Cluster Expansions of Thermal States using Tensor Networks

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- Introduction
- Cluster Expansions
- Results

Introduction

Introduction

- Overview condensed matter physics
  - Macroscopic and microscopic physical properties of matter
    - Metals
    - semiconductors
    - Liquids
    - Bose-Einstein Condensates
    - Magnets
  - Different disciplines
    - Experimental
    - Theoretical
    - Engineering

Introduction

- Overview condensed matter physics
- Strongly correlated materials
  - High T_c Superconductors
  - Quantum spin liquids
  - Strange metals
  - Correlated topological matter

Introduction

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

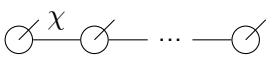
Simulating Quantum Many-body Systems

- Equations are known
- Curse of dimensionality
- Numerical methods

Tensor Networks

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

$$\begin{aligned} C^{i_1 i_2 \cdots i_n} &= w_l C^{i_1} C^{i_2} \cdots C^{i_n} w_r \\ &= \end{aligned} \tag{2}$$



- Matrix Product State
- Relevant corner Hilbert space

Operator Exponential

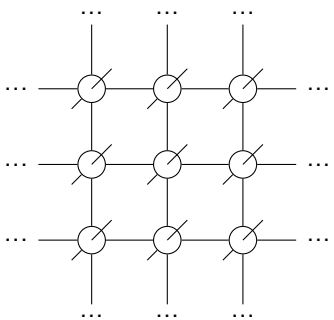
- Time evolution:

$$\hat{H}\,|\Psi(t)\rangle = i\frac{d}{dt}\,|\Psi(t)\rangle \qquad (3)$$

$$|\Psi(t)\rangle = e^{-i\hat{H}t}\,|\Psi(0)\rangle \qquad (4)$$

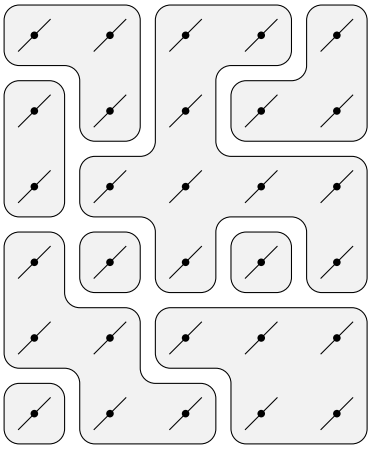
- Statistical ensembles:

$$\hat{\rho} = \frac{e^{-\beta\hat{H}}}{\mathrm{Tr}\left(e^{-\beta\hat{H}}\right)} \qquad (5)$$



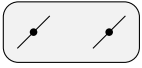
Cluster Expansions

Cluster Expansions



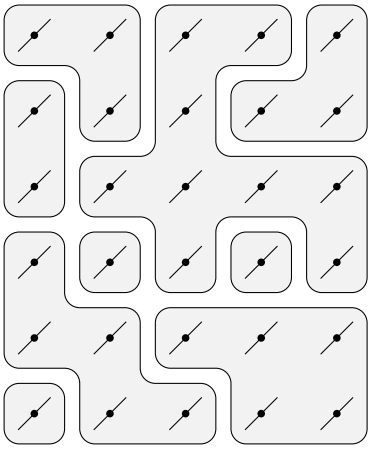
- $e^{-\beta \hat{H}} = \sum_{\{B\}} \bigotimes_i B_i$

