

Introduction

Cluster
Expansions

Results

Conclusion and
Outlook

Cluster Expansions of Thermal States using Tensor Networks

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Simulation

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- Overview condensed matter physics
 - Macroscopic and microscopic physical properties of matter
 - Metals
 - semiconductors
 - Liquids
 - Bose-Einstein Condensates
 - Magnets
 - Different disciplines
 - Experimental
 - Theoretical
 - Engineering

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

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- 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
 - Exact diagonalisation
 - (post-) Hartree Fock methods, DFT methods
 - Monte Carlo methods
 - Tensor Networks

Tensor Networks

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

$$C^{i_1 i_2 \dots i_n} = w_l C^{i_1} C^{i_2} \dots C^{i_n} w_r \quad (2)$$

$=$ 

- MPS
- Relevant corner Hilbert space

Operator exponential

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- (Real) Time evolution:

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

- Statistical ensembles:

$$\hat{O} = \frac{e^{-\beta\hat{H}}}{\text{Tr}(e^{-\beta\hat{H}})} \quad (4)$$

$$\hat{O} = \begin{array}{c} \dots & \dots & \dots \\ \dots - \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \dots \\ | & | & | \\ \dots - \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \dots \\ | & | & | \\ \dots - \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \dots \\ \dots & \dots & \dots \end{array} \quad (5)$$

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Cluster Expansions

Cluster Expansion

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

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

$$(6) \quad e^{H(3)} = \boxed{\diagup \bullet \diagdown \quad \diagup \bullet \diagdown \quad \diagup \bullet \diagdown}$$

$$+ \boxed{\diagup \bullet \diagdown \quad \diagup \bullet \diagdown} \quad \boxed{\diagup \bullet \diagdown}$$

(7)

$$+ \boxed{\diagup \bullet \diagdown} \quad \boxed{\diagup \bullet \diagdown \quad \diagup \bullet \diagdown}$$

$$+ \boxed{\diagup \bullet \diagdown} \quad \boxed{\diagup \bullet \diagdown} \quad \boxed{\diagup \bullet \diagdown}$$

(8)

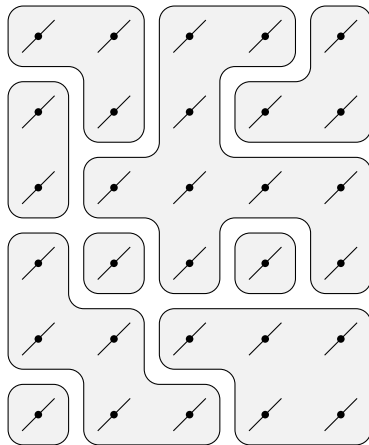
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- $e^{\hat{H}} = \sum_{\{B\}} \bigotimes_i B_i$
- Finite number of blocks
- Encoded by 1 tensor

$$O^{abcd} = \begin{array}{c} \begin{array}{c} b \\ a \quad \bigcirc \quad i \\ j \quad d \quad c \end{array} \end{array} \quad (6)$$

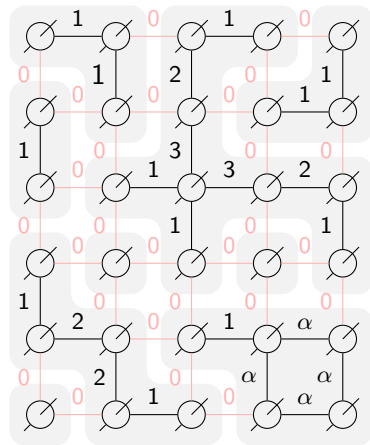
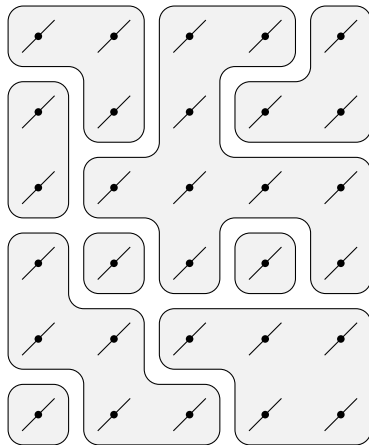
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Cluster Expansion

