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Outlook

Cluster Expansion of Thermal States using Tensor Networks

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Problem Statement

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- Overview condensed matter physics

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

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

Simulating Quantum Many-body Systems

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- Equations are known
- Curse of dimensionality
- Tensor networks

Tensor Networks: Introduction

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$$|\Psi\rangle = \sum_{i_1 i_2 \dots i_n} C^{i_1 i_2 \dots i_n} |i_1\rangle \otimes |i_2\rangle \otimes \dots \otimes |i_n\rangle. \quad (1)$$

$$C^{i_1 i_2 \dots i_n} = \text{Tr}(C^{i_1} C^{i_2} \dots C^{i_n} M). \quad (2)$$

Tensor Networks: Graphical Notation

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

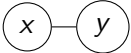
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conventional	Einstein	tensor notation
\vec{x}	x_α	
M	$M_{\alpha\beta}$	
$\vec{x} \cdot \vec{y}$	$x_\alpha y_\alpha$	

Tensor Networks: MPS

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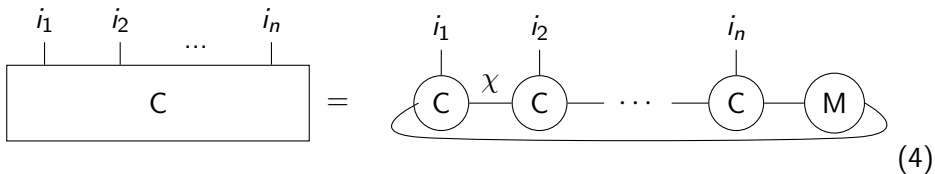
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$$C^{i_1 i_2 \dots i_n} = \text{Tr}(C^{i_1} C^{i_2} \dots C^{i_n} M) \quad (3)$$


$$\text{Diagram illustrating the trace operation in the MPS representation. On the left, a rectangular tensor } C \text{ with indices } i_1, i_2, \dots, i_n \text{ is shown. This is equated to a chain of circular tensors. The first } n \text{ circles are labeled } C \text{ with indices } i_1, i_2, \dots, i_n. \text{ They are connected sequentially by horizontal lines. The last circle in the chain is labeled } M. \text{ A curved line connects the bottom of the first circle back to the bottom of the last circle, representing the trace operation. The entire expression is labeled (4).}$$

Tensor Networks: Operators

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$$\hat{O} = \dots \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \dots \quad (5)$$

$$\hat{O} |\psi\rangle = \dots \text{---} \begin{array}{c} \bigcirc \chi \\ | \\ \bigcirc \chi \end{array} \text{---} \begin{array}{c} \bigcirc \\ | \\ \bigcirc \end{array} \text{---} \begin{array}{c} \bigcirc \\ | \\ \bigcirc \end{array} \text{---} \dots = \dots \text{---} \bigcirc \chi^2 \text{---} \bigcirc \text{---} \bigcirc \text{---} \dots \quad (6)$$

Operator exponential

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

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$$e^{H(1)} = \boxed{\diagup}$$

$$e^{H(2)} = \boxed{\diagup \diagup} + \boxed{\diagup} \boxed{\diagup}$$

(7)

(8)

$$e^{H(3)} = \boxed{\diagup \diagup \diagup} + \boxed{\diagup \diagup} \boxed{\diagup} + \boxed{\diagup} \boxed{\diagup \diagup} + \boxed{\diagup} \boxed{\diagup} \boxed{\diagup}$$

(9)

Cluster Expansion

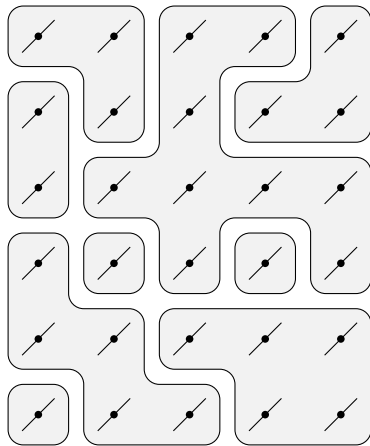
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- $e^{-\beta \hat{H}} = \sum_{\{B_i\}} \bigotimes_i B_i$
- Finite number of blocks
- Encoded by 1 tensor

$$O^{abcd} = \begin{array}{c} \begin{array}{c} b \\ | \\ a \circ i \\ | \\ c \end{array} \\ \begin{array}{c} a \\ | \\ \circ \\ | \\ j \\ | \\ d \end{array} \end{array} \quad (7)$$

$$O^{0010} = \begin{array}{c} \begin{array}{c} 1 \\ | \\ \circ \end{array} \end{array} \quad (8)$$