$e^{-\beta H(1)} =$ 

$e^{-\beta H(2)} =$ 

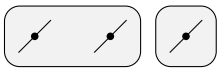
$+$ 

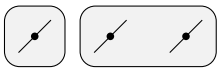
Cluster Expansions



- $e^{-\beta \hat{H}} = \sum_{\{B\}} \bigotimes_i B_i$

$e^{-\beta H(3)} =$ 

$+$ 

$+$ 

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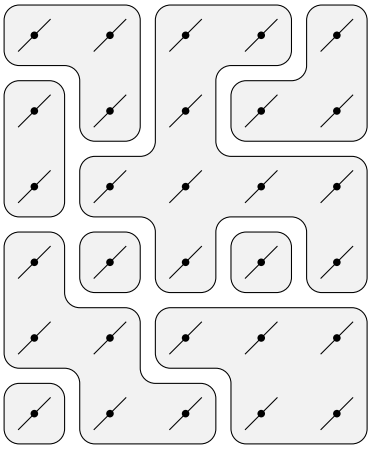
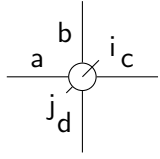
Cluster Expansions

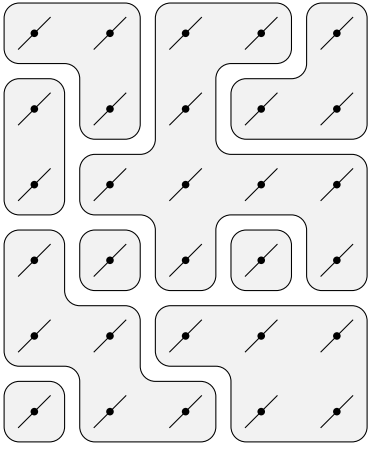


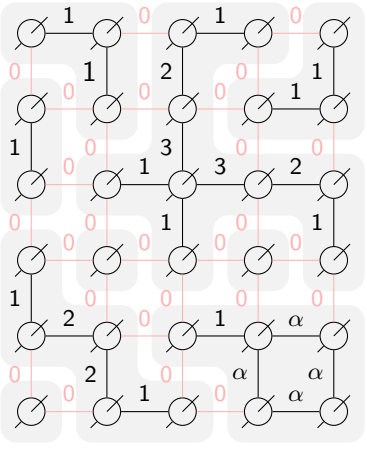
- $e^{-\beta \hat{H}} = \sum_{\{B\}} \bigotimes_i B_i$
- Finite number of blocks: trucate order
- Encoded by 1 tensor

$$O^{abcd} =$$



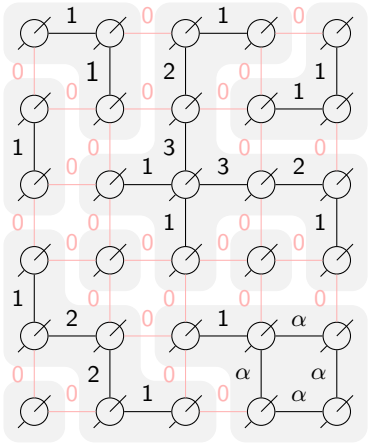
Cluster Expansions





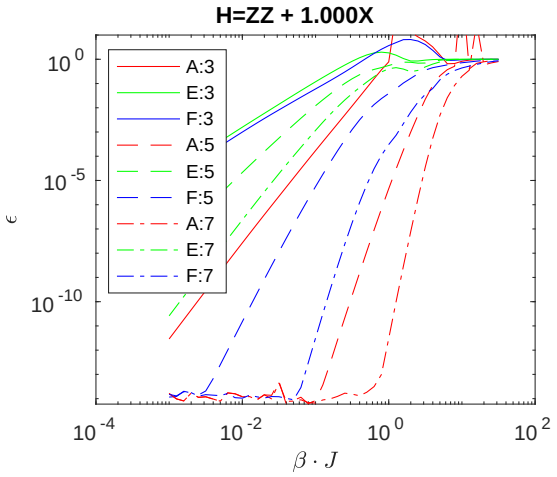
Cluster Expansions

- Multiple choices for encoding
- Size extensive
- Preserves global and internal symmetries
- Tensor Network toolbox



Results

1D: Transverse Field Ising (TFI)



- Relative error ϵ
- Different encodings:
  - A: Small
  - E: Strict
  - F: well-conditioned
- bond dimension