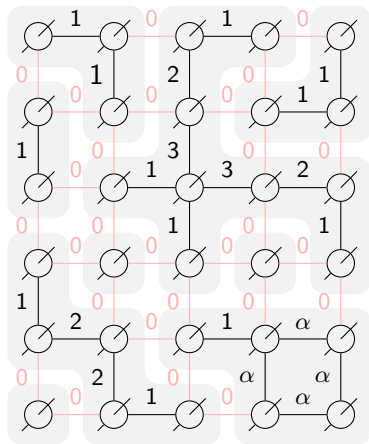
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- Multiple choices for encoding
- Solvers
 - Linear
 - Nonlinear



Advantages

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

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1D exact

2D exact

2D Transverse Ising
model

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Results

1D: Encodings + Error Measure

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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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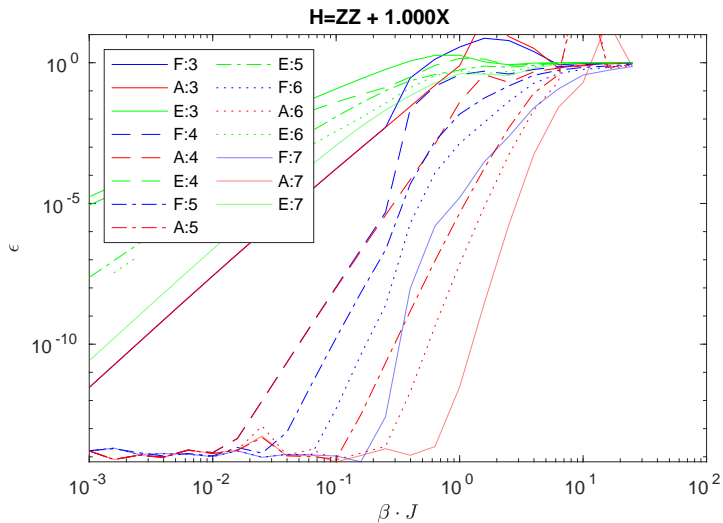
Results

1D exact

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1D: Heisenberg XXX

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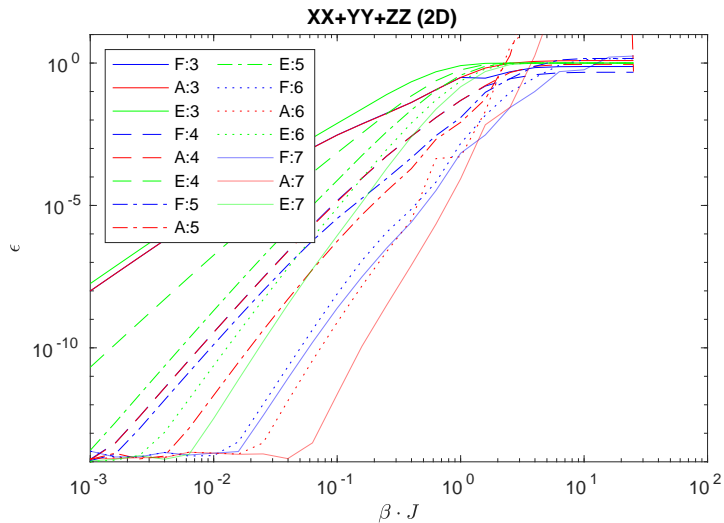
Results

1D exact

2D exact

2D Transverse Ising
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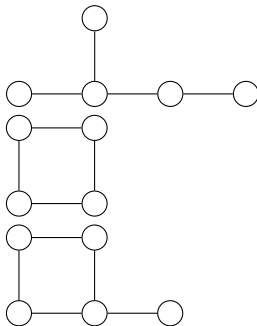
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2D: Encodings + Error Measure

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

- No loops



- +Plaquette

- +Extensions

	χ
no loops	21
plaquette	27
extensions	43

2D: TFI

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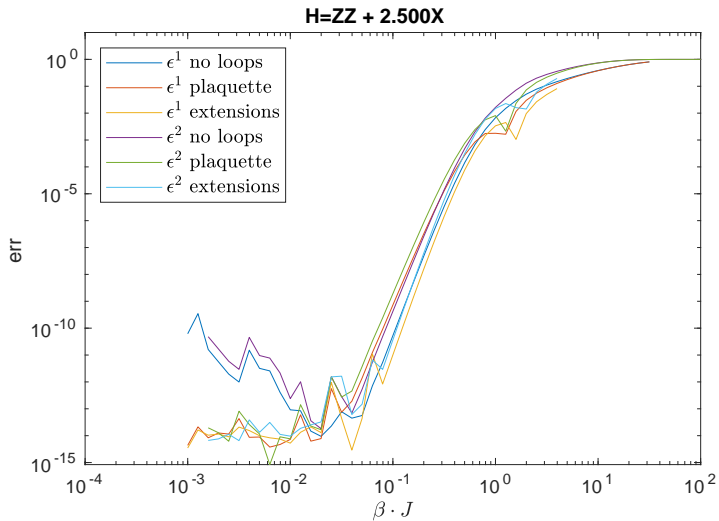
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Conclusion

