Cluster Expansions of Thermal States using Tensor Networks

David Devoogdt

Faculty of Engineering and Architecture
Ghent University

June 22, 2021

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

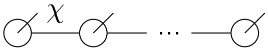
- Equations are known
- Curse of dimensionality
- Numerical methods

Tensor Networks

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

$$C^{i_1 i_2 \cdots i_n} = w_l C^{i_1} C^{i_2} \cdots C^{i_n} w_r \tag{2}$$

=



- MPS
- Relevant corner Hilbert space

Operator Exponential

- (Real) Time evolution:

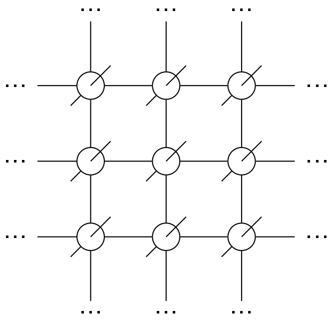
$$\hat{O} = e^{-i\hat{H}t} \tag{3}$$

- Statistical ensembles:

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

Imaginary time ($\beta = it$)

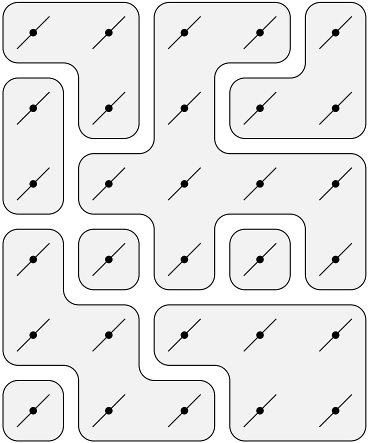
$\hat{O} =$



(5)

Cluster Expansions

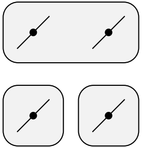
Cluser Exapansions



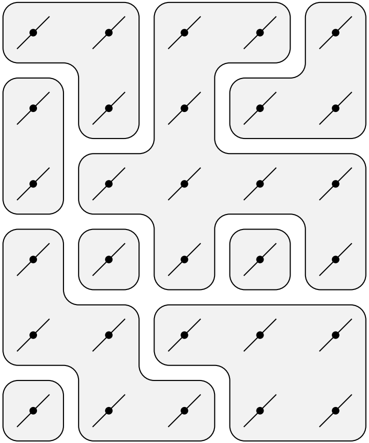
- $e^{\hat{H}} = \sum_{\{B\}} \bigotimes_i B_i$

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

$$e^{H(2)} = \quad + \quad (7)$$

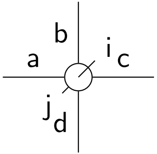


Cluser Exapansions



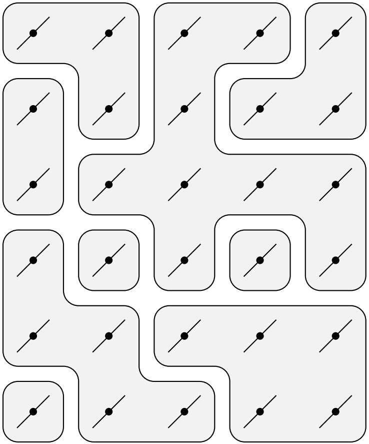
- $e^{\hat{H}} = \sum_{\{B\}} \bigotimes_i B_i$
- Finite number of blocks
- Encoded by 1 tensor

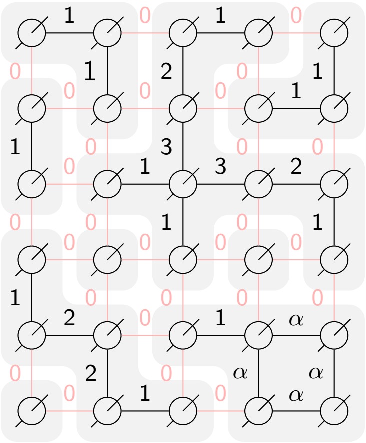
$O^{abcd} =$



(6)

