Cluster Expansion of Thermal States using Tensor Networks

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June 20, 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

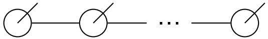
Simulating Quantum Many-body Systems

- Equations are known
- Curse of dimensionality
- Numerical methods
  - Exact diagonalisation
  - (post-) Hartree Fock methods, DFT methods
  - Monte Carlo methods
  - Tensor Networks

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

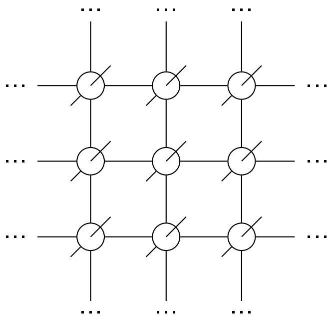
- (Real) Time evolution:

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

- Statistical ensembles:

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

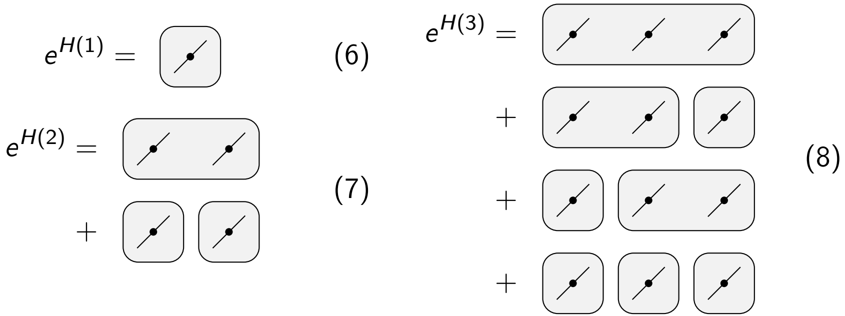
$\hat{O} =$



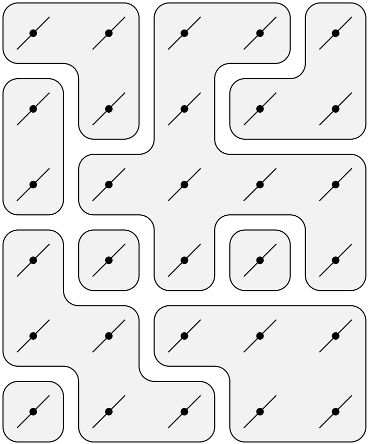
(5)

Cluster Expansion

Cluser Exapansion

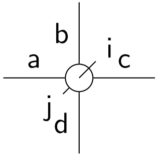


Cluser Exapansion

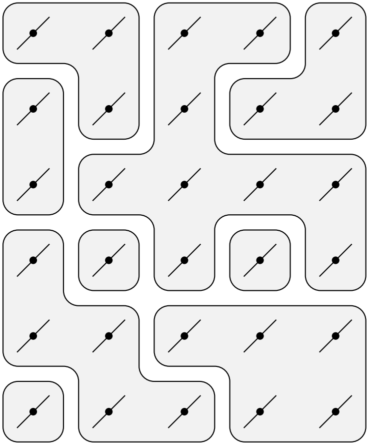


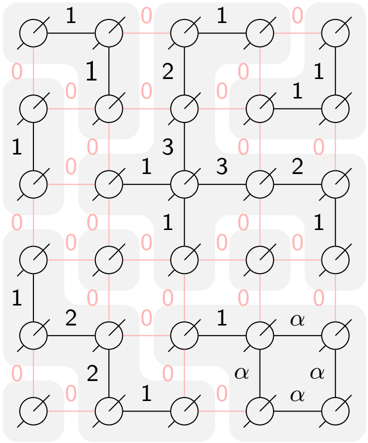
- $e^{\hat{H}} = \sum_{\{B\}} \bigotimes_i B_i$
- Finite number of blocks
- Encoded by 1 tensor