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

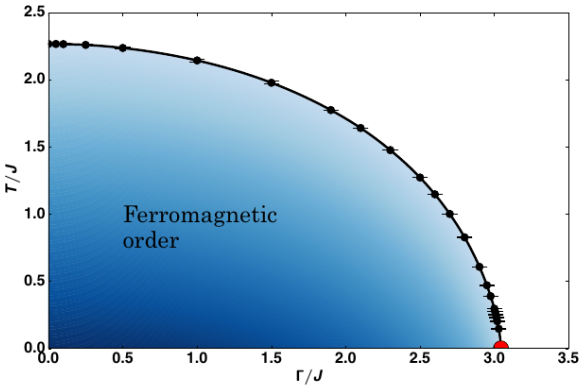
Conclusion

- 2D: similar results
- Real time evolution
- Encoding

2D TFI: Introduction

$$\hat{H} = -J \sum_{\langle ij \rangle} Z_i Z_j + \Gamma \sum_i X_i \tag{6}$$

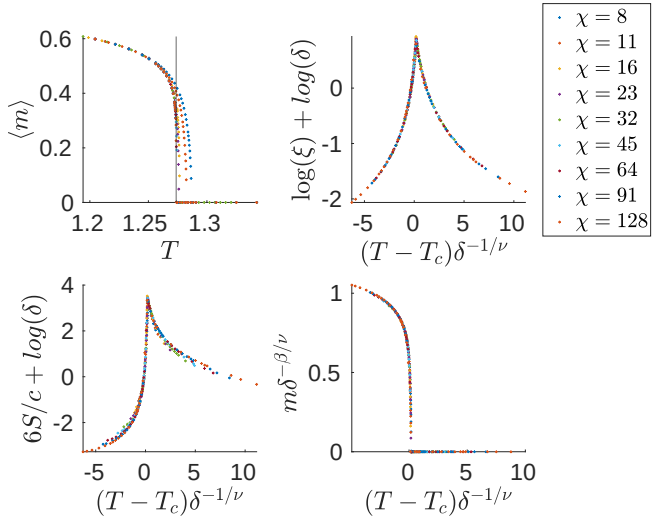
- Different phases
- $\Gamma = 2.5$
- VUMPS
- Order 5



Criticality

- Phase transition
- Power law
- Finite size scaling (χ,δ^{-1})
- Data collapse
  - Observables: m, S and ξ
  - Parameters: T_c

TFI Phase Diagram: $\Gamma = 2.5$



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

Data from [**?**]

Conclusion

Conclusion

- Cluster expansions work extremely well for some encodings
- Stable and fast framework

References I


P. Czarnik and P. Corboz.
Finite correlation length scaling with infinite projected entangled pair states at finite temperature.
Physical Review B, 99:245107, 2019.


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

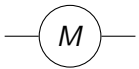
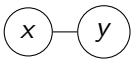
Tensor Networks

Tensor Networks: Introduction

$$|\Psi\rangle = \sum_{i_1 i_2 \cdots i_n} C^{i_1 i_2 \cdots i_n} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle \,. \tag{7}$$

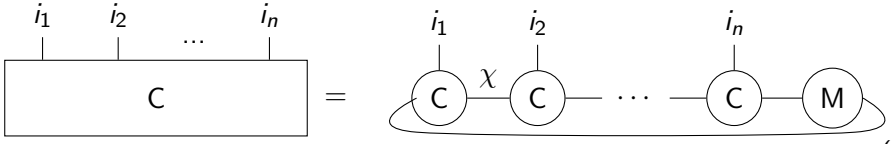
$$C^{i_1 i_2 \cdots i_n} = Tr(C^{i_1} C^{i_2} \cdots C^{i_n} M). \tag{8}$$

