Cluster Expansions of Thermal States using Tensor Networks

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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 [1]
  - 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

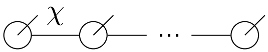
Simulating Quantum Many-body Systems

- Equations are known
- Curse of dimensionality
- Numerical methods

Tensor Networks

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

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



- MPS
- Relevant corner Hilbert space

Operator Exponential

- (Real) Time evolution:

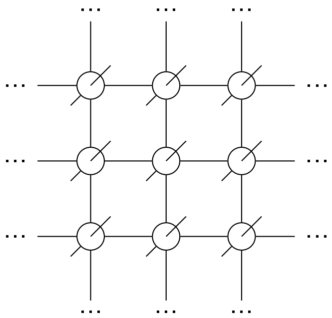
$$\hat{O} = e^{-i\hat{H}t} \tag{3}$$

- Statistical ensembles:

$$\hat{O} = \frac{e^{-\beta\hat{H}}}{\mathrm{Tr}\left(e^{-\beta\hat{H}}\right)} \tag{4}$$

Imaginary time ($\beta = it$)

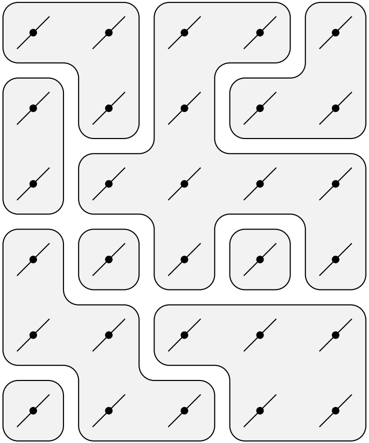
$\hat{O} =$



(5)

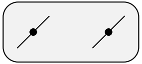
Cluster Expansions

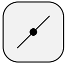
Cluser Exapansions



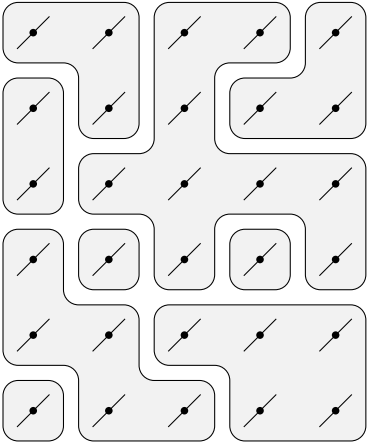
- $e^{\hat{H}} = \sum_{\{B\}} \bigotimes_i B_i$

$e^{H(1)} =$  (6)

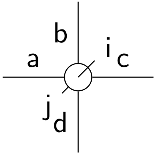
$e^{H(2)} =$ 

$+$   (7)

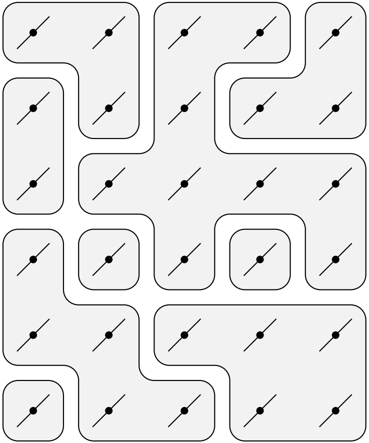
Cluser Exapansions

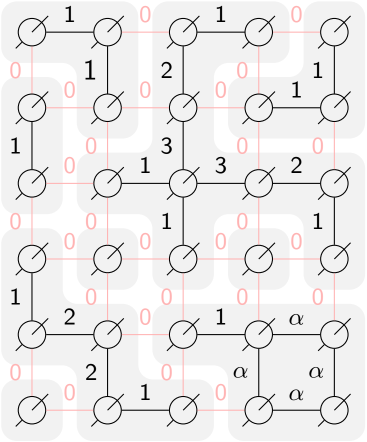


- $e^{\hat{H}} = \sum_{\{B\}} \bigotimes_i B_i$
- Finite number of blocks
- Encoded by 1 tensor

$O^{abcd} =$  (6)

