Cluster Expansion 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

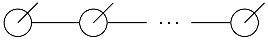
Simulating Quantum Many-body Systems

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

Tensor Networks

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

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



- MPS
- Relevant corner Hilbert space

Operator exponential

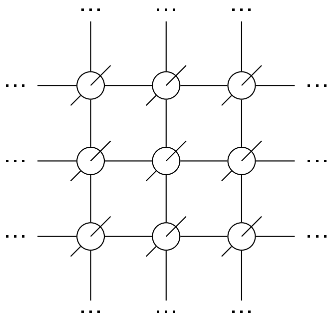
- (Real) Time evolution:

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

- Statistical ensembles:

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

$\hat{O} =$



(5)

Cluster Expansion

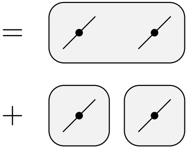
Cluser Exapansion

$$e^{\hat{H}} = \sum_{\{B\}} \bigotimes_i B_i \tag{6}$$

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

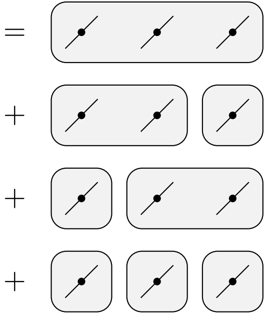
(7)

$$e^{H(2)} =$$



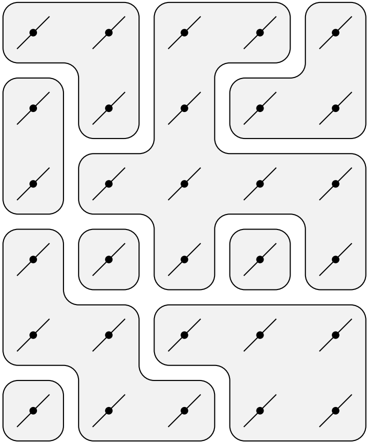
(8)

$$e^{H(3)} =$$



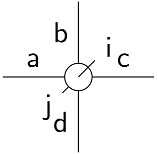
(9)

Cluser Exapansion

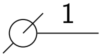


- Finite number of blocks
- Encoded by 1 tensor

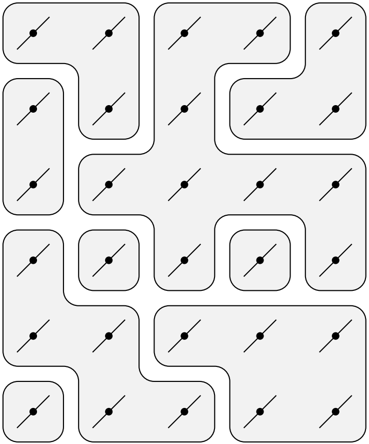
$$O^{abcd} = \quad \text{(6)}$$

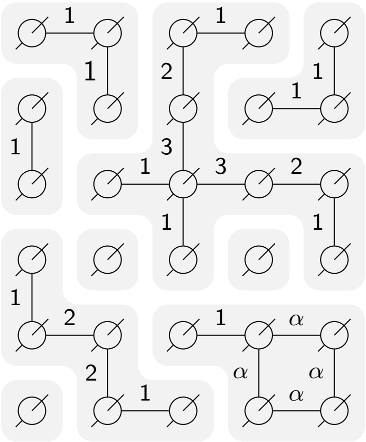


$$O^{0010} = \quad \text{(7)}$$



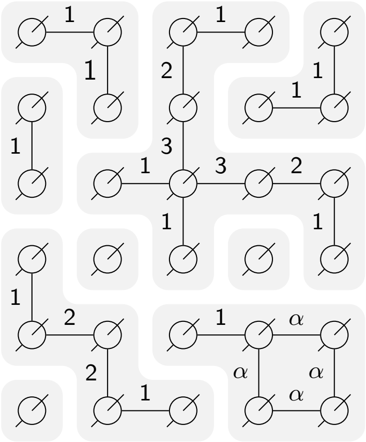
Cluser Exapansion





Cluser Exapansion

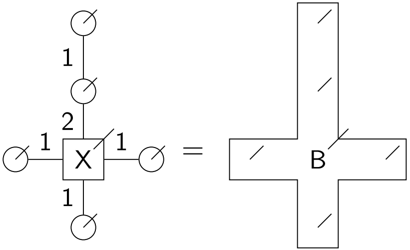
- Multiple choices for encoding
- Doesn't break symmetry
- Thermodynamic limit
- Tensor Network toolbox