Tensor Networks: Graphical Notation

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

Tensor Networks: MPS

$$C^{i_1 i_2 \cdots i_n} = Tr(C^{i_1} C^{i_2} \cdots C^{i_n} M) \tag{9}$$



(10)

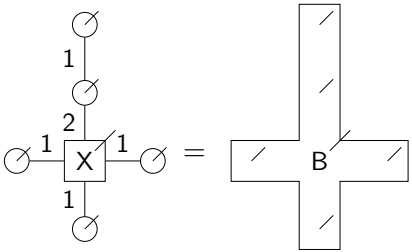
Tensor Networks: Operators

$$\hat{O} = \cdots \cdots \tag{11}$$

$$\hat{O}\,|\Psi\rangle = \cdots \chi \cdots \cdots \chi \cdots = \cdots \chi^2 \cdots \tag{12}$$

Linear Solver

Linear Solver: Inversion Scheme



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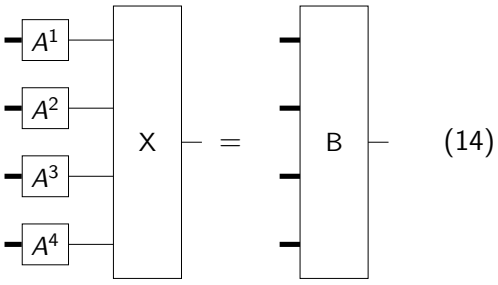
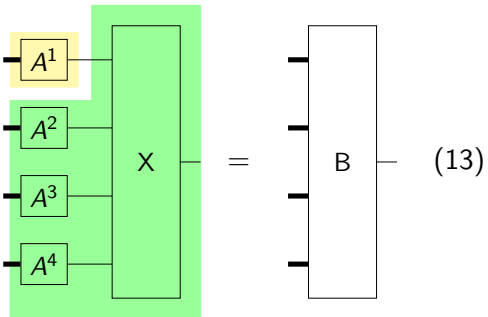


(14)

Linear Solver: Inversion Scheme

- Invert A^i separately
  - Fast
  - Numerically unstable



(13)

Linear Solver: Inversion Scheme

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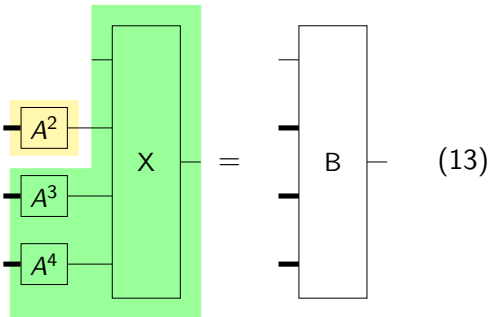
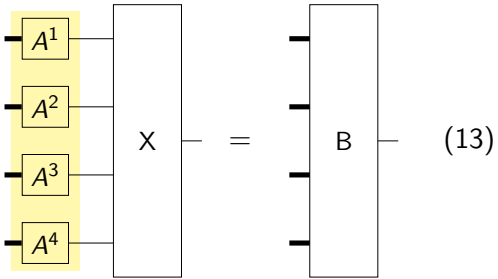


(13)

Linear Solver: Inversion Scheme

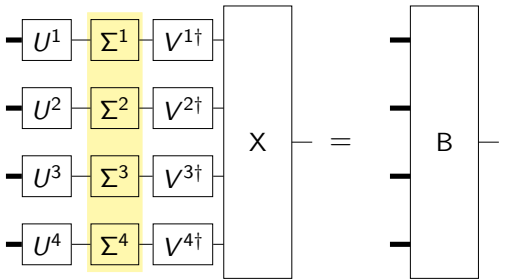
- Invert A^i separately
- Full inversion
  - Slow
  - Stable for pseudoinverse



(13)

Linear Solver: Inversion Scheme

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



(13)

Construction

Notation

$$O^{00} = \quad \overset{i}{\underset{j}{0 \;\bigcirc\; 0}} \quad = \bigcirc \tag{14}$$