Cluster Expansion

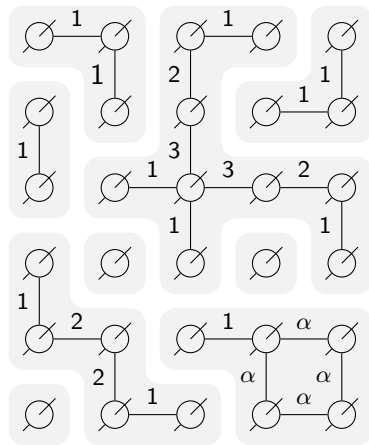
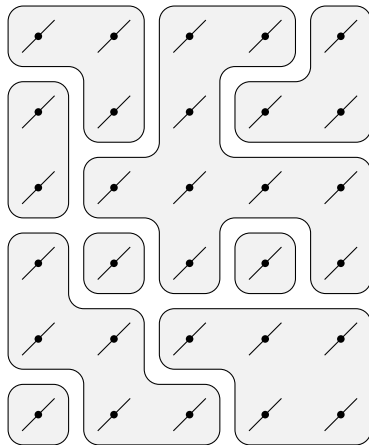
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Cluster Expansion

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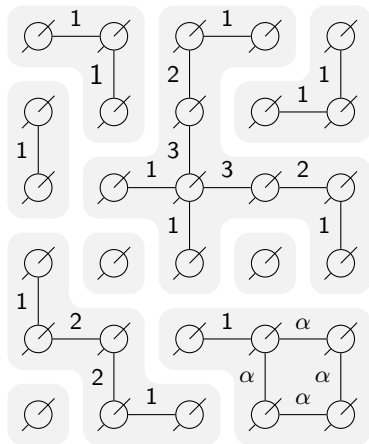
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- Multiple choices for encoding
- Doesn't break symmetry
- Thermodynamic limit
- Tensor Network toolbox



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Linear Solver

Nonlinear Solver

Sequential Linear Solver

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Linear solver

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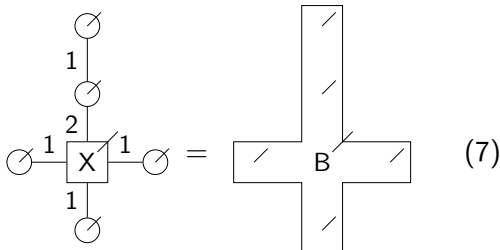
Nonlinear Solver

Sequential Linear Solver

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



Linear Solver: Applicability

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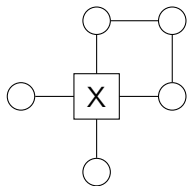
Linear Solver

Nonlinear Solver

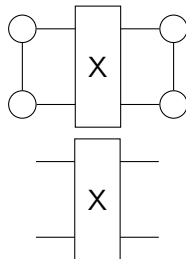
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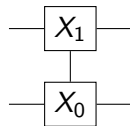


(8)



(9a)

=



(9b)

Nonlinear Solver

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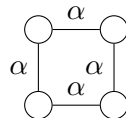
Nonlinear Solver

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- Nonlinear least squares
- Jacobian
- Permutations



(10)