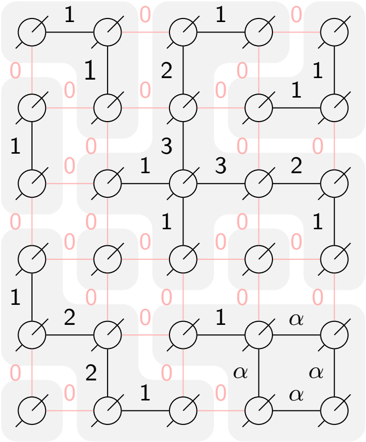
Cluser Exapansions





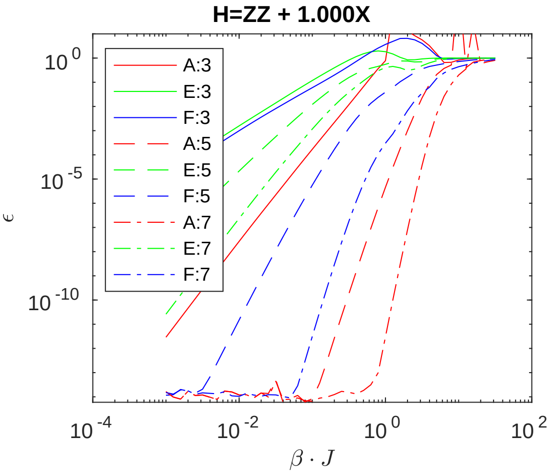
Cluser Exapansions

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

Conclusion

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

2D TFI: Introduction

- Phase Transition
- $\Gamma = 2.5$
- VUMPS
- Order 5

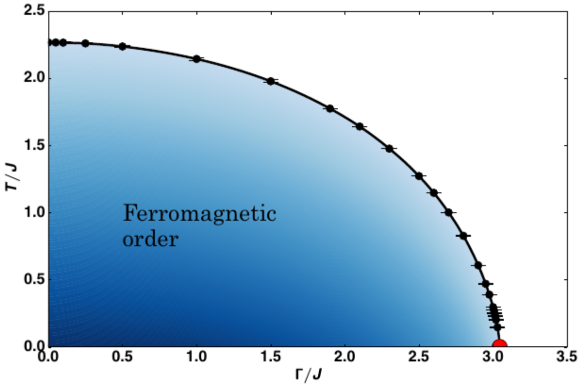
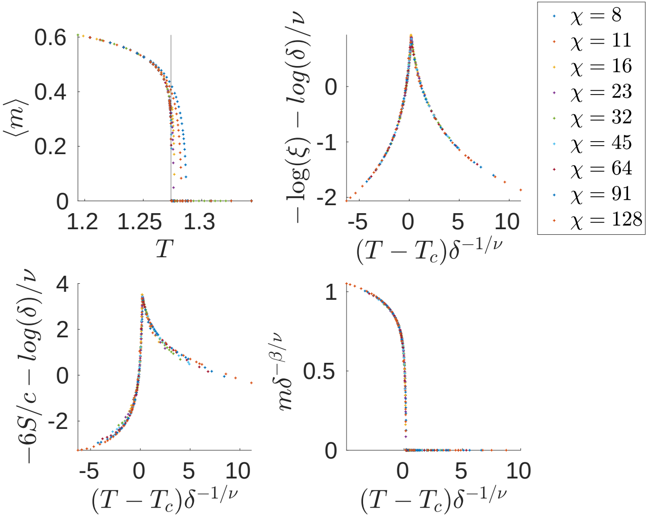


Figure taken from [2]

TFI Phase Diagram: $\Gamma = 2.5$



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

Data from [3]

Conclusion

References I

Introduction
Cluster Expansions
Results
Conclusion

A. Alexandradinata, N. P. Armitage, A. Baydin, W. Bi, Y. Cao, H. J. Changlani, E. Chertkov, E. H. d. S. Neto, L. Delacretaz, I. E. Baggari, G. M. Ferguson, W. J. Gannon, S. A. A. Ghorashi, B. H. Goodge, O. Goulko, G. Grissonnanche, A. Hallas, I. M. Hayes, Y. He, E. W. Huang, A. Kogar, D. Kumah, J. Y. Lee, A. Legros, F. Mahmood, Y. Maximenko, N. Pellatz, H. Polshyn, T. Sarkar, A. Scheie, K. L. Seyler, Z. Shi, B. Skinner, L. Steinke, K. Thirunavukkuarasu, T. V. Trevisan, M. Vogl, P. A. Volkov, Y. Wang, Y. Wang, D. Wei, K. Wei, S. Yang, X. Zhang, Y.-H. Zhang, L. Zhao, A. Zong, The Future of the Correlated Electron Problem (oct 2020).
arXiv:2010.00584.
URL http://arxiv.org/abs/2010.00584

References II

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.