Solvers

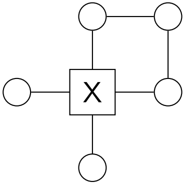
Linear solver

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

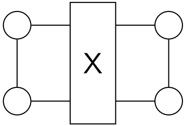


(6)

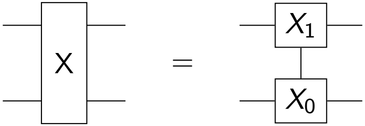
Linear Solver: Applicability



(7)



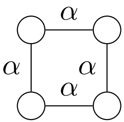
(8a)



(8b)

Nonlinear Solver

- Nonlinear least squares
- Jacobian
- Permutations



(9)

Sequential Linear Solver

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

Results

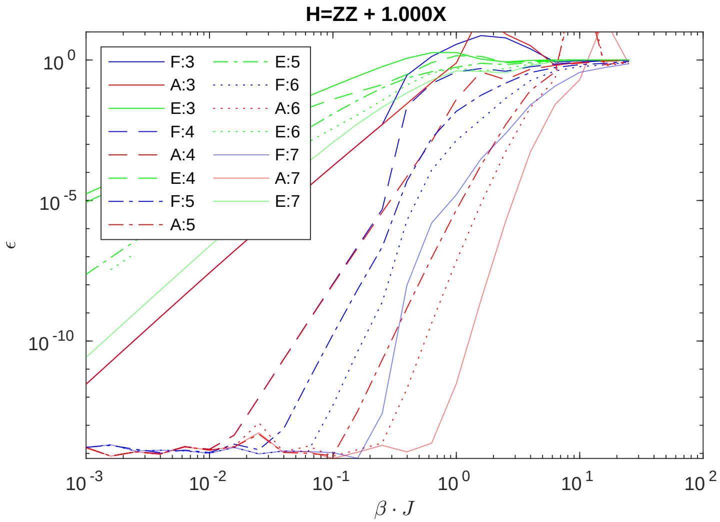
1D: Cluster expansions

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

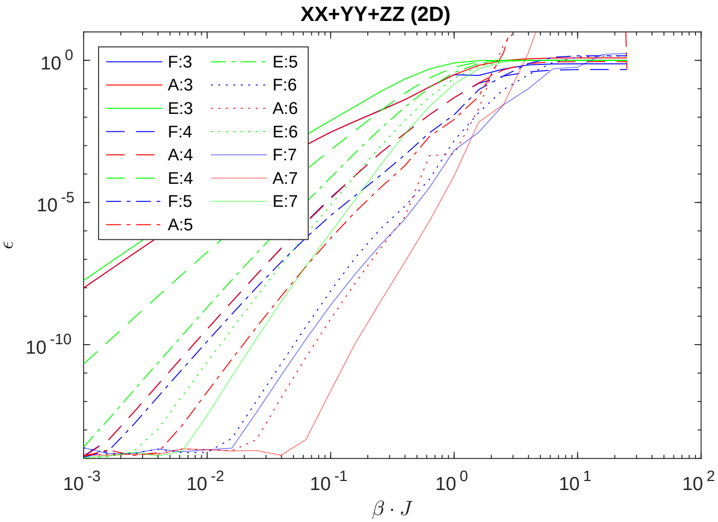
χ

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

1D: Transverse Field Ising

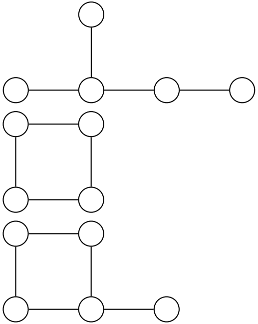


1D: Heisenberg XXX



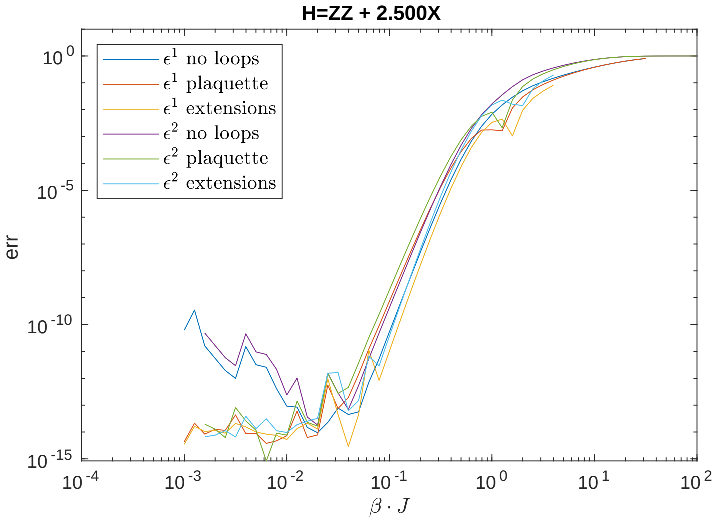
2D: Cluster expansions

- 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 $\Gamma = 2.5$