Sequential Linear Solver

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

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1D exact

2D exact

2D Transverse Ising
model

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1D: Cluster expansions

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1D exact

2D exact

2D Transverse Ising
model

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Outlook

- 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

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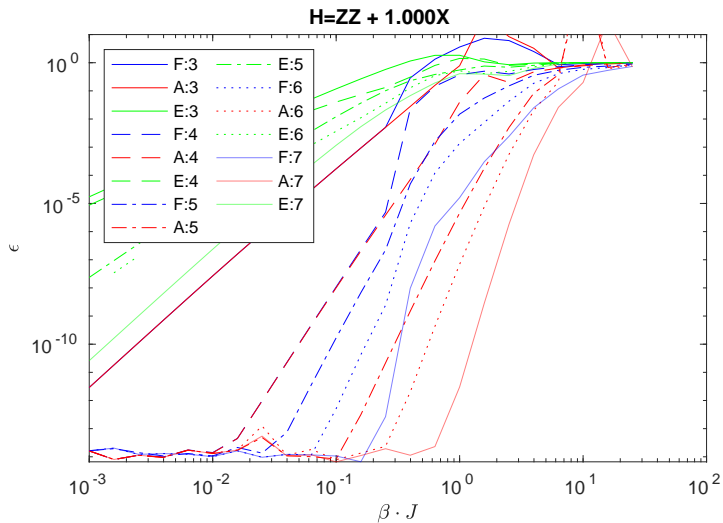
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1D exact

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2D Transverse Ising
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1D: Heisenberg XXX

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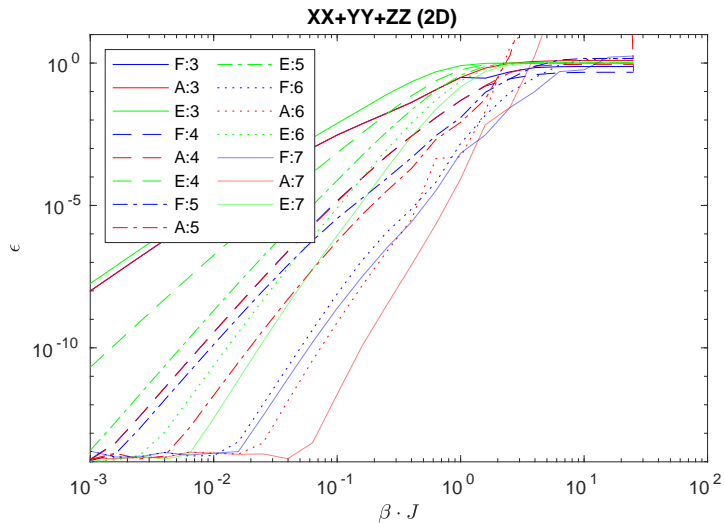
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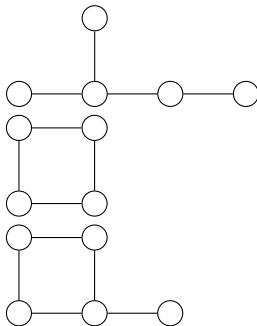
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2D: Cluster expansions

- Relative error ϵ
- Encodings based on A (order 5)

- No loops



- +Plaquette

- +Extensions

	χ
no loops	21
loops	27
extensions	43

2D: TFI

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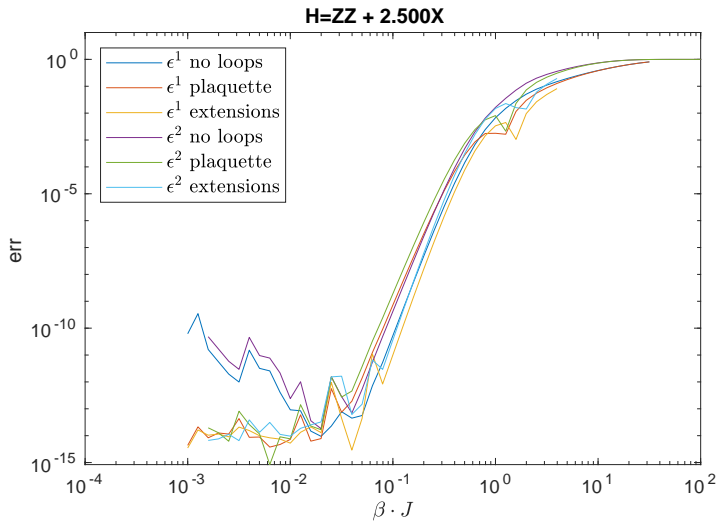
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TFI: Phase Diagram

