Introduction
Cluster Expansions
Results
Conclusion

# Cluster Expansions of Thermal States using Tensor Networks

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- Cluster Expansions
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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

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- 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

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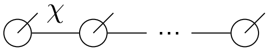
- Equations are known
- Curse of dimensionality
- Numerical methods

# Tensor Networks

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

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

$=$ 


- Matrix Product State
- Relevant corner Hilbert space

# Operator Exponential

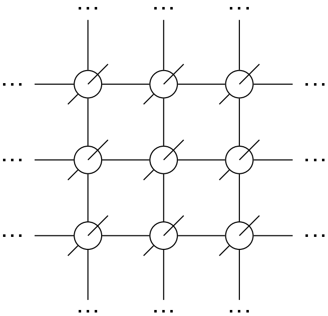
- Time evolution:

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

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

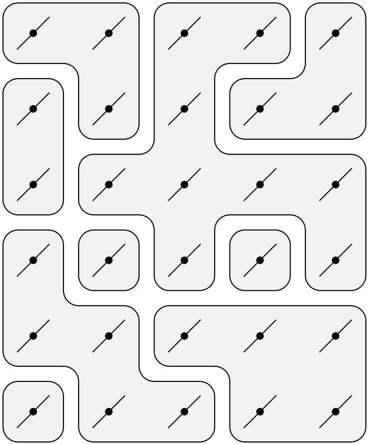
- Statistical ensembles:

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



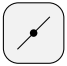
# Cluster Expansions

# Cluster Expansions



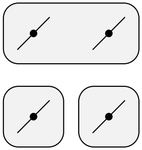
- $e^{-\beta \hat{H}} = \sum_{\{B\}} \bigotimes_i B_i$

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



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

$+$



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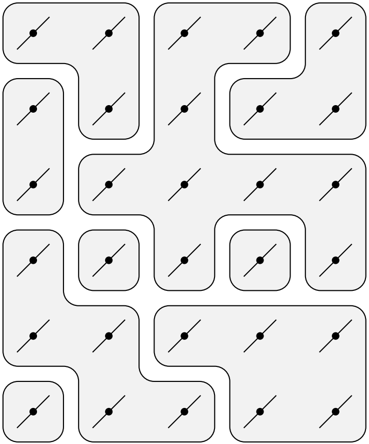
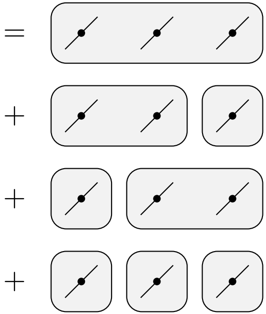
# Cluster Expansions



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

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



# Cluster Expansions

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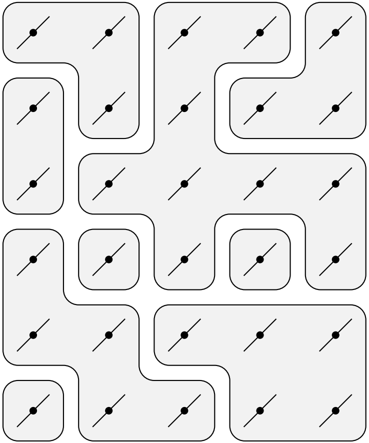
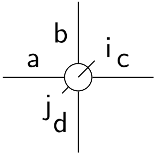


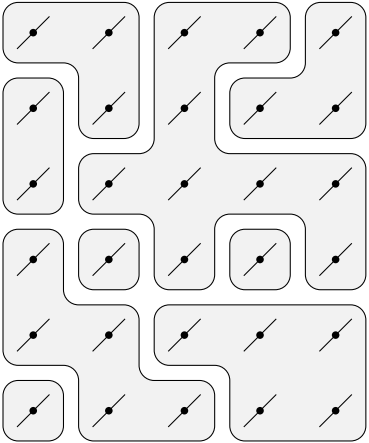
- $e^{-\beta \hat{H}} = \sum_{\{B\}} \bigotimes_i B_i$
- Finite number of blocks: trucate order
- Encoded by 1 tensor