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- Large β -steps
- Real time evolution
- Encoding
- Truncation χ

2D TFI: Introduction

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2D exact

2D Transverse Ising
model

Conclusion and
Outlook

- Phase Transition
- Criticality
- Finite size scaling
 - Observables:
 m , S and ξ
 - Parameters:
 T_c , exponents
- $\Gamma = 2.5$ and $\Gamma = 0$
- VUMPS (χ, δ^{-1})

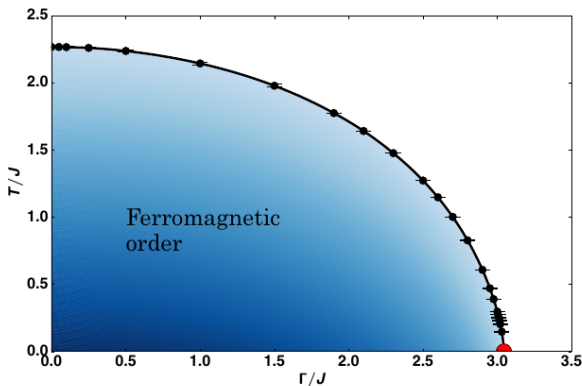


Figure taken from [2]

2D TFI: $\Gamma = 2.5$

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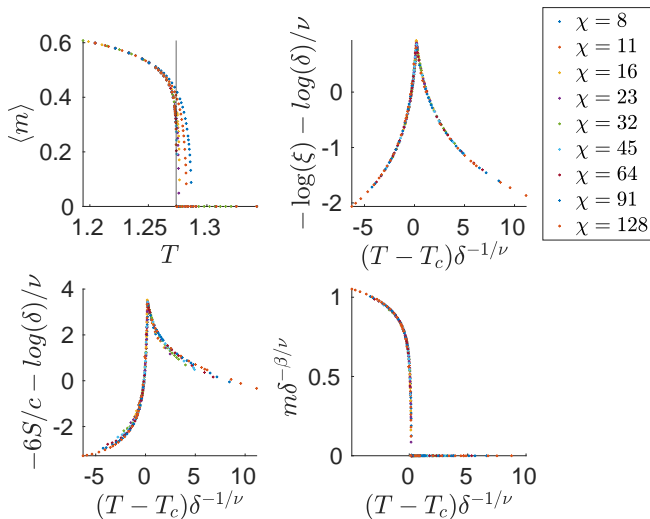
Results

1D exact

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2D Transverse Ising
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	T_c
Fit	1.2736(6)
QMC	1.2737(6)
TN	1.2737(2)

Data from [3]

2D TFI: Classical Ising

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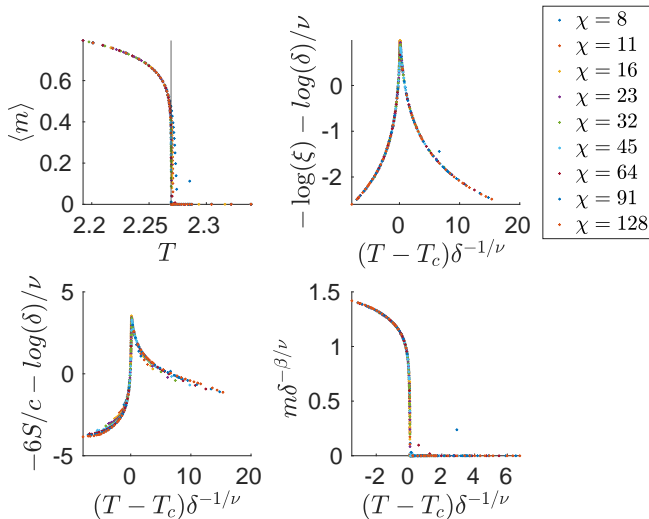
Results

1D exact

2D exact

2D Transverse Ising
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	T_c
Fit	2.691(9)
Exact	2.691853

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Conclusion

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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
- Incorporating internal symmetries
- Lattices

References I



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References II

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 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