P. Czarnik, P. Corboz, Finite correlation length scaling with infinite projected entangled pair states at finite temperature, Physical Review B 99 (2019) 245107.
doi:10.1103/PhysRevB.99.245107.

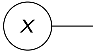
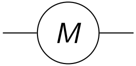
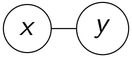
Tensor Networks

Tensor Networks: Introduction

$$|\Psi\rangle = \sum_{i_1 i_2 \cdots i_n} C^{i_1 i_2 \cdots i_n} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle \,. \tag{6}$$

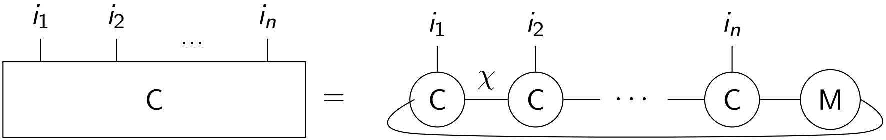
$$C^{i_1 i_2 \cdots i_n} = Tr(C^{i_1} C^{i_2} \cdots C^{i_n} M). \tag{7}$$

Tensor Networks: Graphical Notation

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

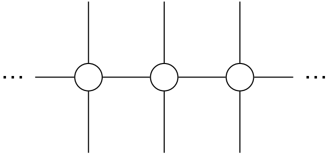
Tensor Networks: MPS

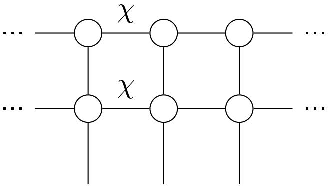
$$C^{i_1 i_2 \cdots i_n} = Tr(C^{i_1} C^{i_2} \cdots C^{i_n} M) \tag{8}$$

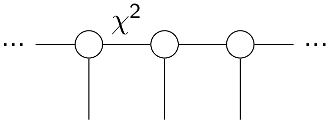


(9)

Tensor Networks: Operators

$\hat{O} =$  (10)

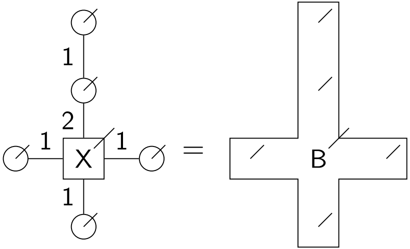
$\hat{O}\,|\Psi\rangle =$ 

$=$ 

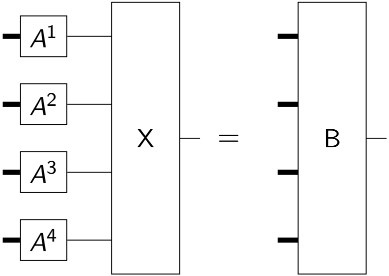
(11)

Linear Solver

Linear Solver: Inversion Scheme



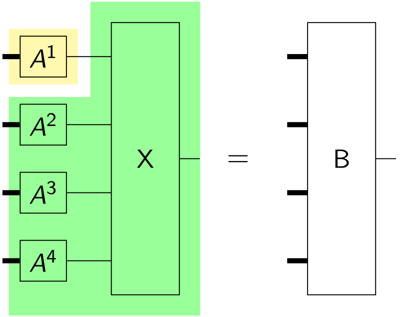
(12)



(13)

Linear Solver: Inversion Scheme

- Invert A^i separately
  - Fast
  - Numerically unstable



(12)

Linear Solver: Inversion Scheme

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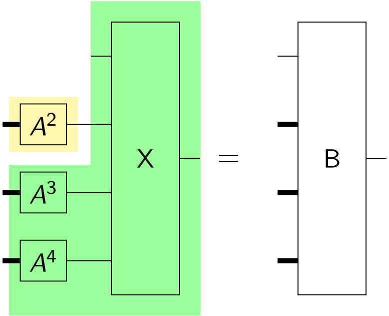
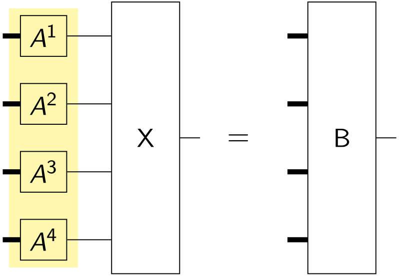