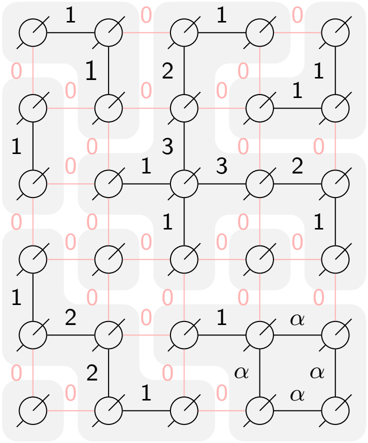
$O^{abcd} =$



# Cluster Expansions







# Cluster Expansions

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Cluster Expansions

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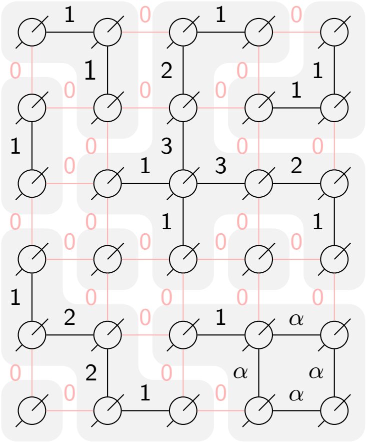
- Multiple choices for encoding
- Size extensive
- Preserves global and internal symmetries
- Tensor Network toolbox



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1D Exact

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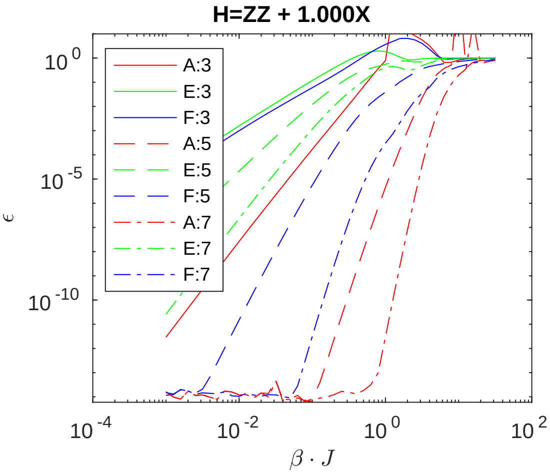
# Results

# 1D: Transverse Field Ising (TFI)




- Relative error $\epsilon$
- 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

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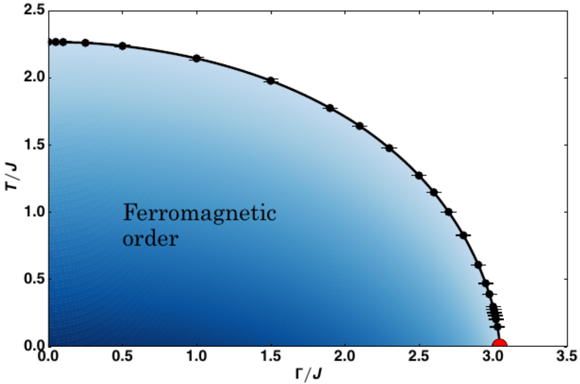
- 2D: similar results
- Real time evolution
- Encoding

# 2D TFI: Introduction

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

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

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# Criticality

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- Phase transition
- Power law
- Finite size scaling $(\chi,\delta^{-1})$
- Data collapse
  - Observables: $m$, $S$ and $\xi$
  - Parameters: $T_c$

# TFI Phase Diagram: $\Gamma = 2.5$

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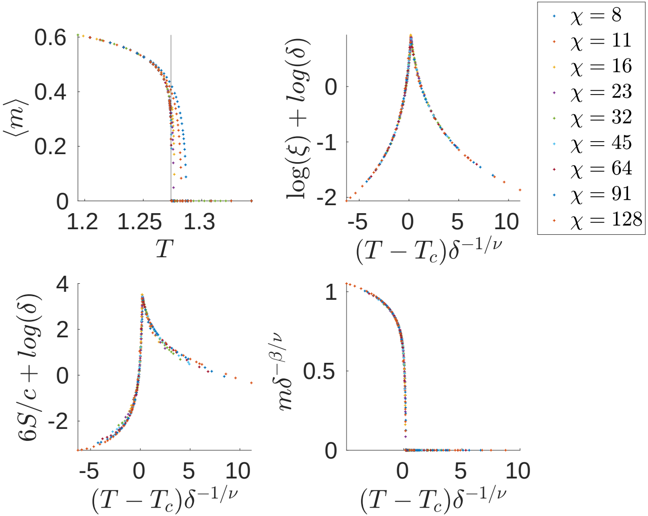


| | $T_c$ |
|---|---|
| Fit | 1.2736(6) |
| QMC | 1.2737(6) |
| TN | 1.2737(2) |

Data from [1]

# Conclusion

# Conclusion

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- 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.