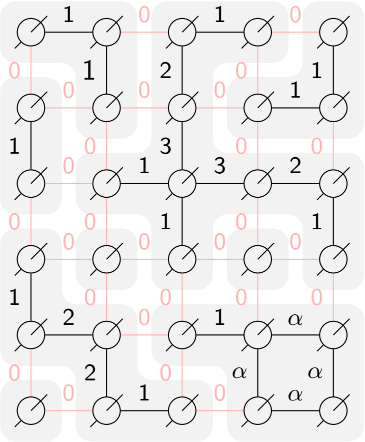
Cluser Exapansions





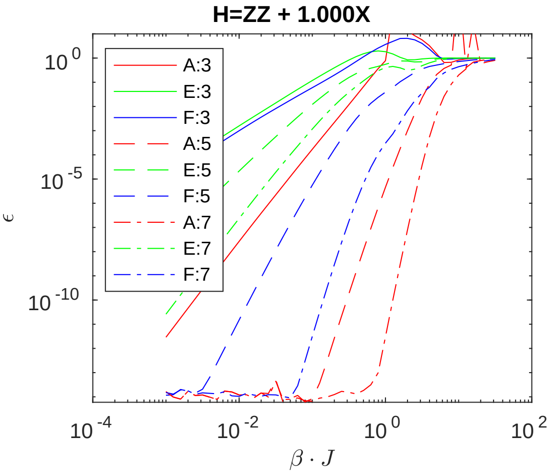
Cluser Exapansions

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

Conclusion

- Large β-steps
- Real time evolution
- Encoding
- Truncation χ

2D TFI: Introduction

- Phase Transition
- Criticality
- Data collapse
  - Observables: m, S and ξ
  - Parameters: T_c, exponents
- $\Gamma = 2.5$
- VUMPS

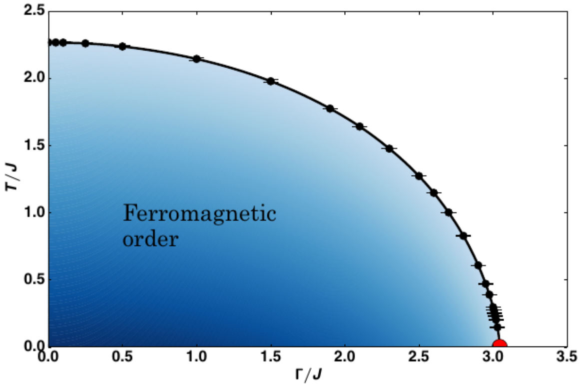
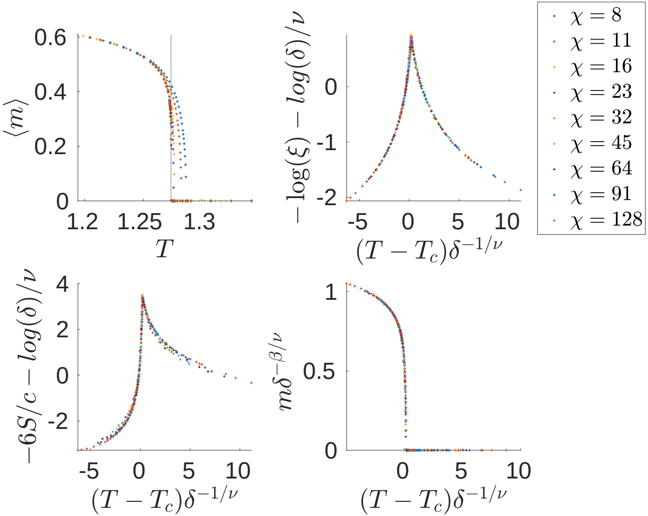


Figure taken from [2]

TFI Phase Diagram: $\Gamma = 2.5$



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

Data from [3]

Conclusion and Outlook

References I

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

Introduction

Cluster Expansions

Results

Conclusion and Outlook

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.

