Cluster Expansion of Thermal States using Tensor Networks

David Devoogdt

Faculty of Engineering and Architecture
Ghent University

June 19, 2021

Introduction

- Overview condensed matter physics

Introduction

- Overview condensed matter physics
- Strongly correlated materials [1]
  - Superconductors
  - Quantum spin liquids
  - Strange metals
  - Quantum Criticality
  - Correlated topological matter

Introduction

- Overview condensed matter physics
- Strongly correlated materials
- How to proceed
  - Material synthesis and discovery
  - Numerical methods
  - Analytical methods

Simulating Quantum Many-body Systems

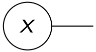
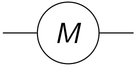
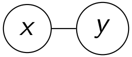
- Equations are known
- Curse of dimensionality
- Tensor networks

Tensor Networks: Introduction

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

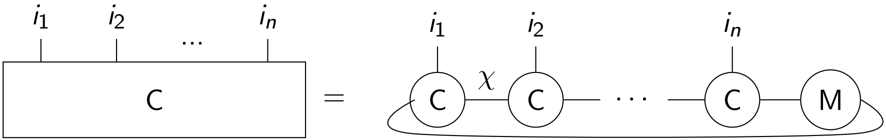
$$C^{i_1 i_2 \cdots i_n} = Tr(C^{i_1} C^{i_2} \cdots C^{i_n} M). \tag{2}$$

Tensor Networks: Graphical Notation

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

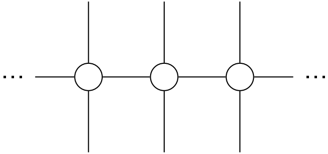
Tensor Networks: MPS

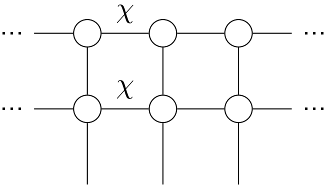
$$C^{i_1 i_2 \cdots i_n} = Tr(C^{i_1} C^{i_2} \cdots C^{i_n} M) \tag{3}$$

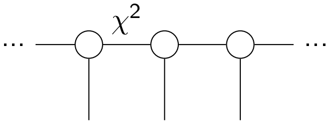


(4)

Tensor Networks: Operators

$\hat{O} =$  (5)

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

$=$ 

(6)

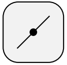
Operator exponential

- (Real) Time evolution: $\hat{O} = e^{-i\hat{H}t}$
- Statistical ensembles: $\hat{O} = e^{-\beta\hat{H}}$