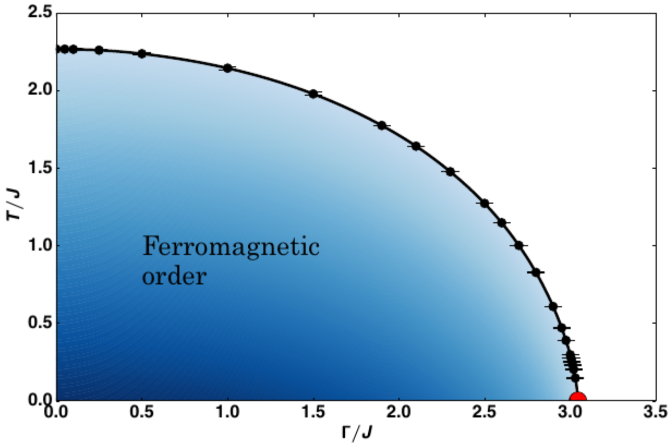
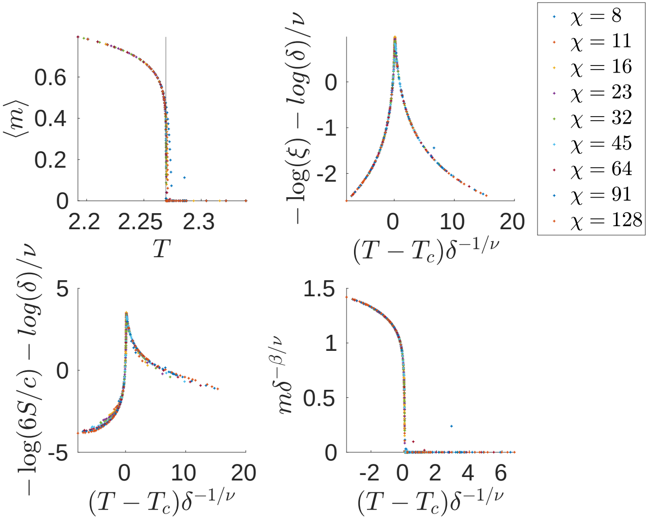


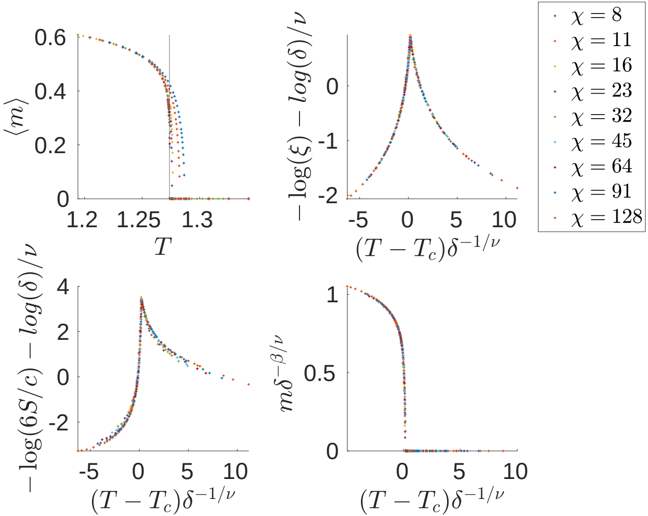
Figure taken from [2]

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

Introduction
Cluster Expansion
Solvers
Results
Conclusion and Outlook

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.
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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.

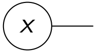
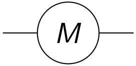
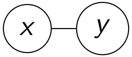
Tensor Networks

Tensor Networks: Introduction

$$|\Psi\rangle = \sum_{i_1 i_2 \cdots i_n} C^{i_1 i_2 \cdots i_n} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle . \tag{10}$$

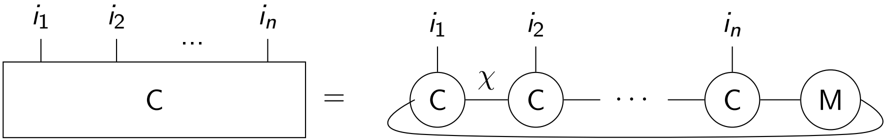
$$C^{i_1 i_2 \cdots i_n} = Tr(C^{i_1} C^{i_2} \cdots C^{i_n} M). \tag{11}$$