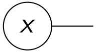
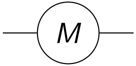
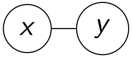
Tensor Networks

Tensor Networks: Introduction

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

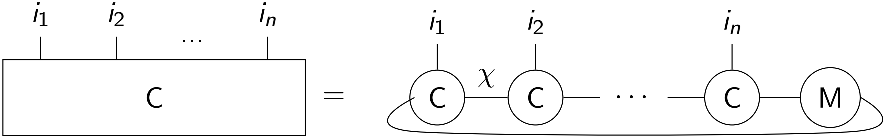
$$C^{i_1 i_2 \cdots i_n} = Tr(C^{i_1} C^{i_2} \cdots C^{i_n} M). \tag{7}$$

Tensor Networks: Graphical Notation

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

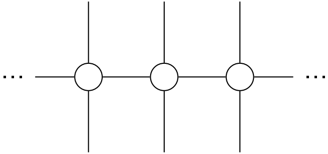
Tensor Networks: MPS

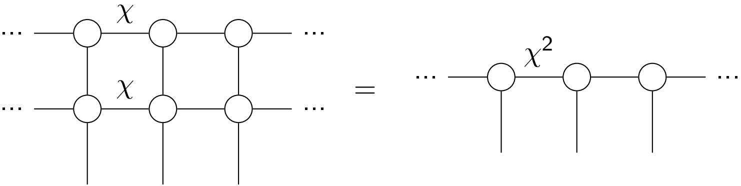
$$C^{i_1 i_2 \cdots i_n} = Tr(C^{i_1} C^{i_2} \cdots C^{i_n} M) \tag{8}$$



(9)

Tensor Networks: Operators

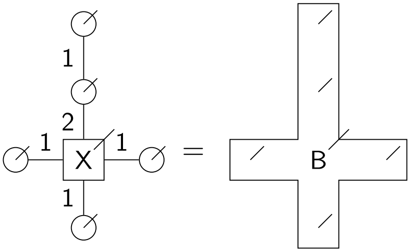
$\hat{O} =$  (10)

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

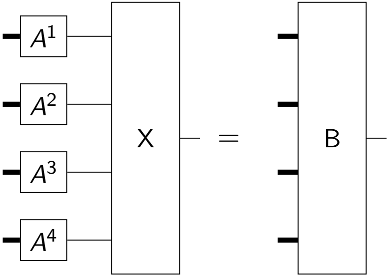
(11)

Linear Solver

Linear Solver: Inversion Scheme



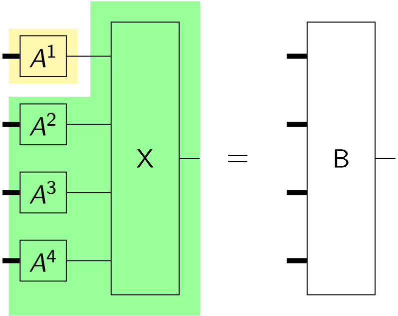
(12)



(13)

Linear Solver: Inversion Scheme

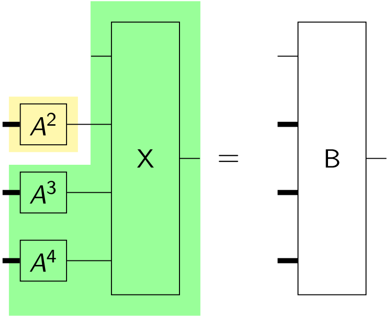
- Invert A^i separately
  - Fast
  - Numerically unstable



(12)

Linear Solver: Inversion Scheme

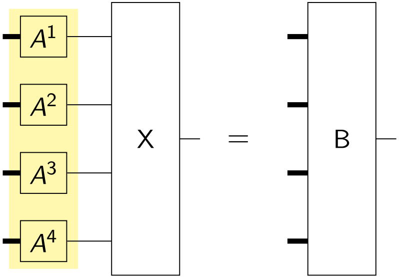
- Invert A^i separately
  - Fast
  - Numerically unstable



(12)

Linear Solver: Inversion Scheme

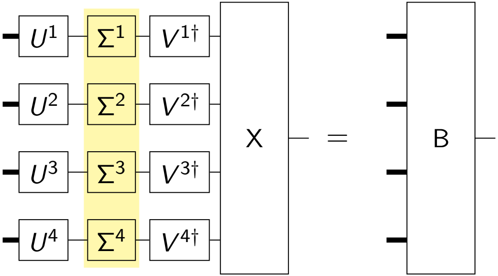
- Invert A^i separately
- Full inversion
  - Slow
  - Stable for pseudoinverse



(12)