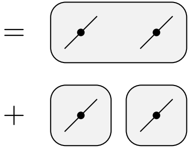
Cluster Expansion

Cluser Exapansion

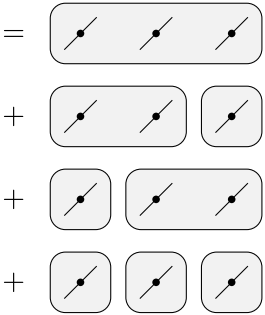
$$e^{H(1)} = \tag{7}$$



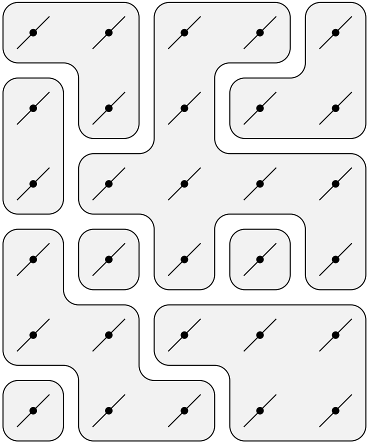
$$e^{H(2)} = \tag{8}$$



$$e^{H(3)} = \tag{9}$$

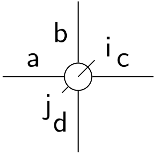


Cluser Exapansion

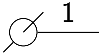


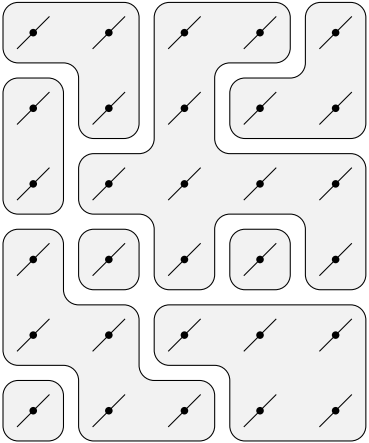
- $e^{-\beta \hat{H}} = \sum_{\{B_i\}} \bigotimes_i B_i$
- Finite number of blocks
- Encoded by 1 tensor

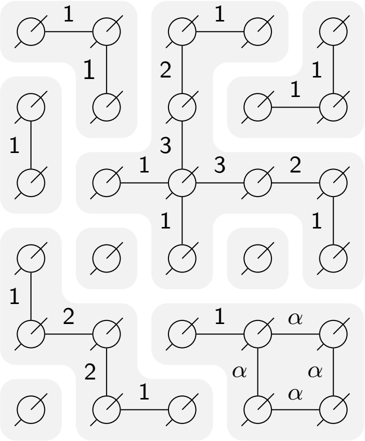
$$O^{abcd} = \quad (7)$$



$$O^{0010} = \quad (8)$$

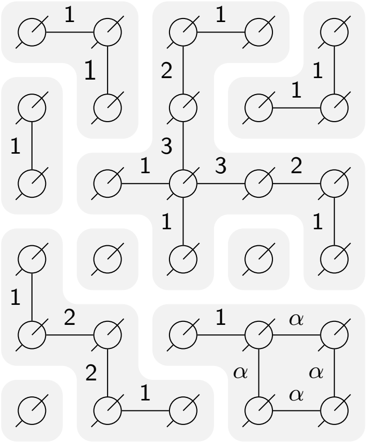





1
1
1
2
1
1
1
3
1
3
2
1
1
1
2
1
α
α
α
2
1
α

Cluser Exapansion

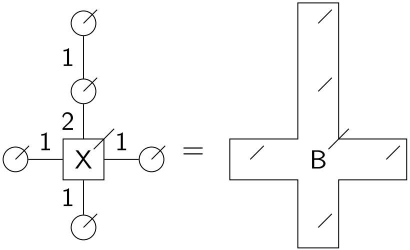
- Multiple choices for encoding
- Doesn't break symmetry
- Thermodynamic limit
- Tensor Network toolbox



Solvers

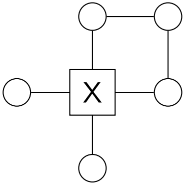
Linear solver

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

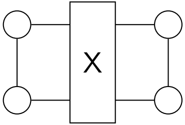


(7)

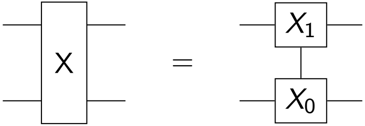
Linear Solver: Applicability



(8)



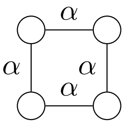
(9a)



(9b)

Nonlinear Solver

- Nonlinear least squares
- Jacobian
- Permutations



(10)