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# Tensor Networks

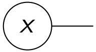
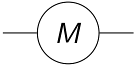
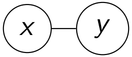
# Tensor Networks: Introduction

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

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

# Tensor Networks: Graphical Notation



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

# Tensor Networks: MPS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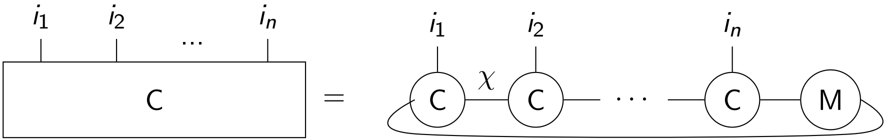
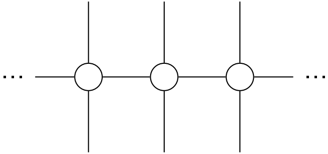
$$C^{i_1 i_2 \cdots i_n} = Tr(C^{i_1} C^{i_2} \cdots C^{i_n} M) \tag{9}$$

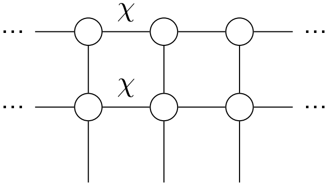


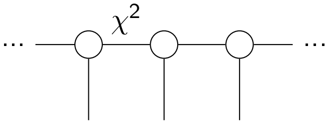

(10)

# Tensor Networks: Operators



$\hat{O} =$  (11)

$\hat{O} \left|\Psi\right\rangle =$ 

$=$ 

(12)

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# Linear Solver

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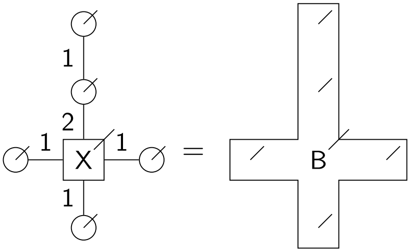
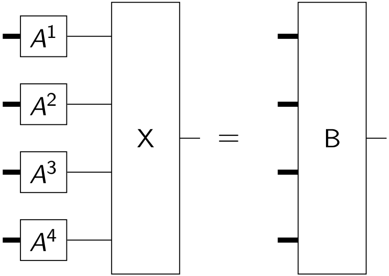
# Linear Solver: Inversion Scheme




(13)




(14)

## Linear Solver: Inversion Scheme

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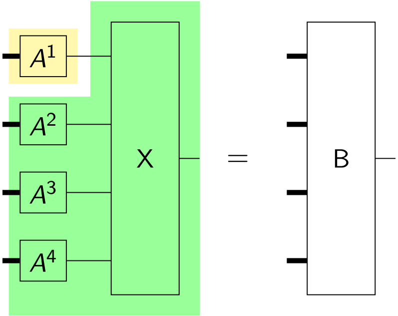
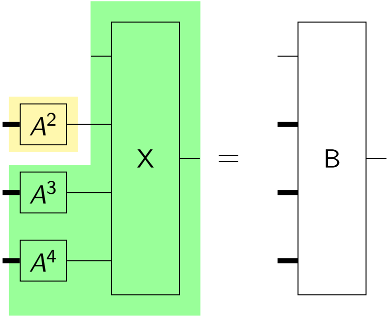
- Invert $A^i$ separately
  - Fast
  - Numerically unstable




(13)

# Linear Solver: Inversion Scheme

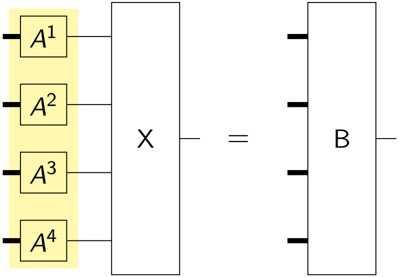
- Invert $A^i$ separately
  - Fast
  - Numerically unstable