$$O^{abcd} = \quad (6)$$



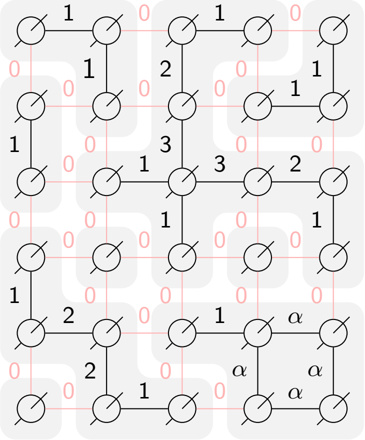
Cluser Exapansion





Cluser Exapansion

- Multiple choices for encoding
- Solvers
  - Linear
  - Nonlinear



Advantages

- Doesn't break symmetry
- Thermodynamic limit
- Tensor Network toolbox

Results

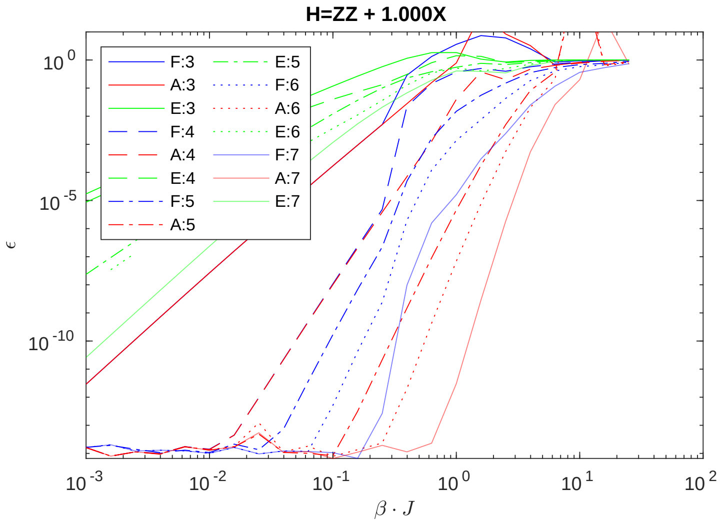
1D: Cluster expansions

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

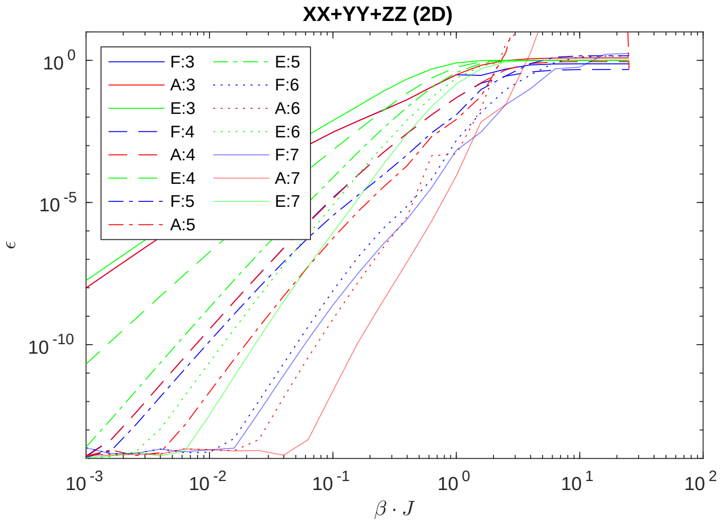
χ

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

1D: Transverse Field Ising

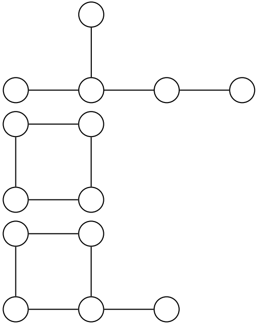


