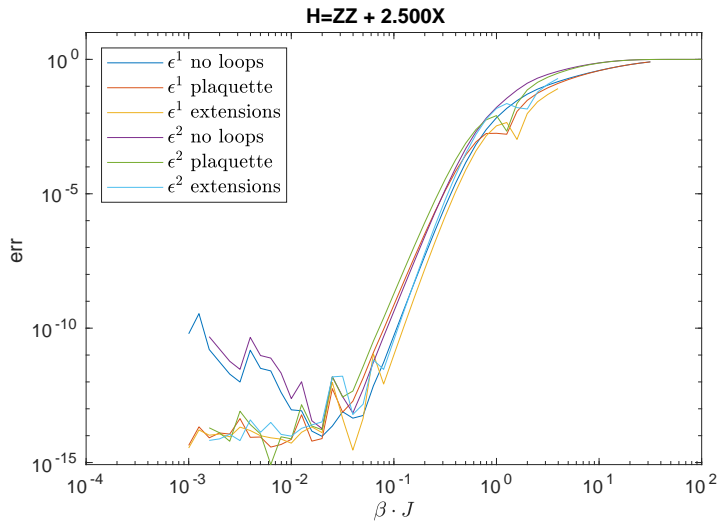
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TFI: Phase Diagram

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- Criticality
- $\Gamma = 0$ and $\Gamma = 2.5$

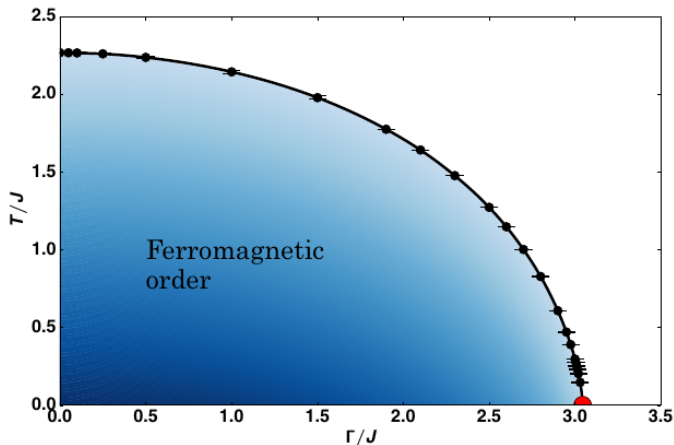
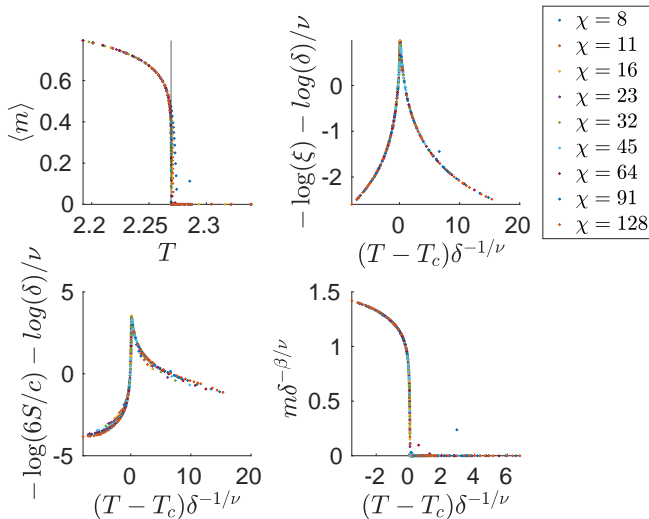


Figure taken from [2]

2D: Classical Ising

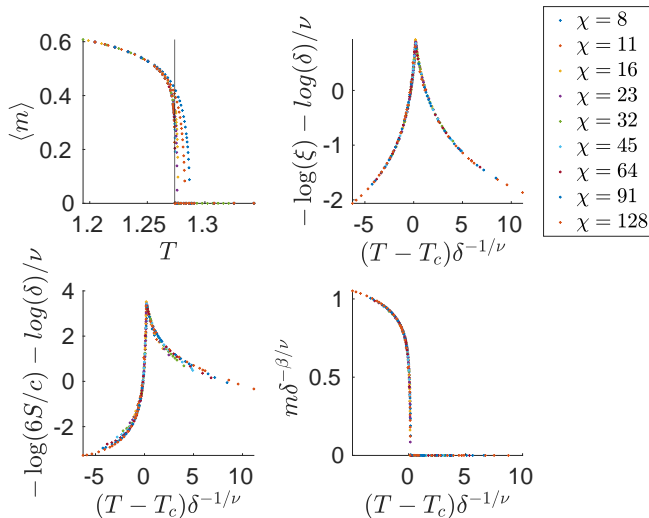
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	T_c
Fit	2.691(9)
Exact	2.691853

2D: TFI $\Gamma = 2.5$

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

References I



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