(13)

# Linear Solver: Inversion Scheme

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

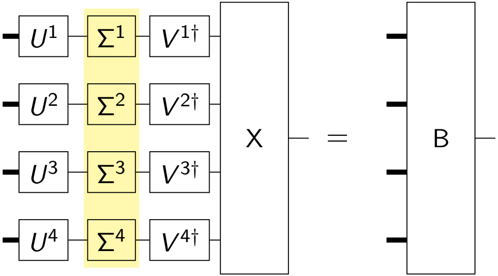



(13)

# Linear Solver: Inversion Scheme



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

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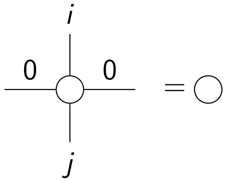
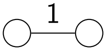
# Construction

# Notation

$O^{00} =$  (14)



$O^{01}O^{10} =$  (15)

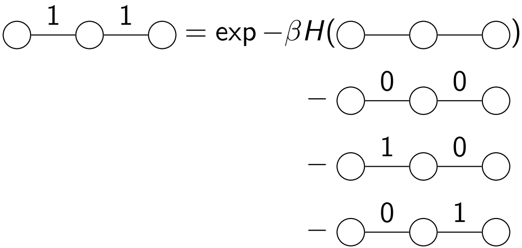
# General idea

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

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

# General idea



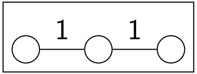



(18)

# General idea

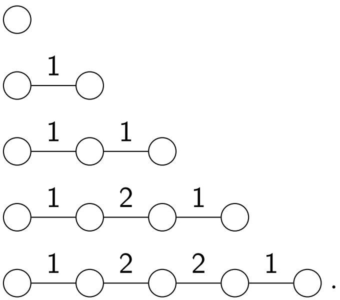
$$\bigcirc \overset{1}{\text{——}} \bigcirc \overset{1}{\text{——}} \bigcirc = \exp -\beta H(\bigcirc\text{——}\bigcirc\text{——}\bigcirc) - \bigcirc\text{——}\bigcirc\text{——}\bigcirc \tag{18}$$

# General idea




(18)

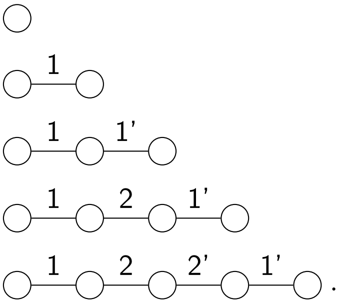
# 1D: Variant A




(19a)
(19b)
(19c)
(19d)
(19e)

# 1D: Variant E






(20a)

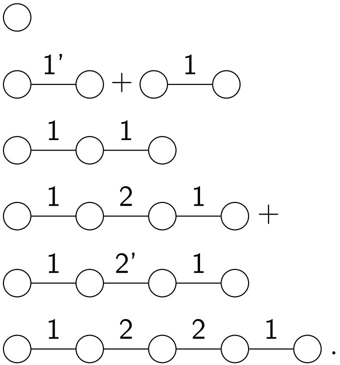
(20b)

(20c)

(20d)

(20e)

# 1D: Variant F




(21a)

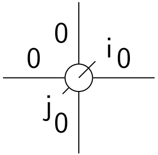
(21b)

(21c)

(21d)

(21e)

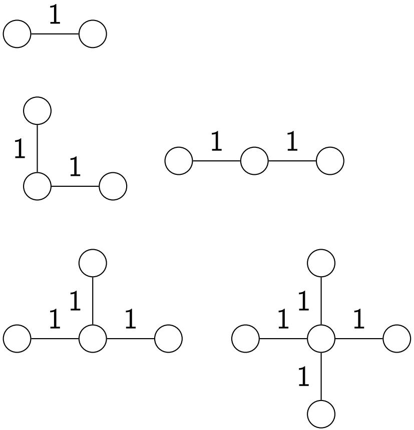
$O^{0000} =$




$$= \bigcirc \tag{22}$$

# 2D: Linear Blocks



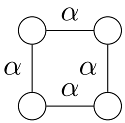



(23a)

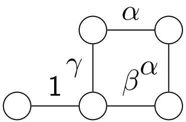
(23b)