Sequential Linear Solver

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

Results

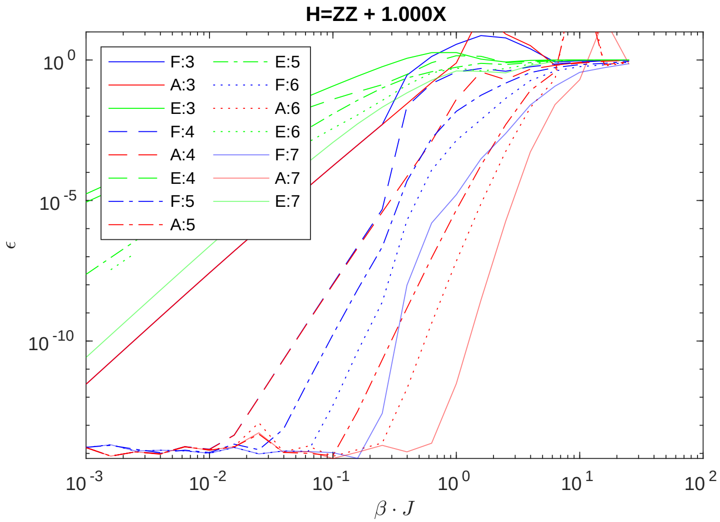
1D: Cluster expansions

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

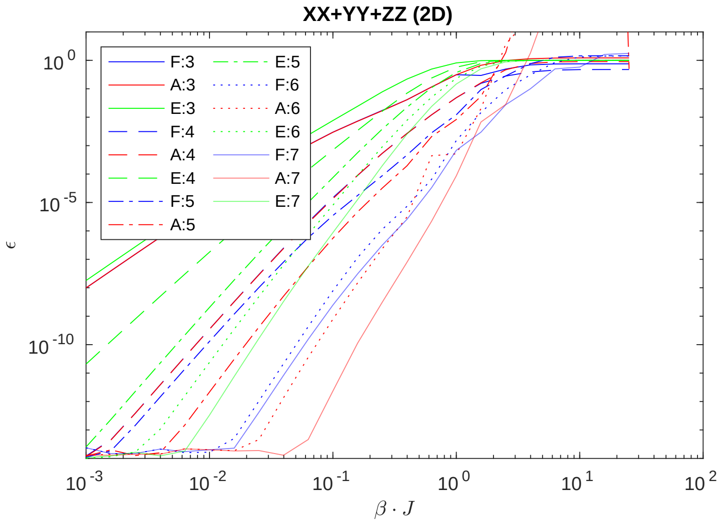
χ

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

1D: Transverse Field Ising

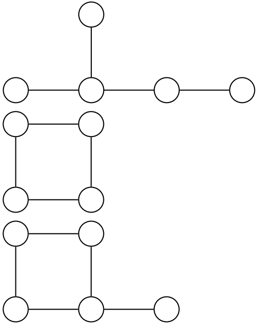


1D: Heisenberg XXX



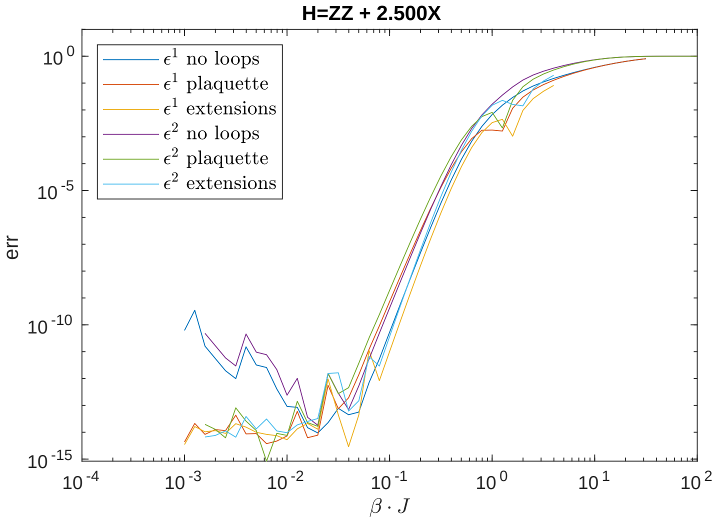
2D: Cluster expansions

- 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 $\Gamma = 2.5$

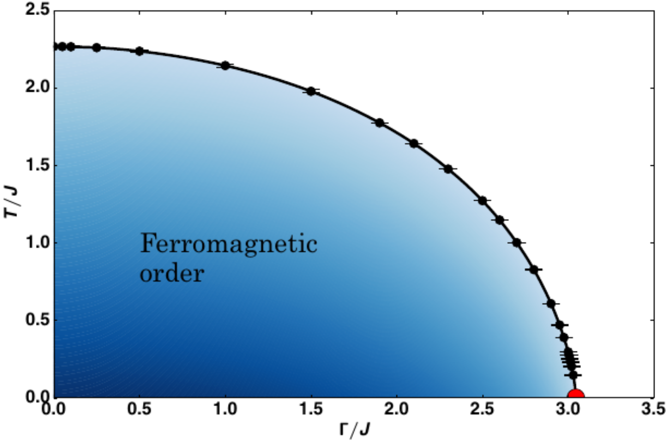