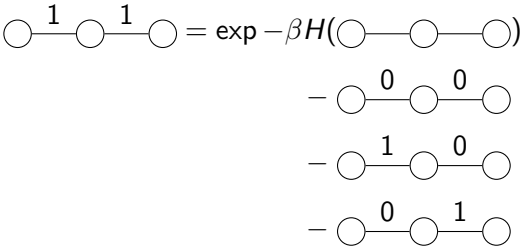
$$O^{01} O^{10} = \bigcirc \overset{1}{\text{———}} \bigcirc \tag{15}$$

General idea

$$\bigcirc = \exp\left(-\beta H(\bigcirc)\right) \tag{16}$$

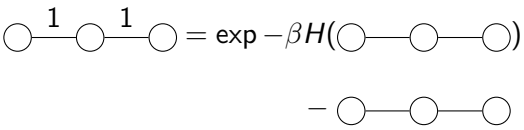
$$\bigcirc\!\!\overset{1}{-}\!\!\bigcirc = \exp -\beta H(\bigcirc\!\!-\!\!\bigcirc - \bigcirc\!\!\overset{0}{-}\!\!\bigcirc) \tag{17}$$

General idea



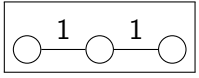
(18)

General idea



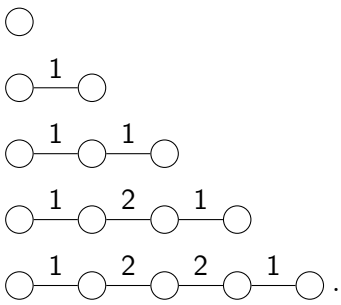
(18)

General idea



(18)

1D: Variant A



(19a)

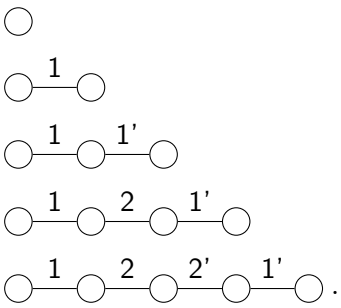
(19b)

(19c)

(19d)

(19e)

1D: Variant E



(20a)

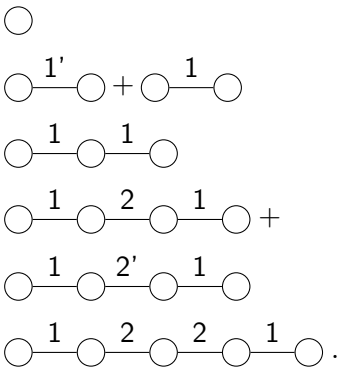
(20b)

(20c)

(20d)

(20e)

1D: Variant F



(21a)

(21b)

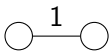
(21c)

(21d)

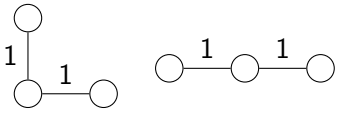
(21e)

$$O^{0000} = \quad = \bigcirc \tag{22}$$

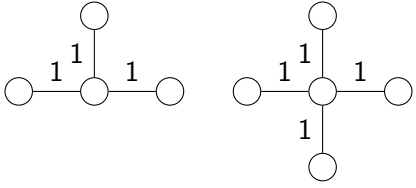
2D: Linear Blocks



(23a)

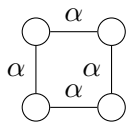


(23b)

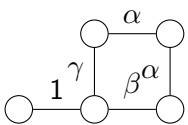


(23c)

2D: Nonlinear Blocks



(24)