(23c)

# 2D: Nonlinear Blocks




(24)

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$g = 0.0$
$g = 2.9$
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# TFI Collapses

# TFI Phase Diagram: Classical Ising

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$g = 2.9$
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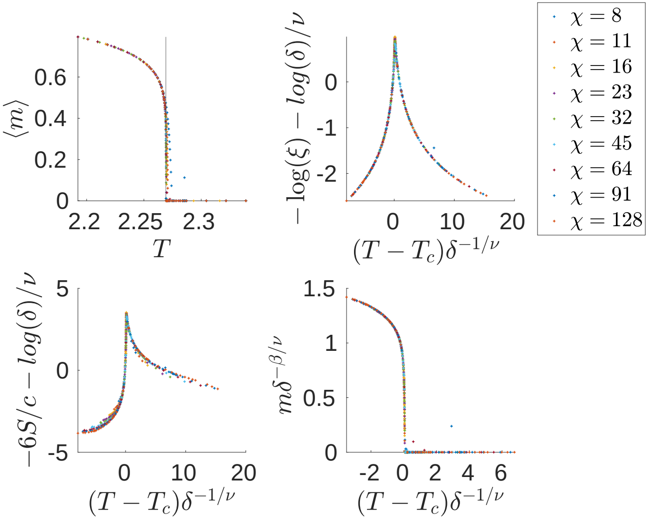
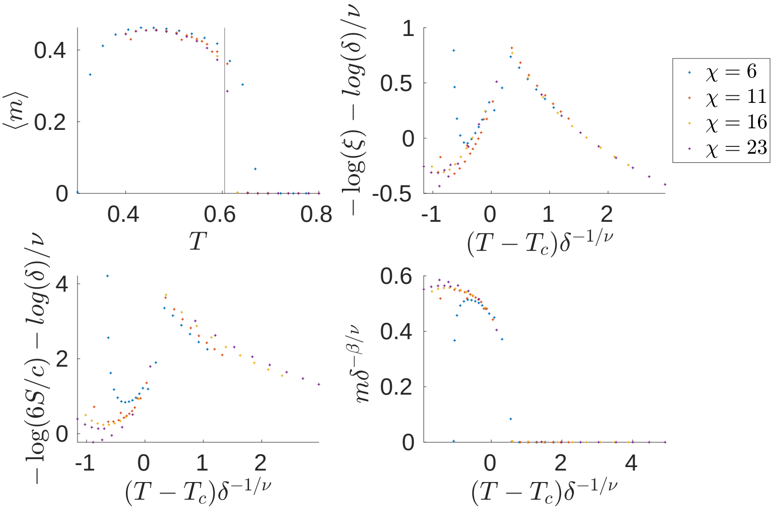



| | $T_c$ |
|---|---|
| Fit | 2.691(9) |
| Exact | 2.691853 |


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

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# Direct Results

# 1D: Transverse Field Ising (TFI): full

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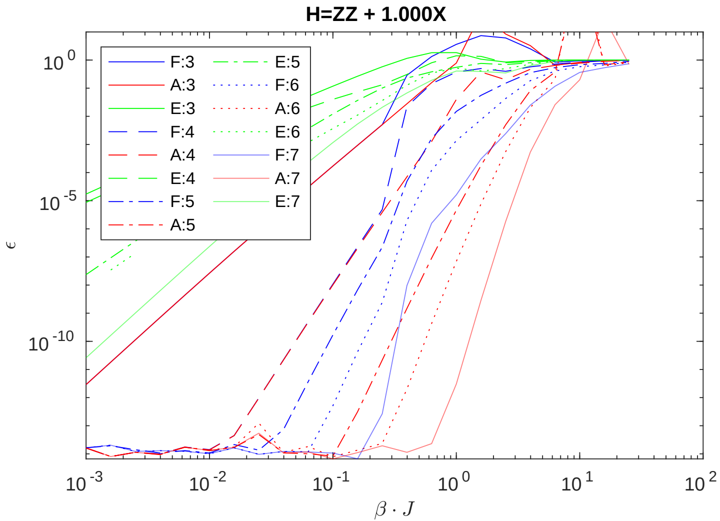