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

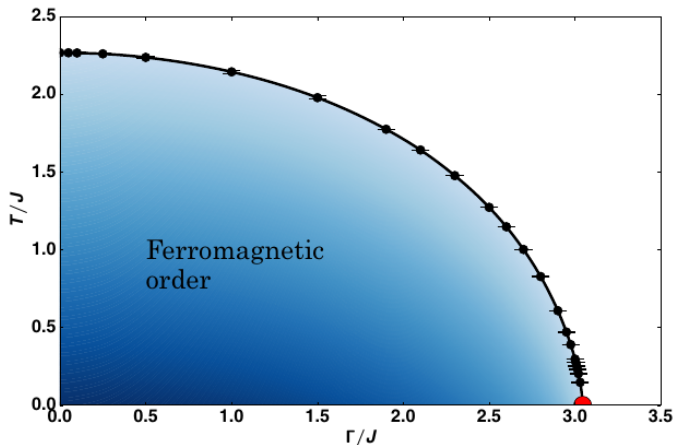
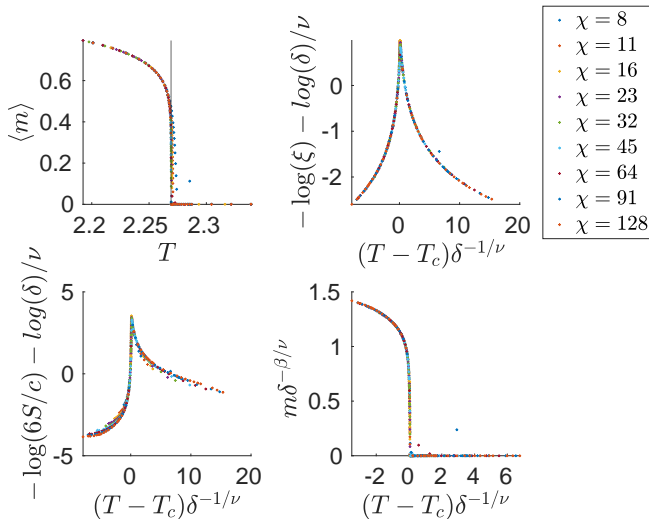


Figure taken from [2]

2D: Classical Ising

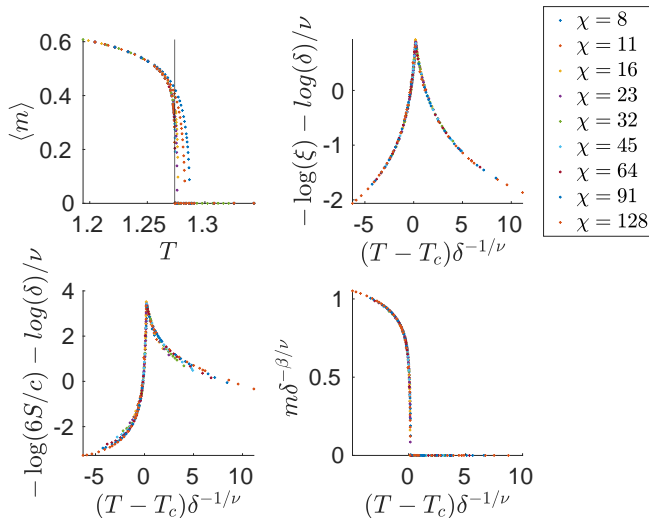
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	T_c
Fit	2.691(9)
Exact	2.691853

2D: TFI $\Gamma = 2.5$

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

Data from [3]

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

Outlook

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- 3D?
- Internal symmetries

References I



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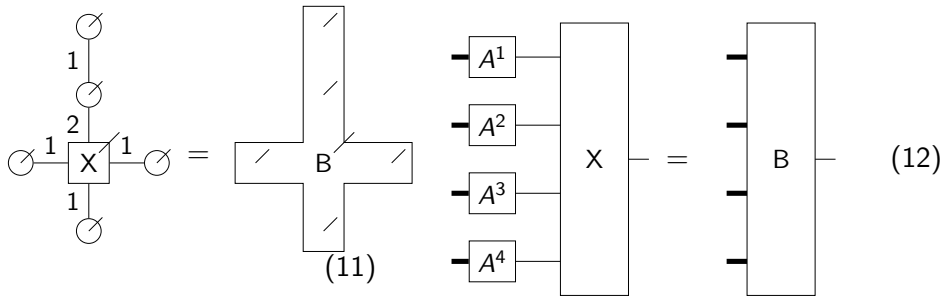
Linear Solver