1D: Heisenberg XXX



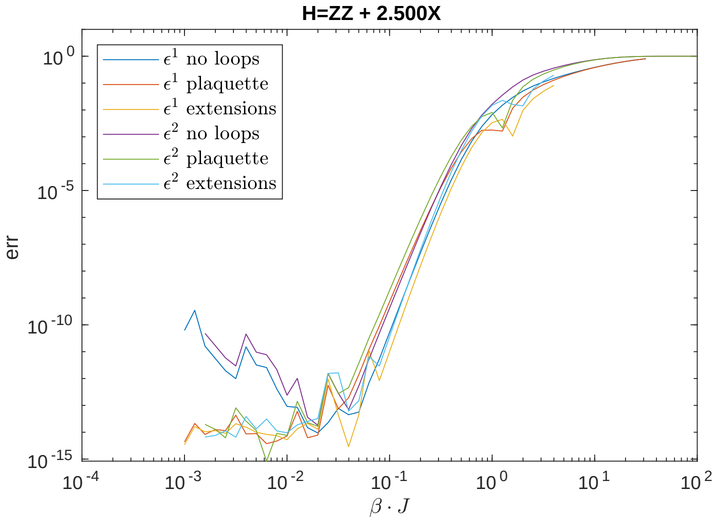
2D: Cluster expansions

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



	χ
no loops	21
loops	27
extensions	43

2D: TFI


H=ZZ + 2.500X
ϵ^1 no loops
ϵ^1 plaquette
ϵ^1 extensions
ϵ^2 no loops
ϵ^2 plaquette
ϵ^2 extensions
err
10^{0}
10^{-5}
10^{-10}
10^{-15}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
$\beta \cdot J$

TFI: Phase Diagram

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

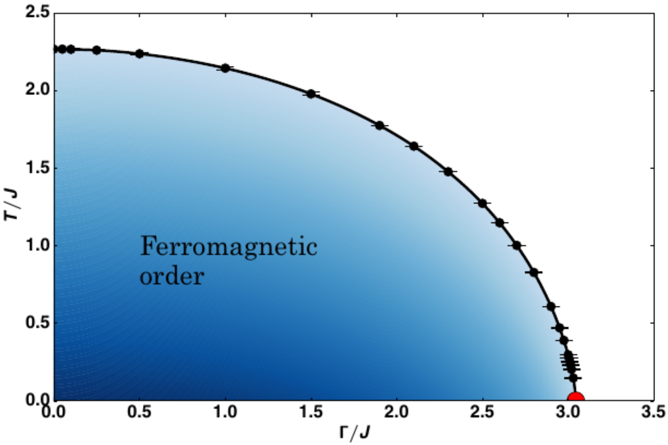
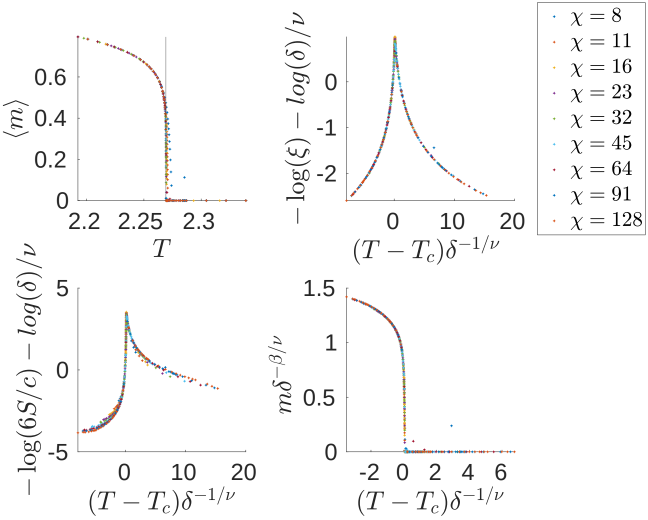