Linear Solver: Inversion Scheme

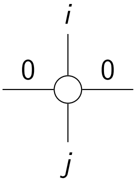
- Invert A^i separately
- Full inversion
- Sparse full inversion
  - $A^i = U^i \Sigma^i V^{i\dagger}$



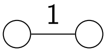
(12)

Construction

Notation

$O^{00} =$ 

$=$  (13)

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

(14)

General idea

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

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

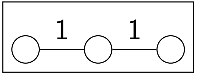
General idea

$$
\begin{aligned}
\bigcirc \overset{1}{\text{——}} \bigcirc \overset{1}{\text{——}} \bigcirc = \exp -\beta H(\bigcirc \text{——} \bigcirc \text{——} \bigcirc) \\
- \bigcirc \overset{0}{\text{——}} \bigcirc \overset{0}{\text{——}} \bigcirc \\
- \bigcirc \overset{1}{\text{——}} \bigcirc \overset{0}{\text{——}} \bigcirc \\
- \bigcirc \overset{0}{\text{——}} \bigcirc \overset{1}{\text{——}} \bigcirc
\end{aligned}
\tag{17}
$$

General idea

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

General idea



(17)

1D: Variant A

$$\bigcirc \tag{18a}$$

$$\bigcirc \overset{1}{\text{——}} \bigcirc \tag{18b}$$

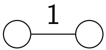
$$\bigcirc \overset{1}{\text{——}} \bigcirc \overset{1}{\text{——}} \bigcirc \tag{18c}$$

$$\bigcirc \overset{1}{\text{——}} \bigcirc \overset{2}{\text{——}} \bigcirc \overset{1}{\text{——}} \bigcirc \tag{18d}$$

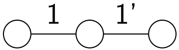
$$\bigcirc \overset{1}{\text{——}} \bigcirc \overset{2}{\text{——}} \bigcirc \overset{2}{\text{——}} \bigcirc \overset{1}{\text{——}} \bigcirc\,. \tag{18e}$$

1D: Variant E

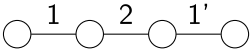
(19a)



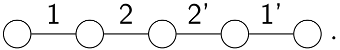
(19b)



(19c)



(19d)



(19e)

1D: Variant F

$$\bigcirc \tag{20a}$$

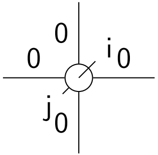
$$\bigcirc\overset{1'}{\text{———}}\bigcirc + \bigcirc\overset{1}{\text{———}}\bigcirc \tag{20b}$$

$$\bigcirc\overset{1}{\text{———}}\bigcirc\overset{1}{\text{———}}\bigcirc \tag{20c}$$

$$\begin{aligned}&\bigcirc\overset{1}{\text{———}}\bigcirc\overset{2}{\text{———}}\bigcirc\overset{1}{\text{———}}\bigcirc +\\ &\bigcirc\overset{1}{\text{———}}\bigcirc\overset{2'}{\text{———}}\bigcirc\overset{1}{\text{———}}\bigcirc\end{aligned} \tag{20d}$$

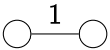
$$\bigcirc\overset{1}{\text{———}}\bigcirc\overset{2}{\text{———}}\bigcirc\overset{2}{\text{———}}\bigcirc\overset{1}{\text{———}}\bigcirc\,. \tag{20e}$$

$$O^{0000} =$$

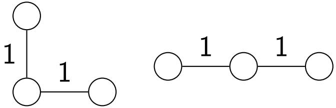


$$= \bigcirc \qquad (21)$$

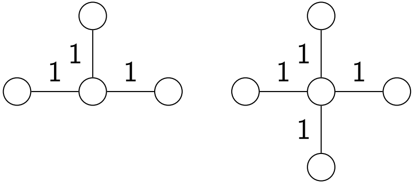
2D: Linear Blocks



(22a)

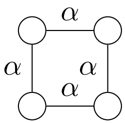


(22b)

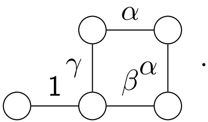


(22c)

