Cluster Expansion of Thermal States using Tensor Networks

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Introduction

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- Overview condensed matter physics

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

Introduction

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

Simulating Quantum Many-body Systems

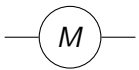
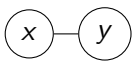
- Equations are known
- Curse of dimensionality
- Tensor networks

Tensor Networks: Introduction

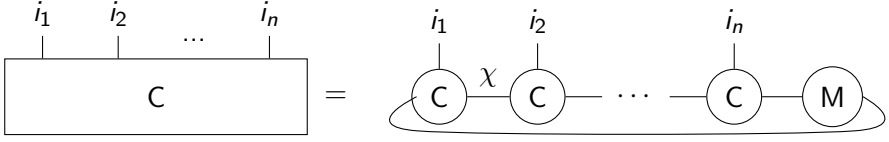
$$|\Psi\rangle = \sum_{i_1 i_2 \cdots i_n} C^{i_1 i_2 \cdots i_n} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle \,. \tag{1}$$

$$C^{i_1 i_2 \cdots i_n} = Tr(C^{i_1} C^{i_2} \cdots C^{i_n} M). \tag{2}$$

Tensor Networks: Graphical Notation

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

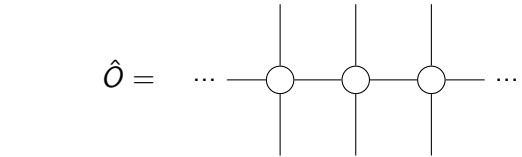
$$C^{i_1 i_2 \cdots i_n} = Tr(C^{i_1} C^{i_2} \cdots C^{i_n} M) \tag{3}$$



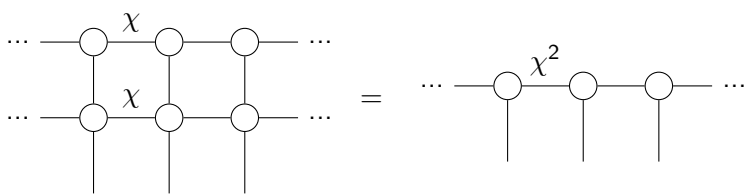
(4)

Tensor Networks: Operators

$$\hat{O} = \quad \cdots \quad \cdots \tag{5}$$



$$\hat{O}\,|\Psi\rangle = \quad \cdots \quad \chi \quad \cdots \quad \cdots \quad \chi \quad \cdots \quad = \quad \cdots \quad \chi^2 \quad \cdots \tag{6}$$

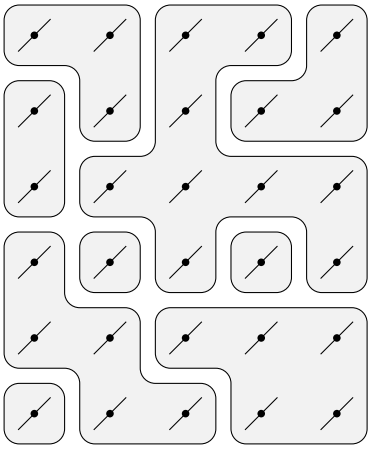


Operator exponential

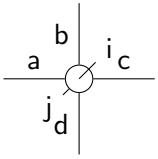
- (Real) Time eveolution: $\hat{O} = e^{-i\hat{H}t}$
- Statistical ensembles: $\hat{O} = e^{-\beta\hat{H}}$

Cluster Expansion

Cluser Exapansion

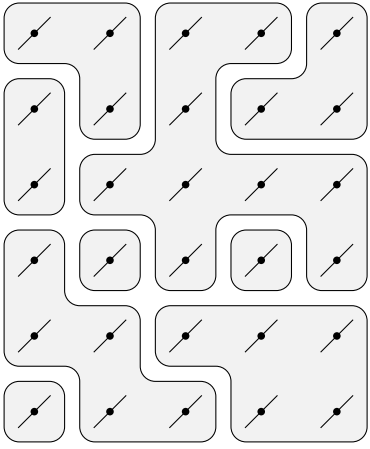


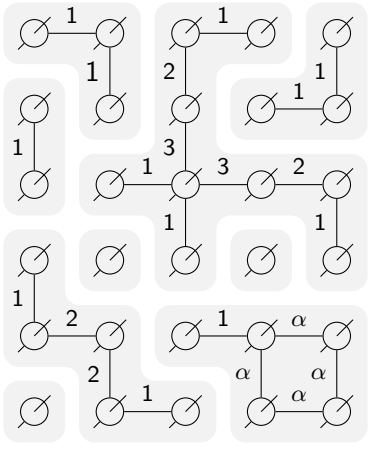
- $e^{-\beta \hat{H}} = \sum_{\{B_i\}} \bigotimes_i B_i$
- Solves local patch exactly
- Increase size patches
- Encoded by 1 tensor