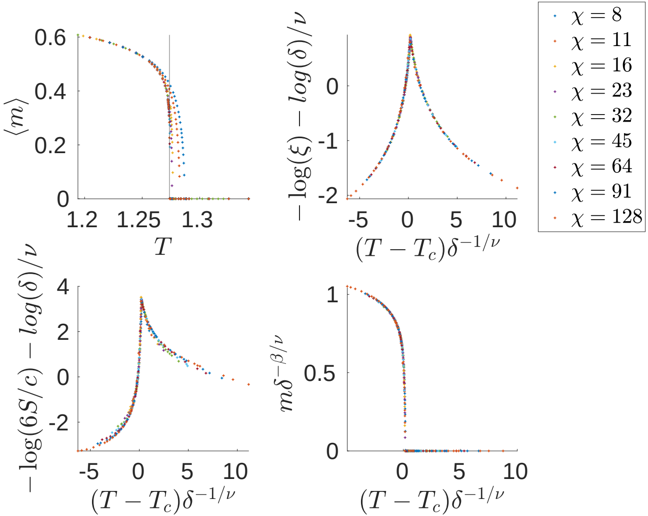
Figure taken from [2]

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

Conclusion

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

Outlook

- 3D?
- Internal symmetries

References I

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arXiv:2010.00584.
URL http://arxiv.org/abs/2010.00584

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- 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.

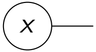
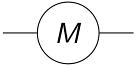
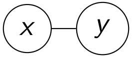
Tensor Networks

Tensor Networks: Introduction

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

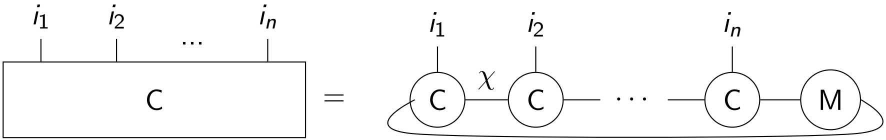
$$C^{i_1 i_2 \cdots i_n} = Tr(C^{i_1} C^{i_2} \cdots C^{i_n} M). \tag{7}$$

Tensor Networks: Graphical Notation

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

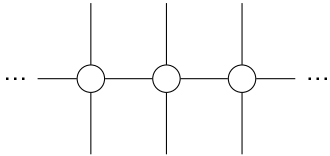
Tensor Networks: MPS

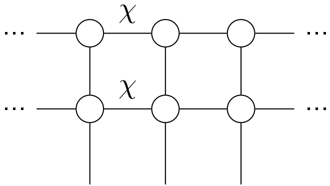
$$C^{i_1 i_2 \cdots i_n} = Tr(C^{i_1} C^{i_2} \cdots C^{i_n} M) \tag{8}$$

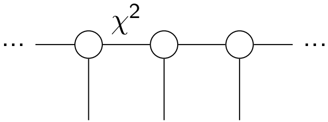


(9)

Tensor Networks: Operators

$\hat{O} =$  (10)

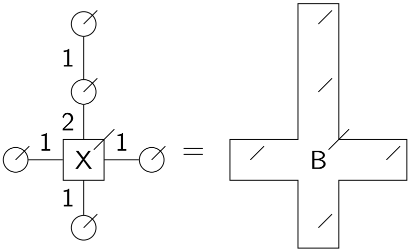
$\hat{O}\,|\Psi\rangle =$ 

$=$ 

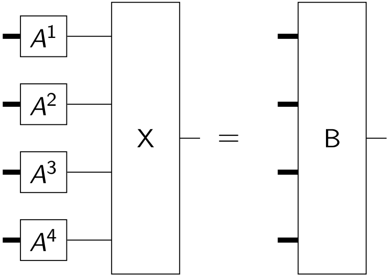
(11)

Linear Solver

Linear Solver: Inversion Scheme



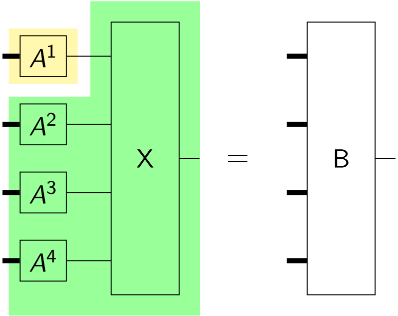
(12)



(13)