(12)

Linear Solver: Inversion Scheme

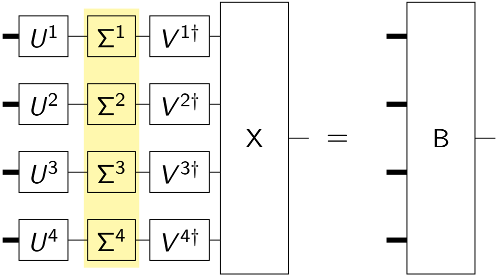
- Invert A^i separately
- Full inversion
  - Slow
  - Stable for pseudoinverse



(12)

Linear Solver: Inversion Scheme

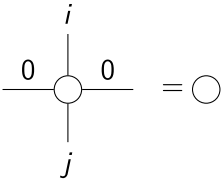
- Invert A^i separately
- Full inversion
- Sparse full inversion
  - $A^i = U^i \Sigma^i V^{i\dagger}$



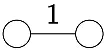
(12)

Construction

Notation

$$O^{00} =$$ 

(13)

$$O^{01}O^{10} =$$ 

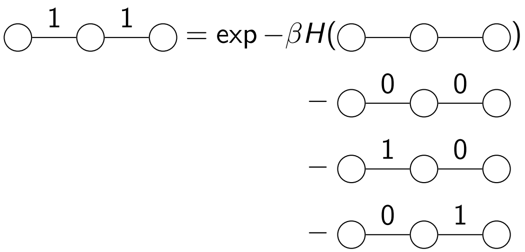
(14)

General idea

$$\bigcirc = \exp\left(-\beta H(\bigcirc)\right) \tag{15}$$

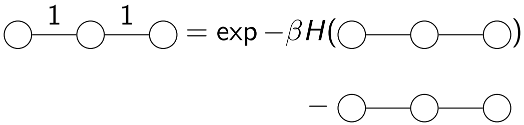
$$\bigcirc\overset{1}{\text{——}}\bigcirc = \exp -\beta H(\bigcirc\text{——}\bigcirc) - \bigcirc\overset{0}{\text{——}}\bigcirc \tag{16}$$

General idea



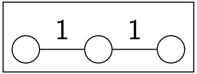
(17)

General idea



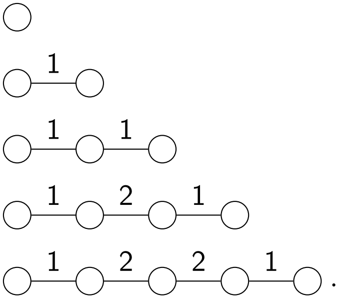
(17)

General idea



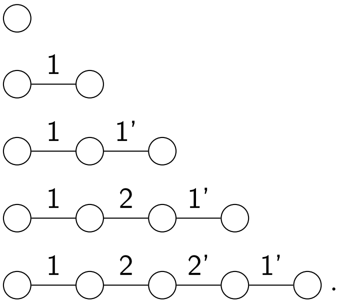
(17)

1D: Variant A



(18a)
(18b)
(18c)
(18d)
(18e)

1D: Variant E



(19a)

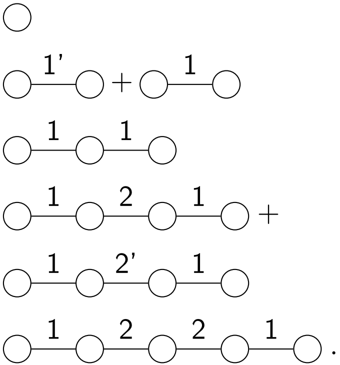
(19b)

(19c)

(19d)

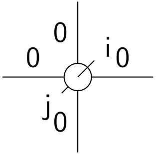
(19e)

1D: Variant F



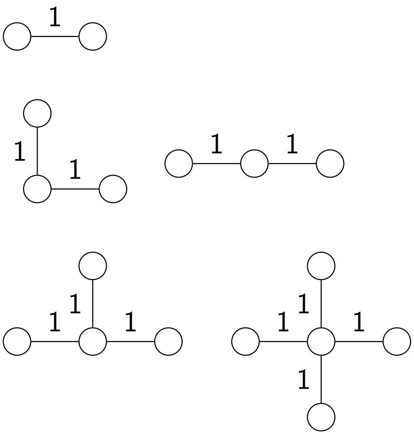
(20a)
(20b)
(20c)
(20d)
(20e)

$$O^{0000} =$$



$$= \bigcirc \tag{21}$$

2D: Linear Blocks

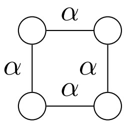


(22a)