(7)

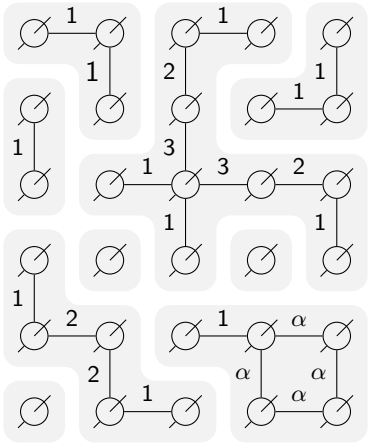
Cluser Exapansion





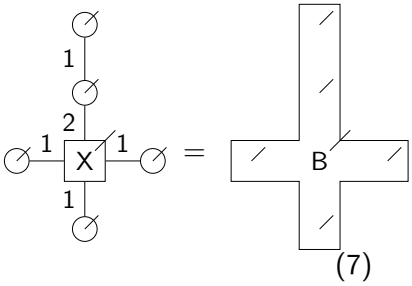
Cluser Exapansion

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

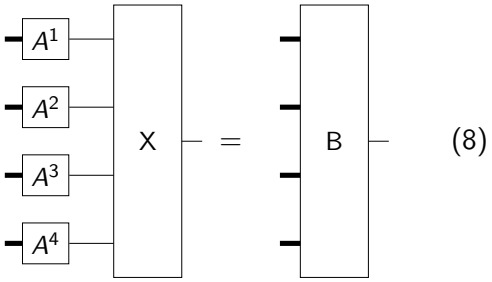


Solvers

Linear Solver: Inversion Scheme



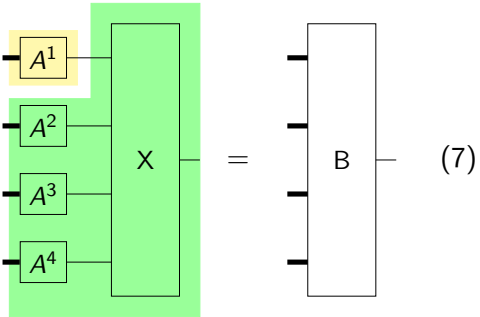
(7)



(8)

Linear Solver: Inversion Scheme

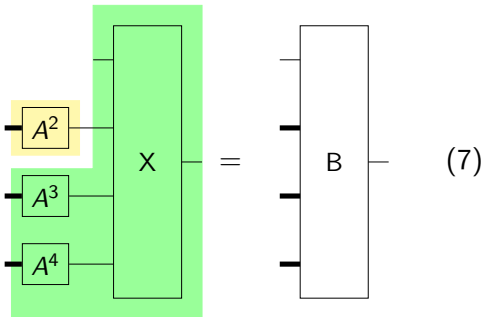
- Invert A^i separately
  - Fast
  - Numerically unstable



(7)

Linear Solver: Inversion Scheme

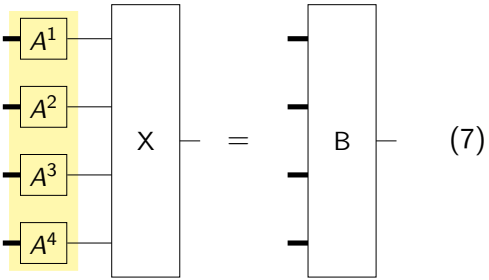
- Invert A^i separately
  - Fast
  - Numerically unstable



(7)

Linear Solver: Inversion Scheme

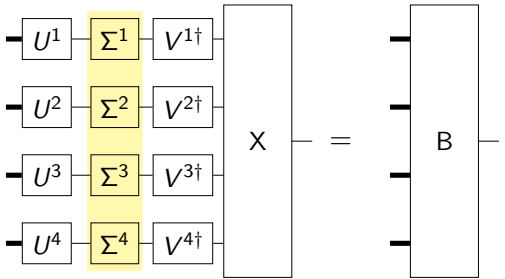
- Invert A^i separately
- Full inversion
  - Slow
  - Stable for pseudoinverse