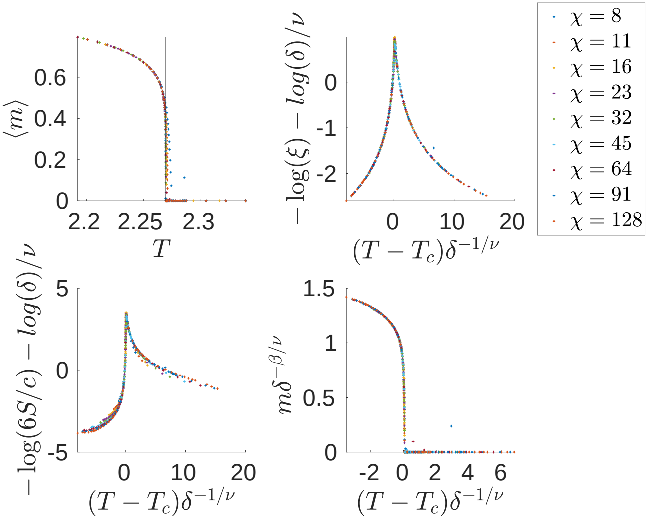


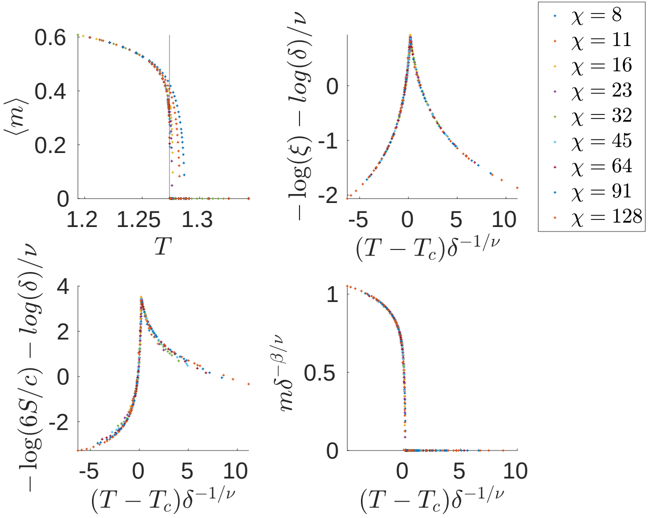
Figure taken from [2]

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

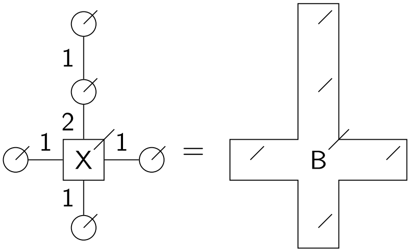
A. Alexandradinata, N. P. Armitage, A. Baydin, W. Bi, Y. Cao, H. J. Changlani, E. Chertkov, E. H. d. S. Neto, L. Delacretaz, I. E. Baggari, G. M. Ferguson, W. J. Gannon, S. A. A. Ghorashi, B. H. Goodge, O. Goulko, G. Grissonnanche, A. Hallas, I. M. Hayes, Y. He, E. W. Huang, A. Kogar, D. Kumah, J. Y. 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