(22b)

(22c)

2D: Nonlinear Blocks



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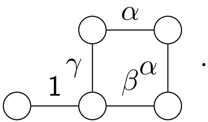
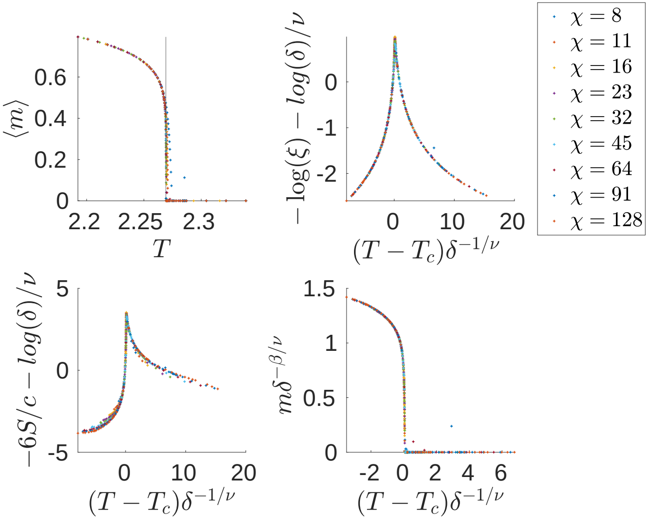


(24)