(7)

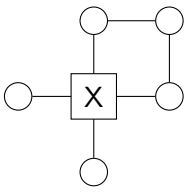
Linear Solver: Inversion Scheme

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

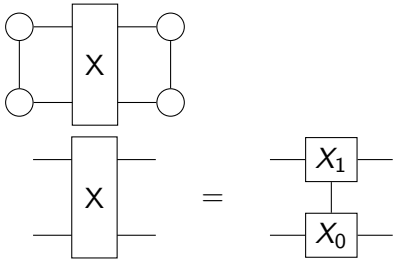


(7)

Linear Solver: Applicability



(8)

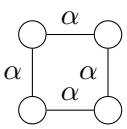


(9a)

(9b)

Nonlinear Solver

- Nonlinear least squares
- Jacobian
- Permutations



(10)

Sequential Linear Solver

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

Results

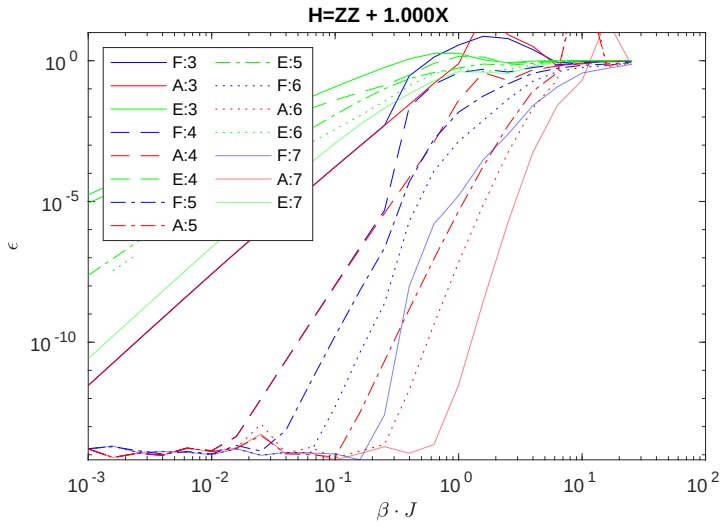
1D: Cluster expansions

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

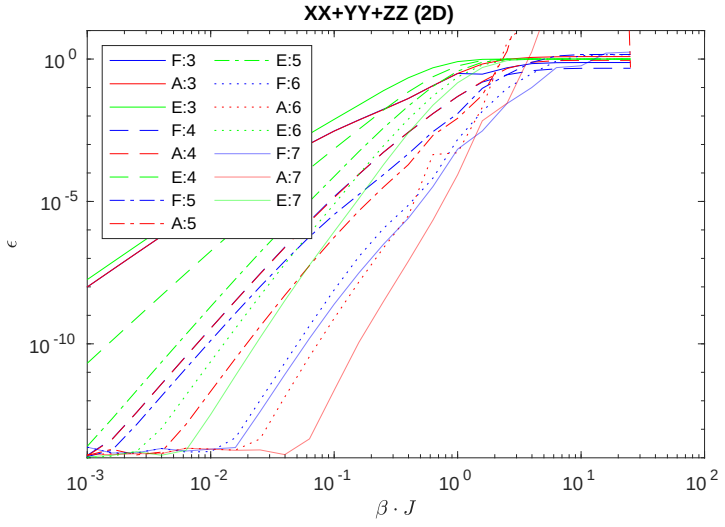
χ

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

1D: Transverse Field Ising

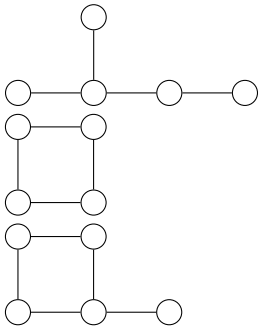


1D: Heisenberg XXX