Linear Solver

Construction

$\Gamma = 2.9$

Solvers

Tensor Networks

Tensor Networks: Introduction

Tensor Networks

Linear Solver

Construction

$\Gamma = 2.9$

Solvers

$$|\Psi\rangle = \sum_{i_1 i_2 \dots i_n} C^{i_1 i_2 \dots i_n} |i_1\rangle \otimes |i_2\rangle \otimes \dots \otimes |i_n\rangle. \quad (6)$$

$$C^{i_1 i_2 \dots i_n} = \text{Tr}(C^{i_1} C^{i_2} \dots C^{i_n} M). \quad (7)$$

Tensor Networks: Graphical Notation



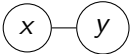
Tensor Networks

Linear Solver

Construction

$\Gamma = 2.9$

Solvers

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

Tensor Networks: MPS

Tensor Networks

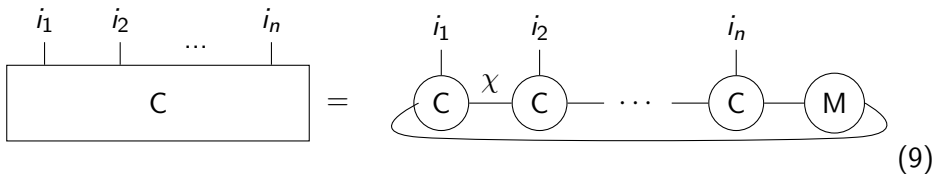
Linear Solver

Construction

$\Gamma = 2.9$

Solvers

$$C^{i_1 i_2 \dots i_n} = \text{Tr}(C^{i_1} C^{i_2} \dots C^{i_n} M) \quad (8)$$


$$\text{Diagram (9): A large rectangle labeled } C \text{ with indices } i_1, i_2, \dots, i_n \text{ at the top is equal to a trace of a product of tensors. The trace is represented by a chain of circles: } C \text{ (with index } i_1 \text{)}, C \text{ (with index } i_2 \text{)}, \dots, C \text{ (with index } i_n \text{)}, \text{ and } M. \text{ A curved line connects the bottom of the first } C \text{ circle to the bottom of the } M \text{ circle, indicating the trace operation.} \quad (9)$$

Tensor Networks: Operators

Tensor Networks

Linear Solver

Construction

$\Gamma = 2.9$

Solvers

$$\hat{O} = \dots \text{---} \bigcirc \text{---} \bigcirc \text{---} \bigcirc \text{---} \dots \quad (10)$$

$$\hat{O} |\psi\rangle = \dots \text{---} \begin{array}{c} \bigcirc \chi \\ | \\ \bigcirc \chi \end{array} \text{---} \begin{array}{c} \bigcirc \\ | \\ \bigcirc \end{array} \text{---} \begin{array}{c} \bigcirc \\ | \\ \bigcirc \end{array} \text{---} \dots = \dots \text{---} \bigcirc \chi^2 \text{---} \bigcirc \text{---} \bigcirc \text{---} \dots \quad (11)$$

Tensor Networks

Linear Solver

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Linear Solver

Linear Solver: Inversion Scheme

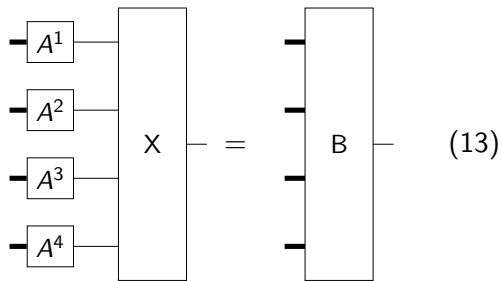
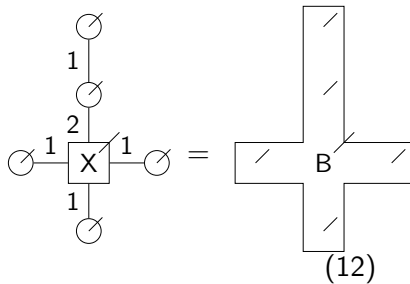
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Linear Solver: Inversion Scheme