Linear Solver: Inversion Scheme

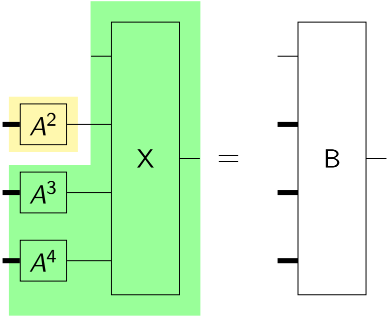
- Invert A^i separately
  - Fast
  - Numerically unstable



(12)

Linear Solver: Inversion Scheme

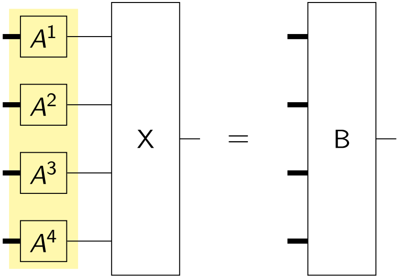
- Invert A^i separately
  - Fast
  - Numerically unstable



(12)

Linear Solver: Inversion Scheme

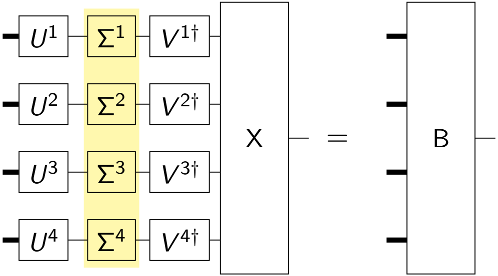
- Invert A^i separately
- Full inversion
  - Slow
  - Stable for pseudoinverse



(12)

Linear Solver: Inversion Scheme

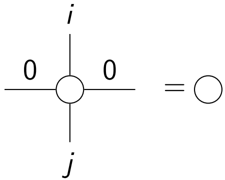
- Invert A^i separately
- Full inversion
- Sparse full inversion
  - $A^i = U^i \Sigma^i V^{i\dagger}$



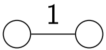
(12)

Construction

Notation

$O^{00} =$ 

(13)

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

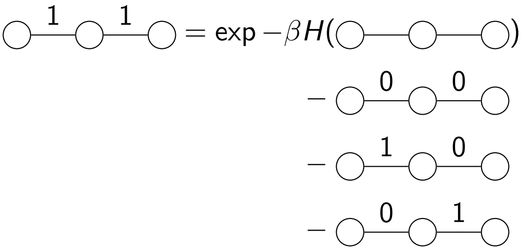
(14)

General idea

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

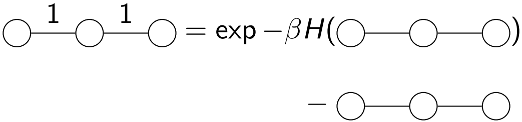
$$\bigcirc\overset{1}{\text{——}}\bigcirc = \exp -\beta H(\bigcirc\text{——}\bigcirc) - \bigcirc\overset{0}{\text{——}}\bigcirc \tag{16}$$

General idea



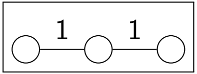
(17)

General idea



(17)

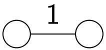
General idea



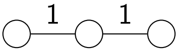
(17)

1D: Variant A

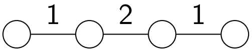
(18a)



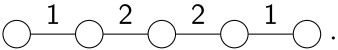
(18b)



(18c)

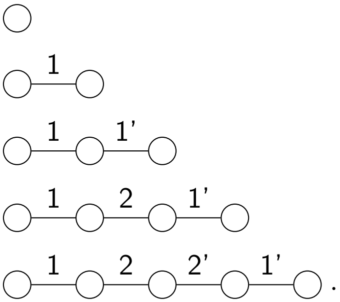


(18d)



(18e)

1D: Variant E



(19a)

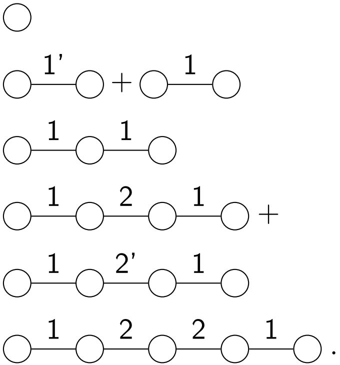
(19b)