Construction

Linear Solver

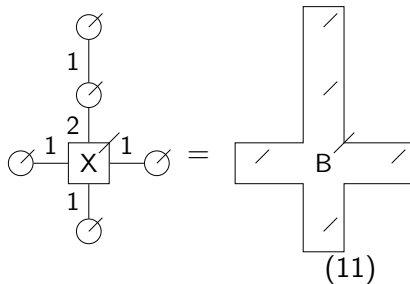
Linear Solver: Inversion Scheme

Linear Solver
Construction

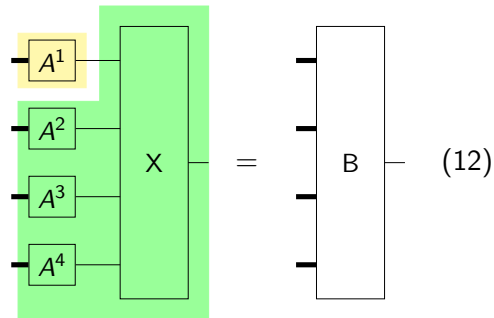


Linear Solver: Inversion Scheme

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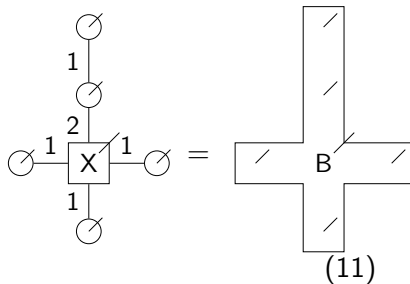


- Invert A^i separately
 - Fast
 - Numerically unstable

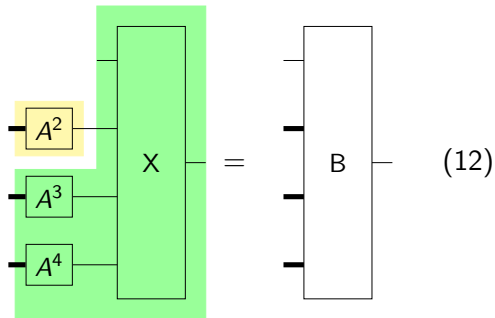


Linear Solver: Inversion Scheme

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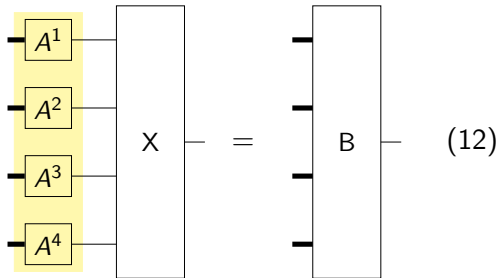
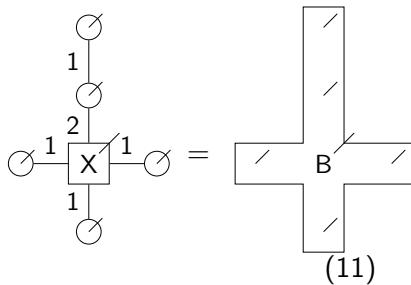


- Invert A^i separately
 - Fast
 - Numerically unstable



Linear Solver: Inversion Scheme

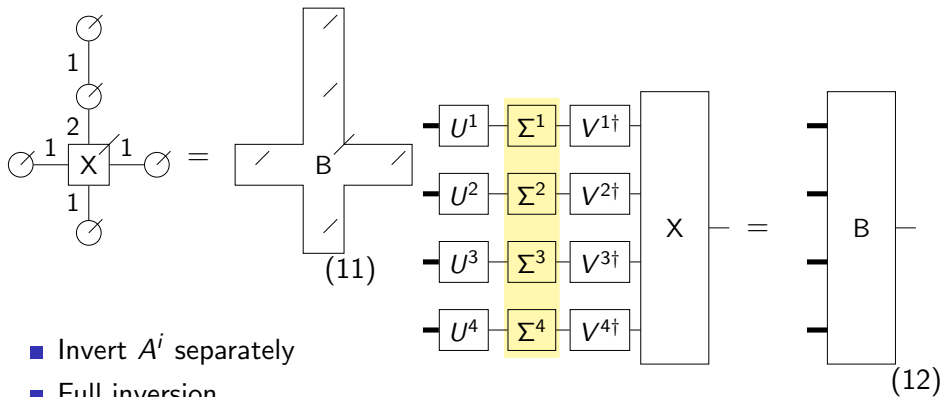
Linear Solver
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- Invert A^i separately
- Full inversion
 - Slow
 - Stable for pseudoinverse