2D: Nonlinear Blocks



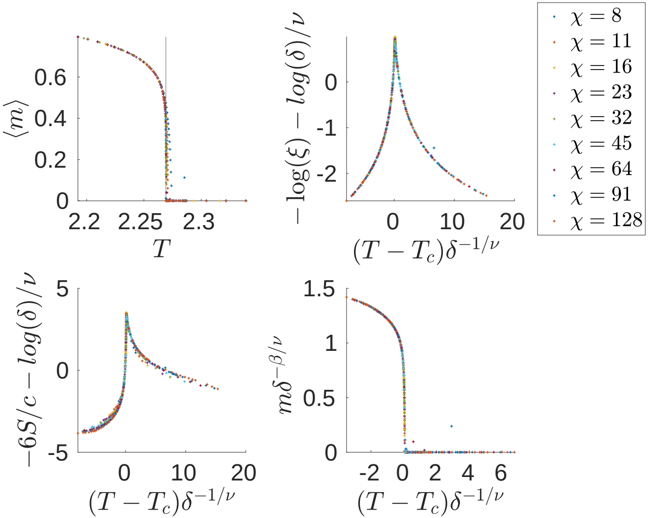
(23)



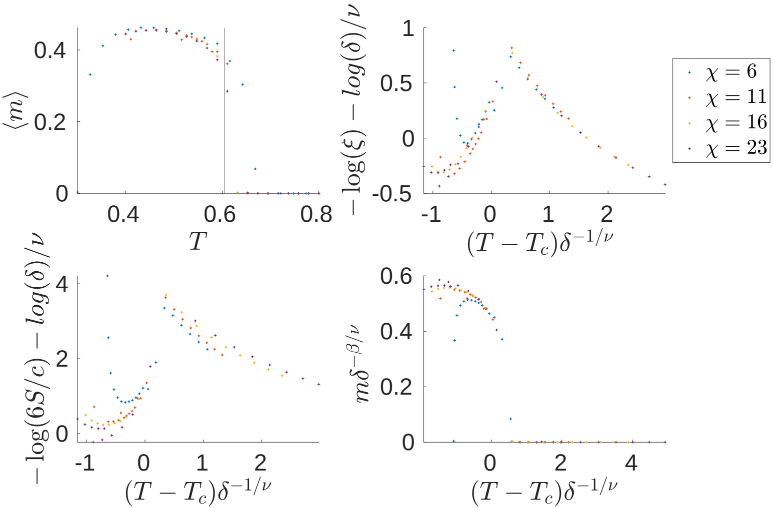
(24)