Tensor Networks

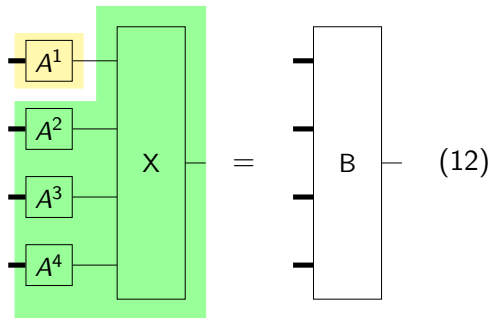
Linear Solver

Construction

$\Gamma = 2.9$

Solvers

- Invert A^i separately
 - Fast
 - Numerically unstable



Linear Solver: Inversion Scheme

Tensor Networks

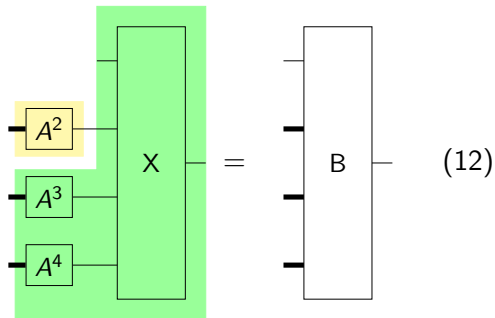
Linear Solver

Construction

$\Gamma = 2.9$

Solvers

- Invert A^i separately
 - Fast
 - Numerically unstable



Linear Solver: Inversion Scheme

Tensor Networks

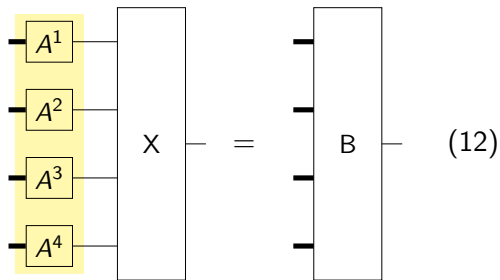
Linear Solver

Construction

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Solvers

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



Linear Solver: Inversion Scheme

Tensor Networks

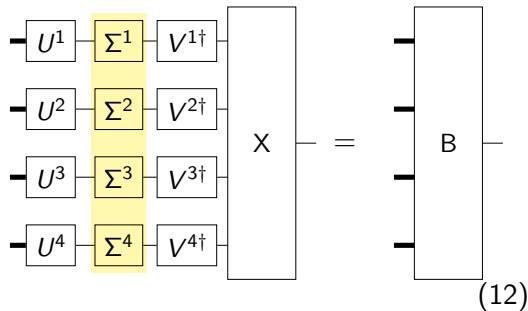
Linear Solver

Construction

$\Gamma = 2.9$

Solvers

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



Tensor Networks

Linear Solver

Construction

1D

2D

$\Gamma = 2.9$

Solvers

Construction

Notation

Tensor Networks

Linear Solver

Construction

1D

2D

$\Gamma = 2.9$

Solvers

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

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

General idea

Tensor Networks

Linear Solver

Construction

1D

2D

$\Gamma = 2.9$

Solvers

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

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

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

General idea

Tensor Networks

Linear Solver

Construction

1D

2D

$\Gamma = 2.9$

Solvers

$$\begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{cc} 1 & 1 \\ 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{array} = \exp -\beta H(\text{---} \text{---} \text{---}) \quad (17)$$

General idea

Tensor Networks

Linear Solver

Construction

1D

2D

$\Gamma = 2.9$

Solvers

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

General idea

Tensor Networks

Linear Solver

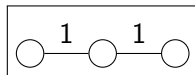
Construction

1D

2D

$\Gamma = 2.9$

Solvers



(17)

1D: Variant A

Tensor Networks

Linear Solver

Construction

1D

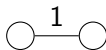
2D

$\Gamma = 2.9$

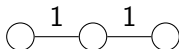
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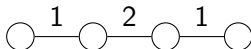
(18a)



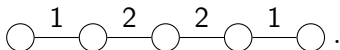
(18b)



(18c)



(18d)



(18e)

1D: Variant E

Tensor Networks

Linear Solver

Construction

1D

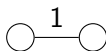
2D

$\Gamma = 2.9$

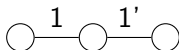
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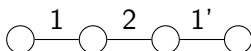
(19a)



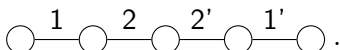
(19b)



(19c)



(19d)



(19e)

1D: Variant F

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1D

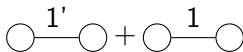
2D

$\Gamma = 2.9$

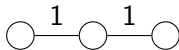
Solvers



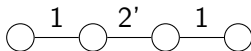
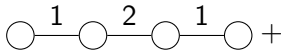
(20a)



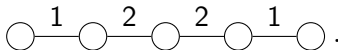
(20b)



(20c)



(20d)



(20e)