# 1D: Heisenberg XXX


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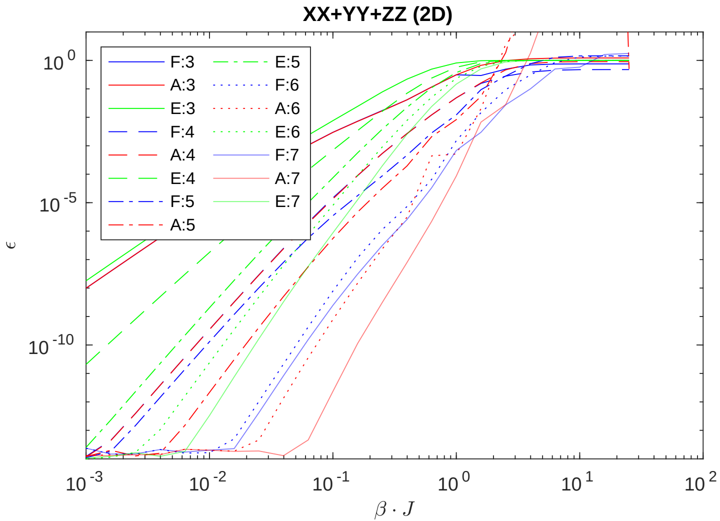

# 2D: Encodings + Error Measure


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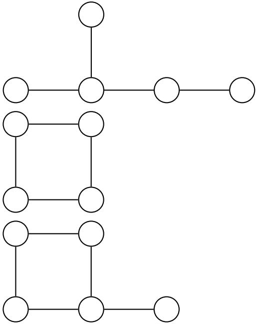
- Relative error $\epsilon$ more challenging
- Encodings based on A (order 5)
  - No loops
  - +Plaquette
  - +Extensions



| | $\chi$ |
|---|---|
| no loops | 21 |
| plaquette | 27 |
| extensions | 43 |

# 2D: Transverse Field Ising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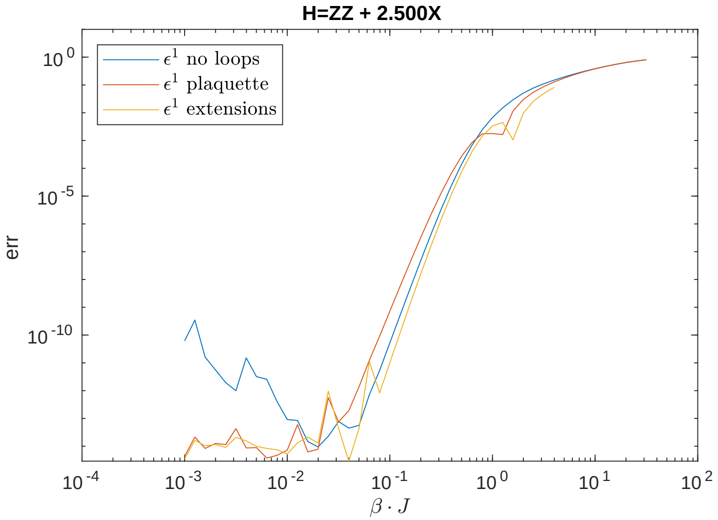

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# Solvers

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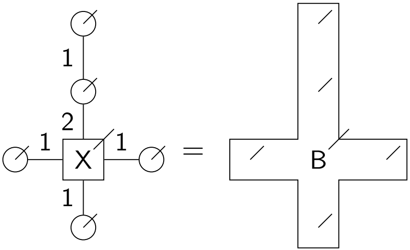
Nonlinear Solver
Sequential Linear Solver

# Linear solver

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




(26)

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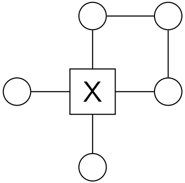
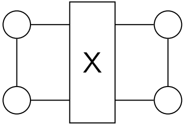
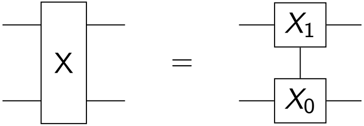
# Linear Solver: Applicability




(27)



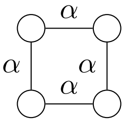

(28a)




(28b)

# Nonlinear Solver

- Nonlinear least squares
- Jacobian
- Permutations




(29)

# Sequential Linear Solver

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