TFI Collapses

TFI Phase Diagram: Classical Ising

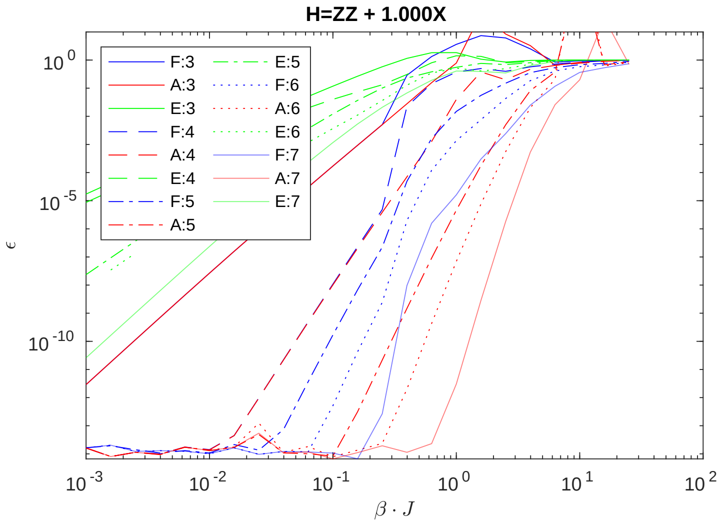


	T_c
Fit	2.691(9)
Exact	2.691853

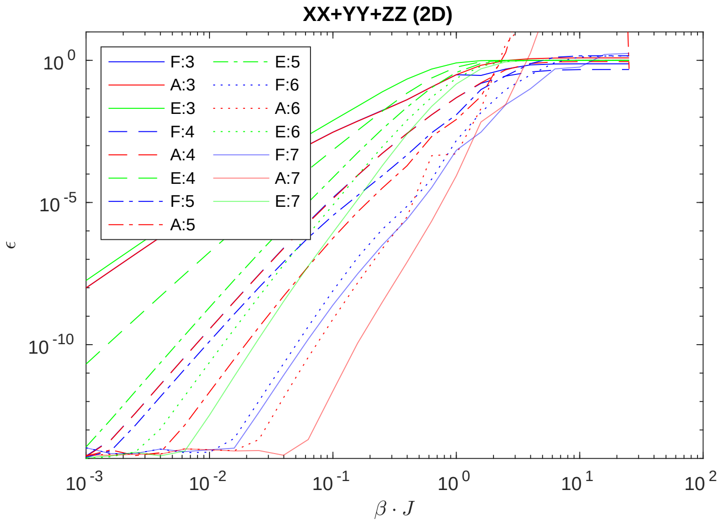

$\langle m \rangle$
0.4
0.2
0
0.4
0.6
0.8
T
$-\log(\xi) - \log(\delta)/\nu$
1
0.5
0
-0.5
-1
0
1
2
$(T - T_c)\delta^{-1/\nu}$
$\chi = 6$
$\chi = 11$
$\chi = 16$
$\chi = 23$
$-\log(6S/c) - \log(\delta)/\nu$
4
2
0
-1
0
1
2
$(T - T_c)\delta^{-1/\nu}$
$m\delta^{-\beta/\nu}$
0.6
0.4
0.2
0
0
2
4
$(T - T_c)\delta^{-1/\nu}$

Direct Results

1D: Transverse Field Ising (TFI): full

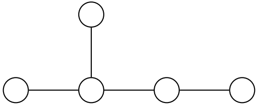


1D: Heisenberg XXX

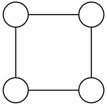


2D: Encodings + Error Measure

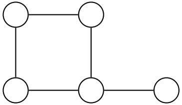
- Relative error ϵ more challenging
- Encodings based on A (order 5)
  - No loops



  - +Plaquette

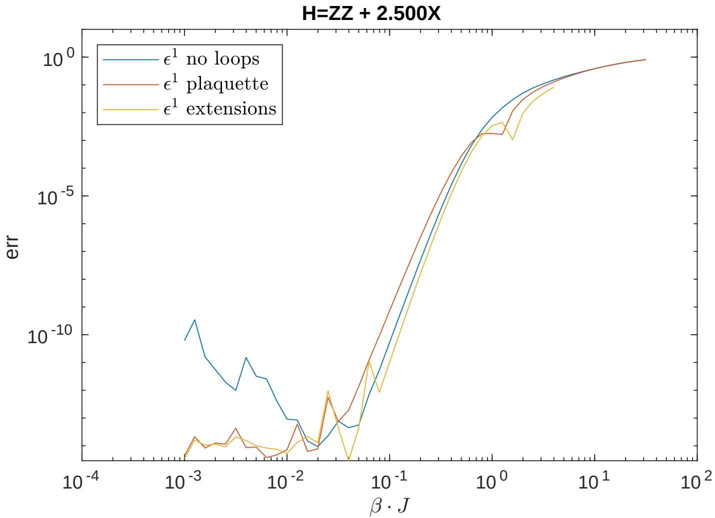


  - +Extensions



	χ
no loops	21
plaquette	27
extensions	43

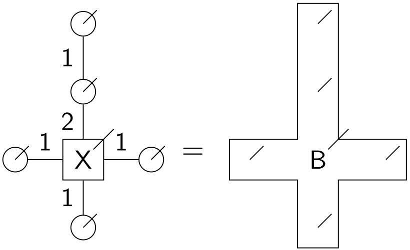
2D: Transverse Field Ising



Solvers

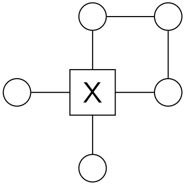
Linear solver

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

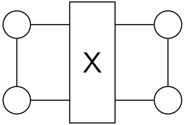


(25)

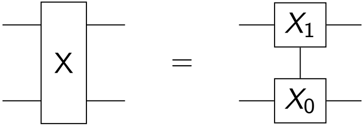
Linear Solver: Applicability



(26)



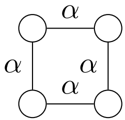
(27a)



(27b)

Nonlinear Solver

- Nonlinear least squares
- Jacobian
- Permutations



(28)

Sequential Linear Solver

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