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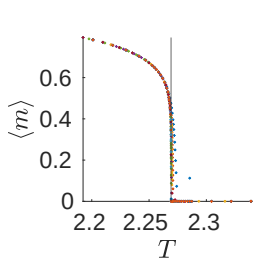
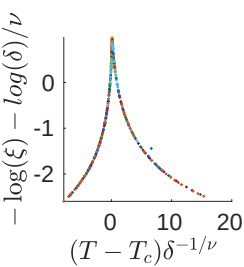
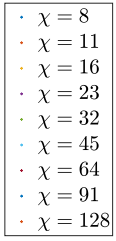
(25)

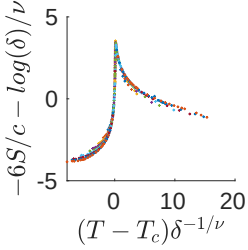
TFI Collapses

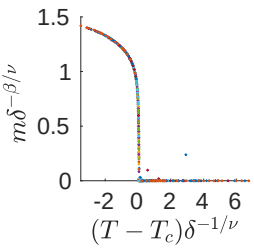
TFI Phase Diagram: Classical Ising



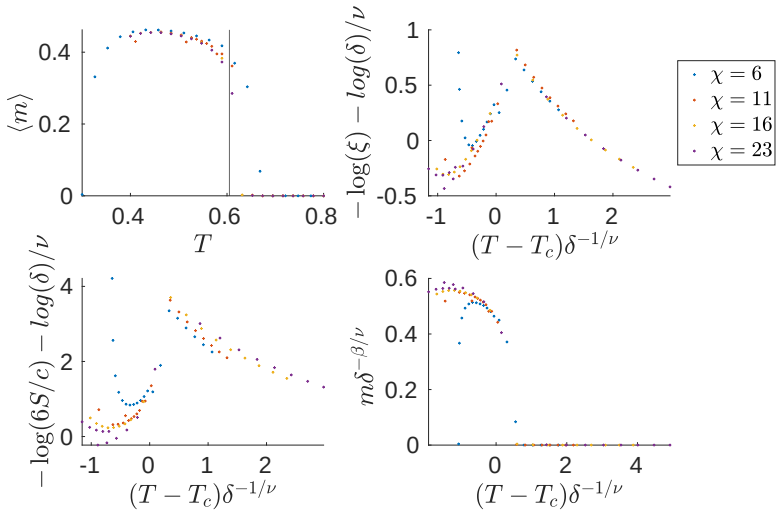






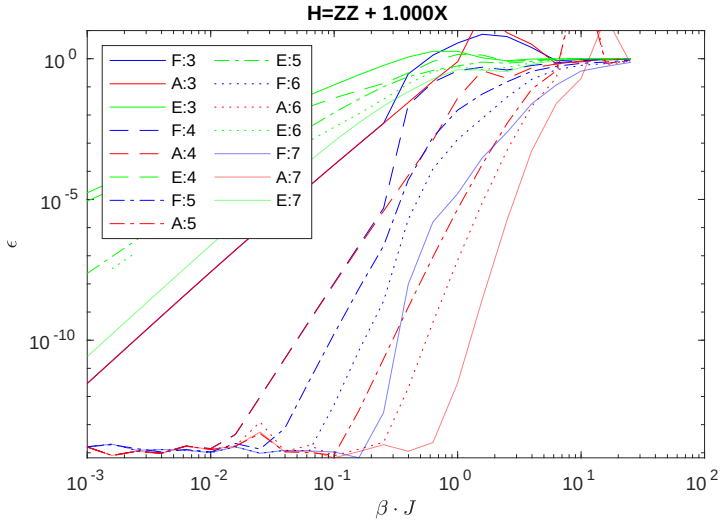


	T_c
Fit	2.691(9)
Exact	2.691853

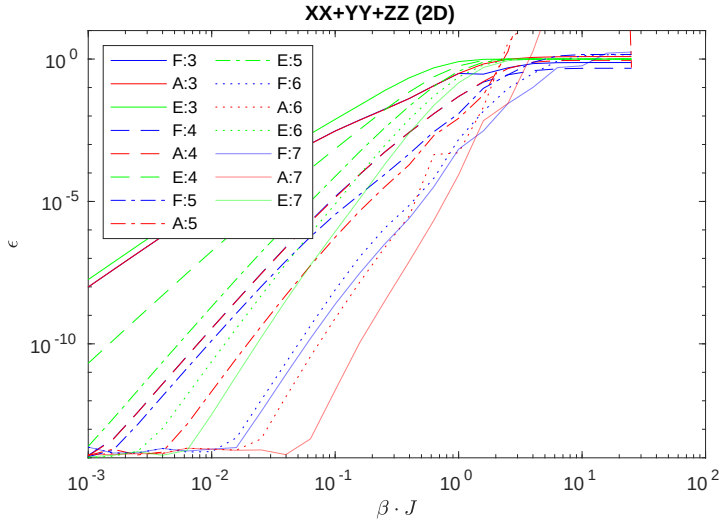


Direct Results

1D: Transverse Field Ising (TFI): full

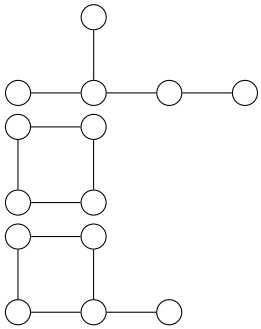


1D: Heisenberg XXX



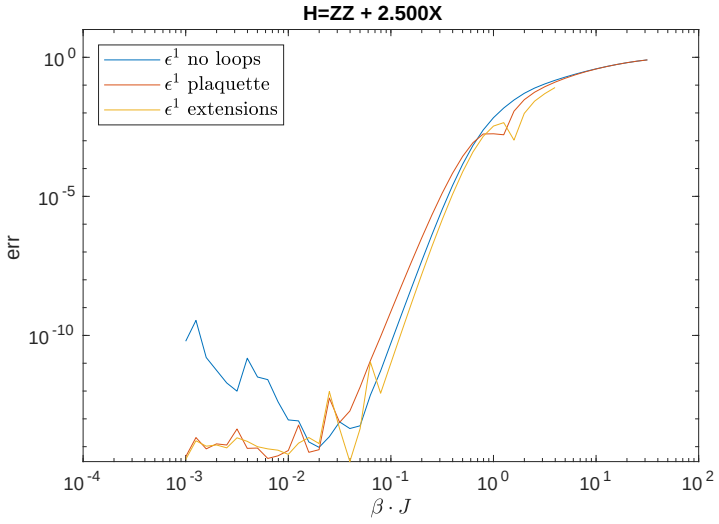