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

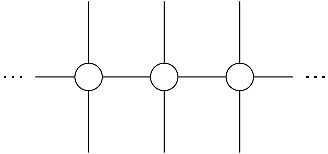
$$C^{i_1 i_2 \cdots i_n} = Tr(C^{i_1} C^{i_2} \cdots C^{i_n} M) \tag{12}$$



(13)

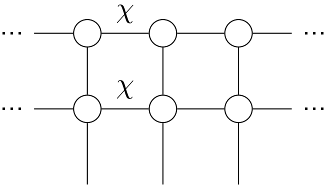
Tensor Networks: Operators

$\hat{O} =$

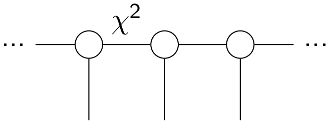


(14)

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



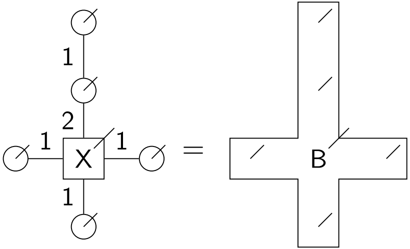
$=$



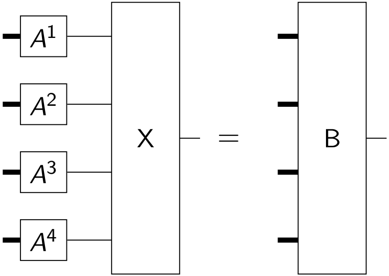
(15)

Linear Solver

Linear Solver: Inversion Scheme



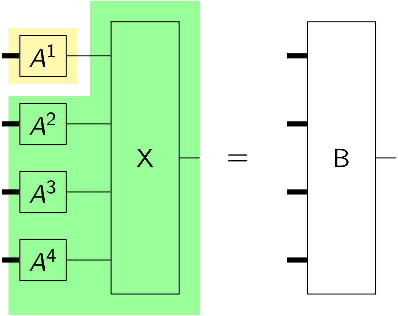
(16)



(17)

Linear Solver: Inversion Scheme

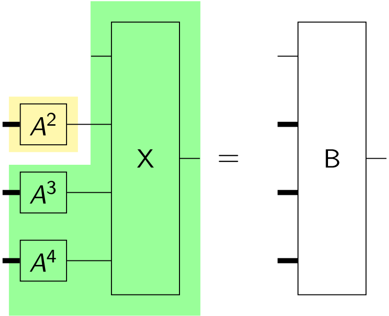
- Invert A^i separately
  - Fast
  - Numerically unstable



(16)

Linear Solver: Inversion Scheme

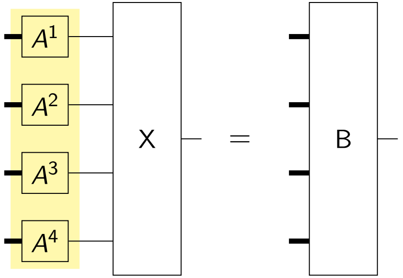
- Invert A^i separately
  - Fast
  - Numerically unstable



(16)

Linear Solver: Inversion Scheme

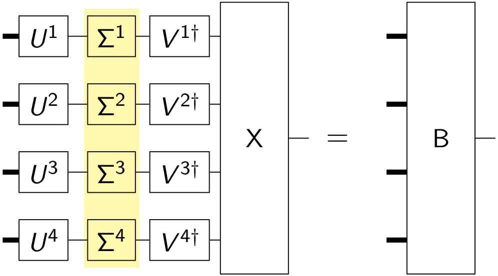
- Invert A^i separately
- Full inversion
  - Slow
  - Stable for pseudoinverse



(16)

Linear Solver: Inversion Scheme

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

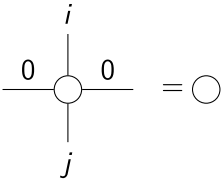


(16)

Construction

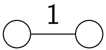
Notation

$$O^{00} =$$



(17)

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



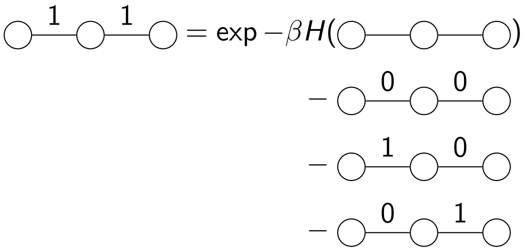
(18)