(19c)

(19d)

(19e)

1D: Variant F



(20a)

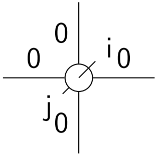
(20b)

(20c)

(20d)

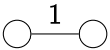
(20e)

$$O^{0000} =$$

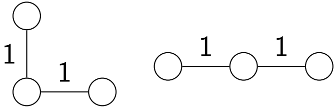


$$= \bigcirc \qquad (21)$$

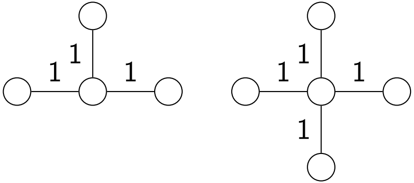
2D: Linear Blocks



(22a)

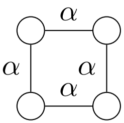


(22b)

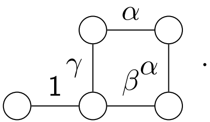


(22c)

2D: Nonlinear Blocks

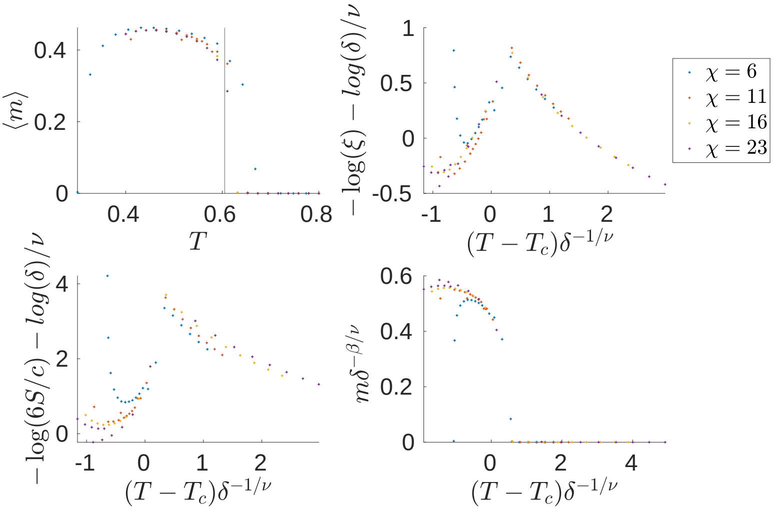


(23)



(24)

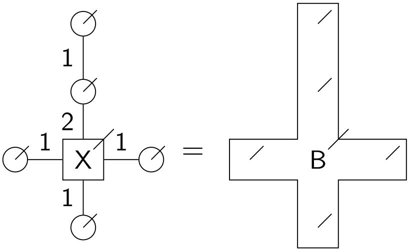
$\Gamma = 2.9$


$\langle m \rangle$
T
$-\log(\xi) - log(\delta)/\nu$
$(T - T_c)\delta^{-1/\nu}$
$\chi = 6$
$\chi = 11$
$\chi = 16$
$\chi = 23$
$-\log(6S/c) - log(\delta)/\nu$
$(T - T_c)\delta^{-1/\nu}$
$m\delta^{-\beta/\nu}$
$(T - T_c)\delta^{-1/\nu}$

Solvers

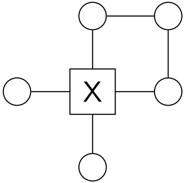
Linear solver

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

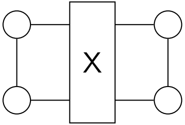


(25)

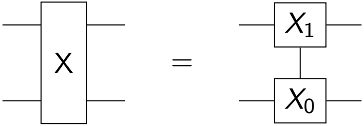
Linear Solver: Applicability



(26)



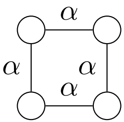
(27a)



(27b)

Nonlinear Solver

- Nonlinear least squares
- Jacobian
- Permutations



(28)

Sequential Linear Solver

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