TFI Collapses

TFI Phase Diagram: Classical Ising



	T_c
Fit	2.691(9)
Exact	2.691853

Tensor Networks

Linear Solver

Construction

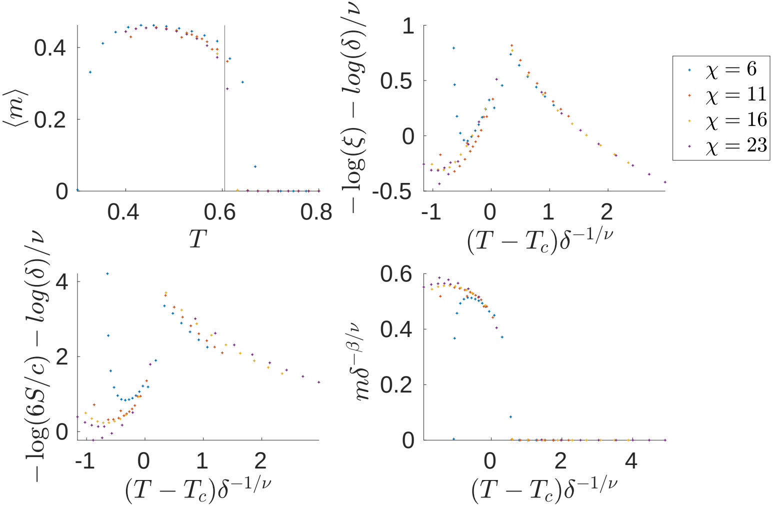
TFI Collapses

$g = 0.0$

$g = 2.9$

Direct Results

Solvers



Direct Results

1D: Transverse Field Ising (TFI): full

Tensor Networks

Linear Solver

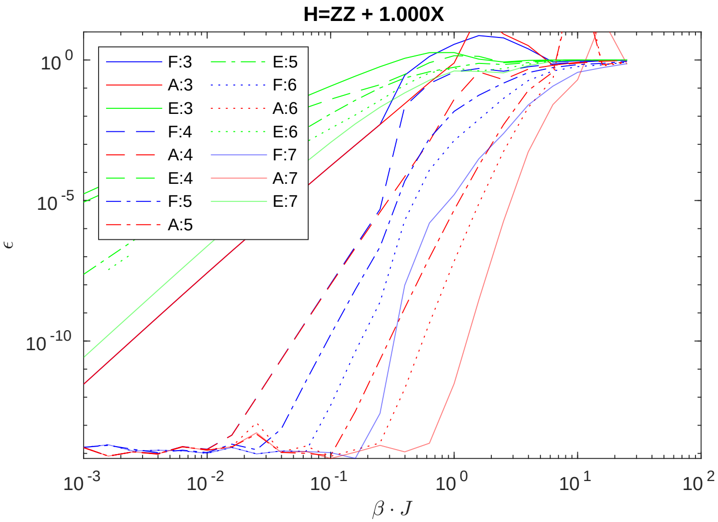
Construction

TFI Collapses

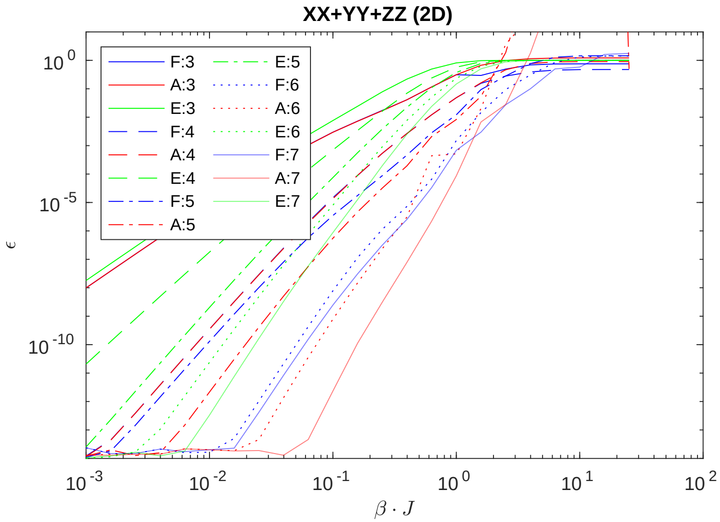
Direct Results

2D Exact

Solvers

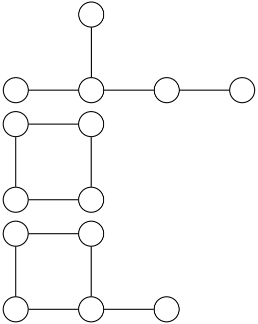


1D: Heisenberg XXX



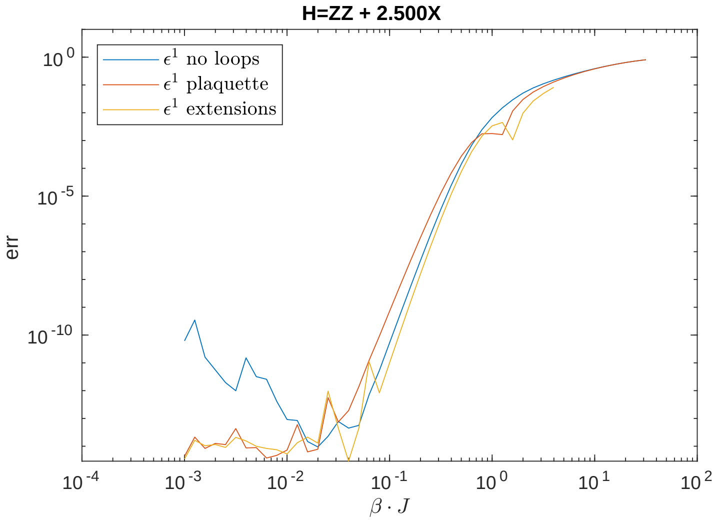
2D: Encodings + Error Measure

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



	χ
no loops	21
plaquette	27
extensions	43

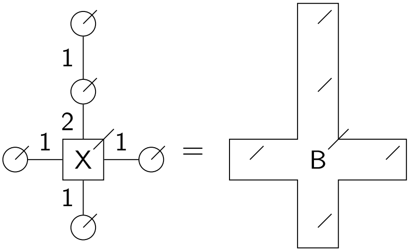
2D: Transverse Field Ising



Solvers

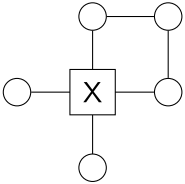
Linear solver

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

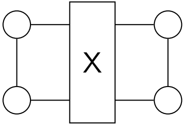


(25)

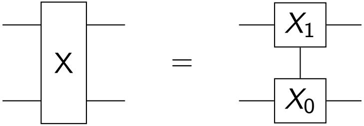
Linear Solver: Applicability



(26)



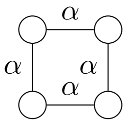
(27a)



(27b)

Nonlinear Solver

- Nonlinear least squares
- Jacobian
- Permutations



(28)

Sequential Linear Solver

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