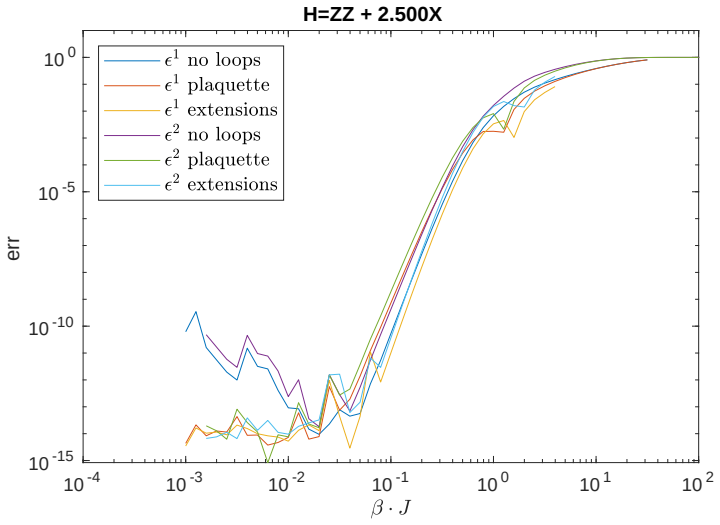
2D: Cluster expansions

- Relative error ϵ
- Encodings based on A (order 5)
  - No loops
  - +Plaquette
  - +Extensions



	χ
no loops	21
loops	27
extensions	43

2D: TFI



TFI: Phase Diagram

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

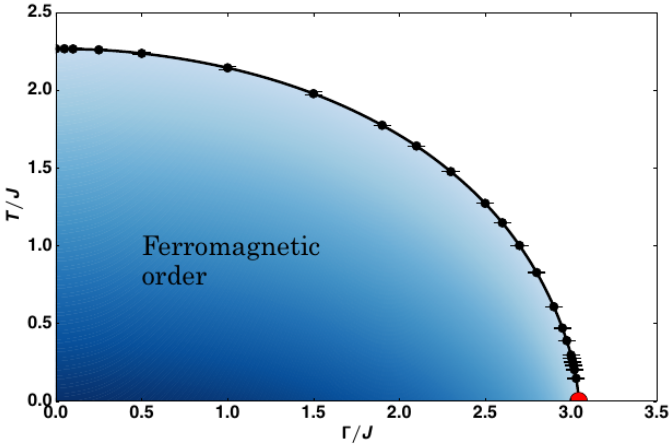
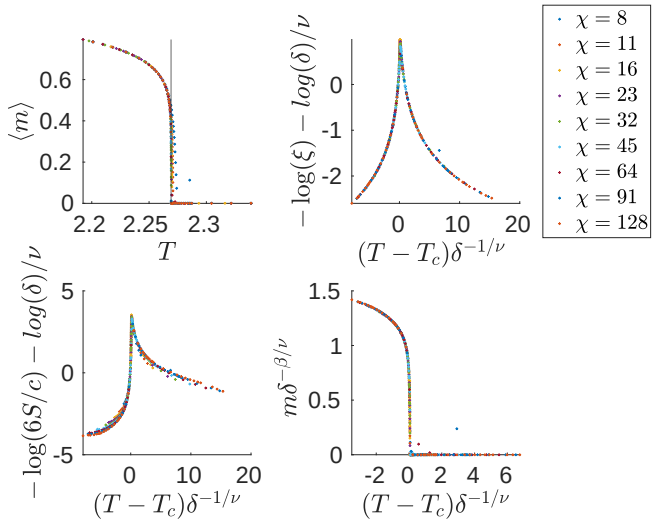


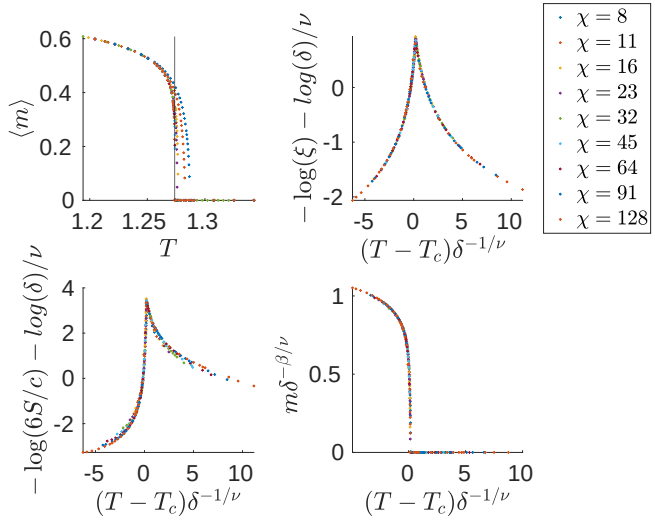
Figure taken from [2]

2D: Classical Ising



	T_c
Fit	2.691(9)
Exact	2.691853

2D: TFI $\Gamma = 2.5$



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

Data from [3]

Conclusion and Outlook

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

References I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