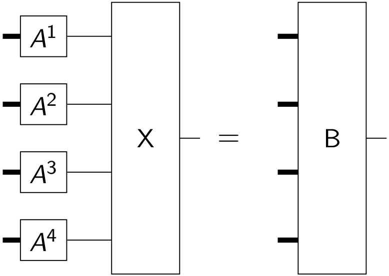
- S. Hesselmann, S. Wessel, Thermal Ising transitions in the vicinity of two-dimensional quantum critical points, PHYSICAL REVIEW B 93 (2016) 155157. doi:10.1103/PhysRevB.93.155157.
- P. Czarnik, P. Corboz, Finite correlation length scaling with infinite projected entangled pair states at finite temperature, Physical Review B 99 (2019) 245107. doi:10.1103/PhysRevB.99.245107.

Linear Solver

Linear Solver: Inversion Scheme

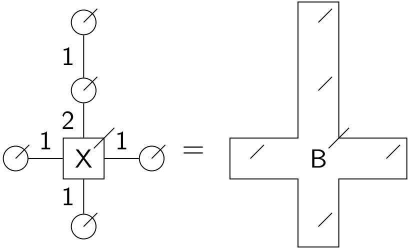


(11)

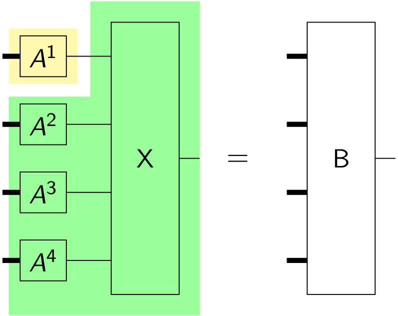


(12)

Linear Solver: Inversion Scheme



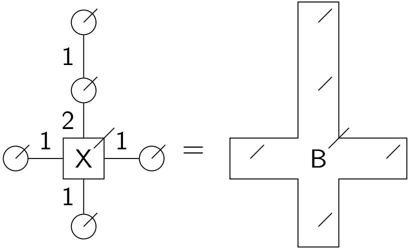
(11)



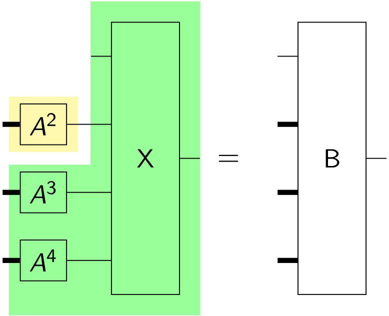
(12)

- Invert A^i separately
  - Fast
  - Numerically unstable

Linear Solver: Inversion Scheme



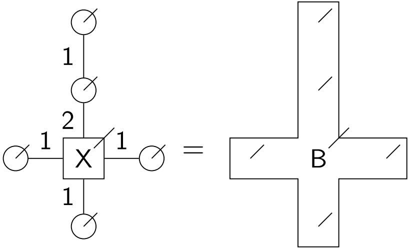
(11)



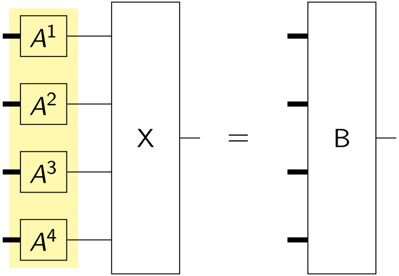
(12)

- Invert A^i separately
  - Fast
  - Numerically unstable

Linear Solver: Inversion Scheme



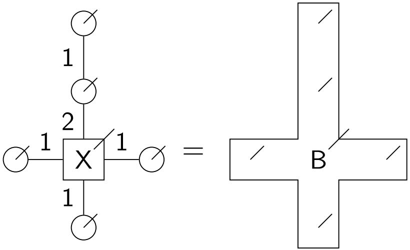
(11)