Tensor Networks

Linear Solver

Construction

1D

2D

$\Gamma = 2.9$

Solvers

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

2D: Linear Blocks

Tensor Networks

Linear Solver

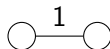
Construction

1D

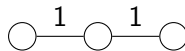
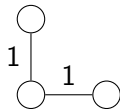
2D

$\Gamma = 2.9$

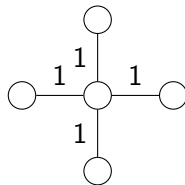
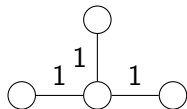
Solvers



(22a)



(22b)



(22c)

2D: Nonlinear Blocks

Tensor Networks

Linear Solver

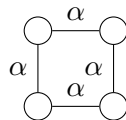
Construction

1D

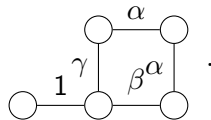
2D

$\Gamma = 2.9$

Solvers



(23)



(24)

Tensor Networks

Linear Solver

Construction

$\Gamma = 2.9$

Solvers

$$\Gamma = 2.9$$

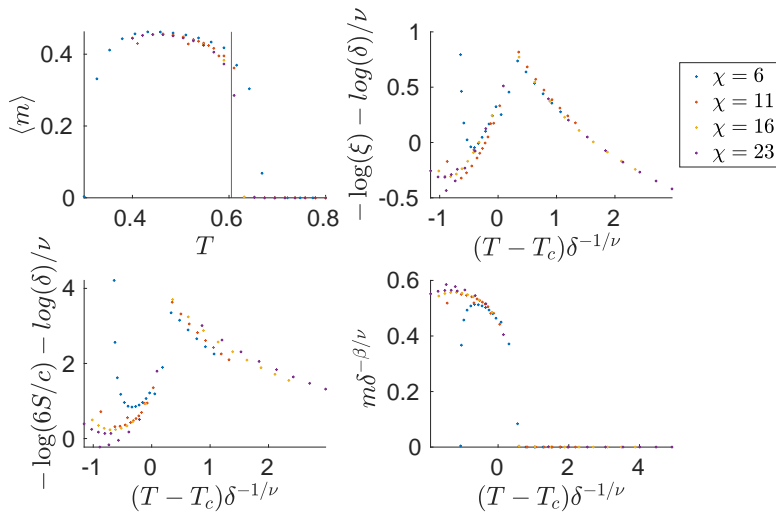
Tensor Networks

Linear Solver

Construction

$\Gamma = 2.9$

Solvers



Tensor Networks

Linear Solver

Construction

$\Gamma = 2.9$

Solvers

Linear Solver

Nonlinear Solver

Sequential Linear Solver

Solvers

Linear solver

Tensor Networks

Linear Solver

Construction

$\Gamma = 2.9$

Solvers

Linear Solver

Nonlinear Solver

Sequential Linear Solver

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

The diagram shows a square box labeled 'X' with four legs extending from its sides. Each leg is labeled with the number '1' and ends in a small circle with a diagonal slash. This box is equated to a square box labeled 'B' with four legs extending from its sides. Each leg of box 'B' is labeled with a diagonal slash. The entire equation is labeled (25) on the right.

$$\text{Diagram of } X \text{ with 4 legs of index 1} = \text{Diagram of } B \text{ with 4 legs of index 1} \quad (25)$$

Linear Solver: Applicability

Tensor Networks

Linear Solver

Construction

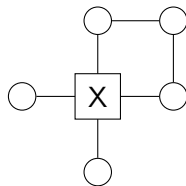
$\Gamma = 2.9$

Solvers

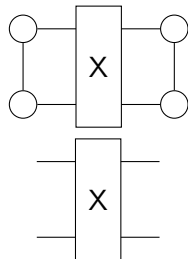
Linear Solver

Nonlinear Solver

Sequential Linear Solver

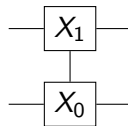


(26)



(27a)

=



(27b)

Nonlinear Solver

Tensor Networks

Linear Solver

Construction

$\Gamma = 2.9$

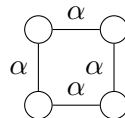
Solvers

Linear Solver

Nonlinear Solver

Sequential Linear Solver

- Nonlinear least squares
- Jacobian
- Permutations



(28)

Sequential Linear Solver

Tensor Networks

Linear Solver

Construction

$\Gamma = 2.9$

Solvers

Linear Solver

Nonlinear Solver

Sequential Linear Solver

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