Linear Solver: Inversion Scheme

Linear Solver
Construction



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

Linear Solver

Construction

1D

2D

Construction

Notation

Linear Solver

Construction

1D

2D

$$O^{00} = \begin{array}{c} i \\ | \\ 0 \text{ --- } \bigcirc \text{ --- } 0 \\ | \\ j \end{array} = \bigcirc \quad (13)$$

$$O^{01} O^{10} = \bigcirc \text{ --- } 1 \text{ --- } \bigcirc \quad (14)$$

General idea

Linear Solver

Construction

1D

2D

$$\bigcirc = \exp(-\beta H(\bigcirc)) \quad (15)$$

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

General idea

Linear Solver

Construction

1D

2D

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

$$- \text{---} \overset{0}{\bigcirc} \text{---} \overset{0}{\bigcirc} \text{---} \bigcirc$$

$$- \text{---} \overset{1}{\bigcirc} \text{---} \bigcirc \text{---} \overset{0}{\bigcirc}$$

$$- \text{---} \overset{0}{\bigcirc} \text{---} \bigcirc \text{---} \overset{1}{\bigcirc}$$

(17)

General idea

Linear Solver

Construction

1D

2D

$$\begin{array}{c} \text{---} \text{1} \text{---} \text{1} \text{---} \\ \text{---} \end{array} \text{---} \text{---} \text{---} = \exp -\beta H(\text{---} \text{---} \text{---}) \quad (17)$$

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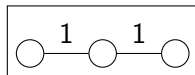
General idea

Linear Solver

Construction

1D

2D



(17)

1D: Variant A

Linear Solver

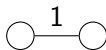
Construction

1D

2D



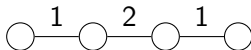
(18a)



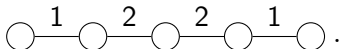
(18b)



(18c)



(18d)



(18e)

1D: Variant E

Linear Solver

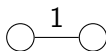
Construction

1D

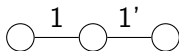
2D



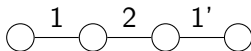
(19a)



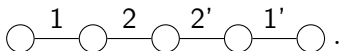
(19b)



(19c)



(19d)



(19e)

1D: Variant F

Linear Solver

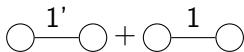
Construction

1D

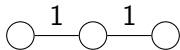
2D



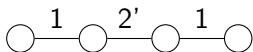
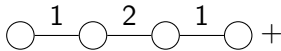
(20a)



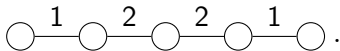
(20b)



(20c)



(20d)



(20e)

Linear Solver

Construction

1D

2D

$$O^{0000} = \begin{array}{c} \begin{array}{c} 0 \\ 0 \end{array} \begin{array}{c} | \\ \circ \\ | \end{array} \begin{array}{c} i_0 \\ 0 \end{array} \\ \begin{array}{c} 0 \\ j_0 \end{array} \end{array} = \bigcirc \quad (21)$$

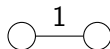
2D: Linear Blocks

Linear Solver

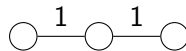
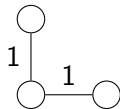
Construction

1D

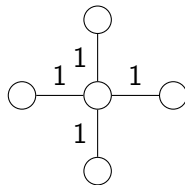
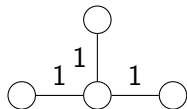
2D



(22a)



(22b)



(22c)

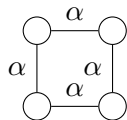
2D: Nonlinear Blocks

Linear Solver

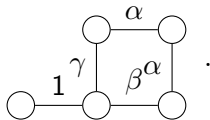
Construction

1D

2D



(23)



(24)