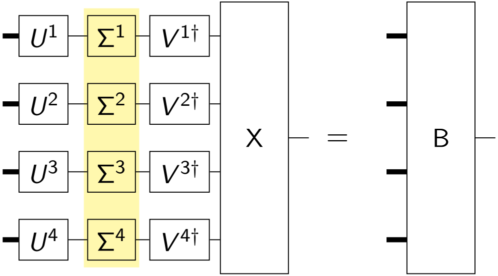
(12)

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

Linear Solver: Inversion Scheme



(11)



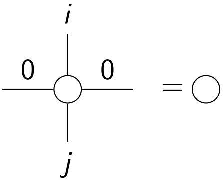
(12)

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

Construction

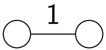
Notation

$O^{00} =$



(13)

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



(14)

General idea

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

$$\begin{aligned} \bigcirc \overset{1}{\textbf{—}} \bigcirc &= \exp -\beta H(\bigcirc \textbf{—} \bigcirc) \\ &\quad - \bigcirc \overset{0}{\textbf{—}} \bigcirc \end{aligned} \tag{16}$$

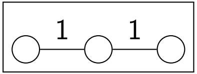
General idea

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

General idea

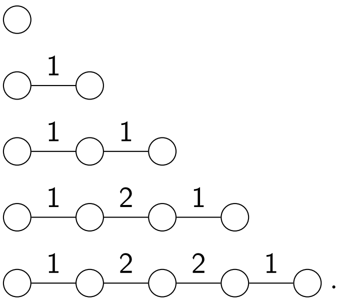
$$\bigcirc\overset{1}{\text{——}}\bigcirc\overset{1}{\text{——}}\bigcirc = \exp -\beta H(\bigcirc\text{——}\bigcirc\text{——}\bigcirc)$$
$$- \bigcirc\text{——}\bigcirc\text{——}\bigcirc \tag{17}$$

General idea



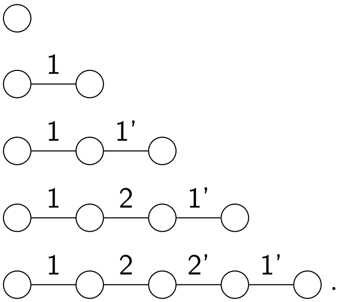
(17)

1D: Variant A



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

1D: Variant E



(19a)

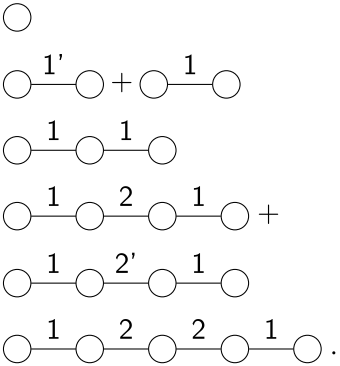
(19b)

(19c)

(19d)

(19e)

1D: Variant F



(20a)

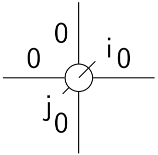
(20b)

(20c)

(20d)

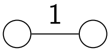
(20e)

$$O^{0000} =$$

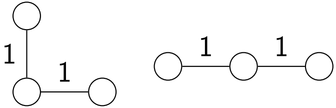


$$= \bigcirc \qquad (21)$$

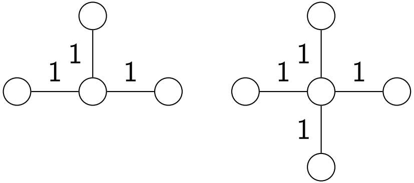
2D: Linear Blocks



(22a)

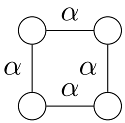


(22b)

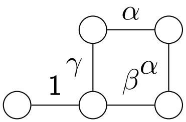


(22c)

2D: Nonlinear Blocks



(23)



.

(24)