2D: Encodings + Error Measure

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



	χ
no loops	21
plaquette	27
extensions	43

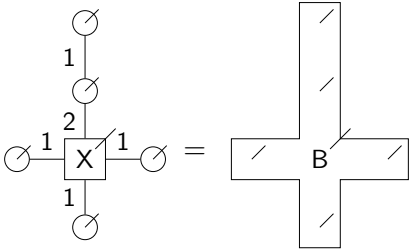
2D: Transverse Field Ising



Solvers

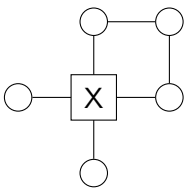
Linear solver

- $AX = B$
- Invert leg per leg
- Pseudoinverse

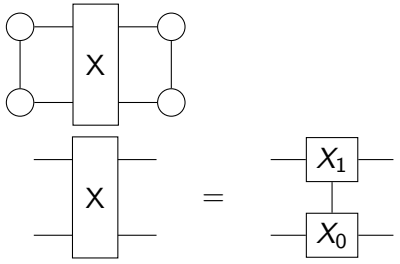


(26)

Linear Solver: Applicability



(27)

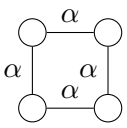


(28a)

(28b)

Nonlinear Solver

- Nonlinear least squares
- Jacobian
- Permutations



(29)

Sequential Linear Solver

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