General idea

$$\bigcirc = \exp\left(-\beta H(\bigcirc)\right) \tag{19}$$

$$\begin{aligned} \bigcirc\overset{1}{\text{——}}\bigcirc &= \exp -\beta H(\bigcirc\text{——}\bigcirc) \\ &\quad -\bigcirc\overset{0}{\text{——}}\bigcirc \end{aligned} \tag{20}$$

General idea

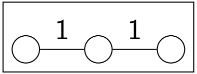


(21)

General idea

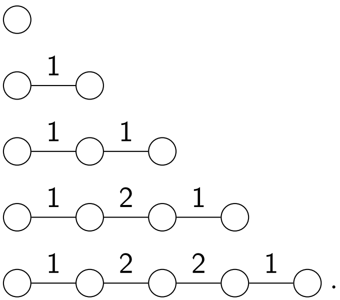
$$\bigcirc \overset{1}{\text{—}} \bigcirc \overset{1}{\text{—}} \bigcirc = \exp -\beta H(\bigcirc \text{—} \bigcirc \text{—} \bigcirc) - \bigcirc \text{—} \bigcirc \text{—} \bigcirc \tag{21}$$

General idea



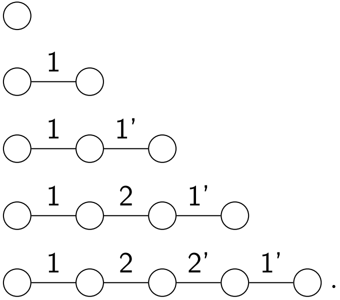
(21)

1D: Variant A



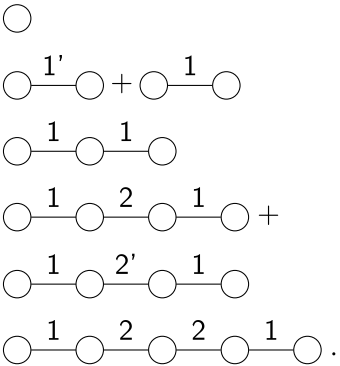
(22a)
(22b)
(22c)
(22d)
(22e)

1D: Variant E



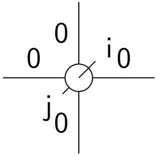
(23a)
(23b)
(23c)
(23d)
(23e)

1D: Variant F



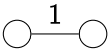
(24a)
(24b)
(24c)
(24d)
(24e)

$O^{0000} =$

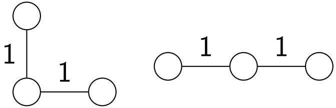


$= \bigcirc$ (25)

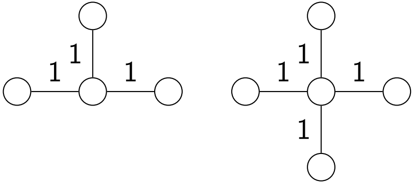
2D: Linear Blocks



(26a)

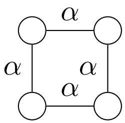


(26b)



(26c)

2D: Nonlinear Blocks



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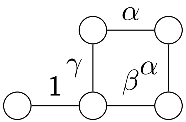

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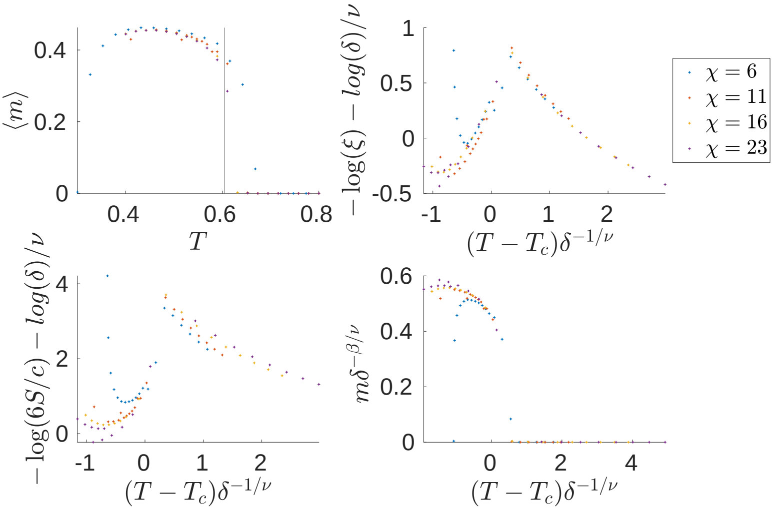
(28)

$\Gamma = 2.9$


$\langle m \rangle$
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
$(T - T_c)\delta^{-1/\nu}$