

Introduction

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Conclusion and
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PEPO cluster expansion of tensor exponential

David Devoogdt

Faculty of Engineering and Architecture
Ghent University

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Problem Statement
Graphical notation
Cluster expansion

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Statistical Quantum mechanics

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$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{Z} \quad (1)$$

$$Z = \text{Tr}(e^{-\beta \hat{H}})$$
$$\langle X \rangle = \text{Tr}(\rho \hat{X}) \quad (2)$$

Graphical notation

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$$\begin{array}{c} i \\ 0 \quad | \quad 0 \\ \hline \bigcirc \\ | \\ j \end{array} = \bigcirc \quad (3)$$

$$\begin{array}{ccc} i_1 & & i_2 \\ 0 \quad | \quad 1 \quad | \quad 0 \\ \hline \bigcirc & \text{---} & \bigcirc \\ | & & | \\ j_1 & & j_2 \end{array} = \bigcirc \text{---} 1 \text{---} \bigcirc \quad (4)$$

$$\begin{array}{ccccc} i_1 & & i_2 & & i_3 \\ 0 \quad | & & | & & | \quad 0 \\ \hline \bigcirc & \text{---} & \bigcirc & \text{---} & \bigcirc \\ | & & | & & | \\ j_1 & & j_2 & & j_3 \end{array} = \bigcirc \text{---} \bigcirc \text{---} \bigcirc \quad (5)$$

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$$\hat{H} = \left(\sum_{\langle ij \rangle} H_2^i H_2^j + \sum_i H_1^i \right) \quad (6)$$

$$\begin{aligned} H(\bigcirc - \bigcirc - \bigcirc) &= H_1 \otimes 1 \otimes 1 \\ &+ 1 \otimes H_1 \otimes 1 \\ &+ 1 \otimes 1 \otimes H_1 \\ &+ H_2 \otimes H_2 \otimes 1 \\ &+ 1 \otimes H_2 \otimes H_2 \end{aligned} \quad (7)$$

General idea

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$$\bigcirc = \exp(-\beta H(\bigcirc)) \quad (8)$$

$$\begin{array}{c} \text{1} \\ \bigcirc \text{---} \bigcirc \end{array} = \exp -\beta H(\begin{array}{c} \bigcirc \text{---} \bigcirc \\ \text{0} \\ \text{---} \bigcirc \text{---} \bigcirc \end{array}) \quad (9)$$

General idea

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

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Advantages

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- size extensive
- symmetry
- fast

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Variant A

Variant C

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Construction 1D

Variant A

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Variant A

Variant C

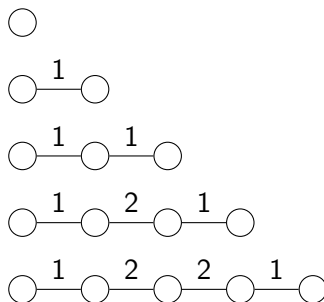
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Variant C

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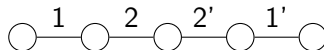
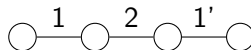
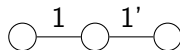
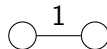
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Error measure

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$$\epsilon(\text{map}) = \frac{\|\exp - \beta H(\text{map}) - \text{MPO}(\text{map})\|}{\|\exp - \beta H(\text{map})\|} \quad (13)$$

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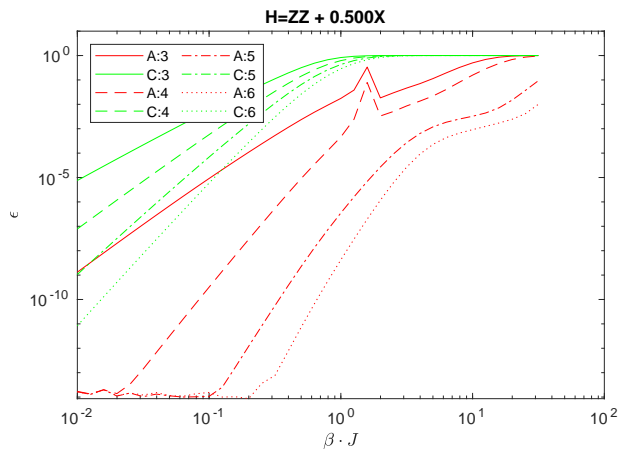
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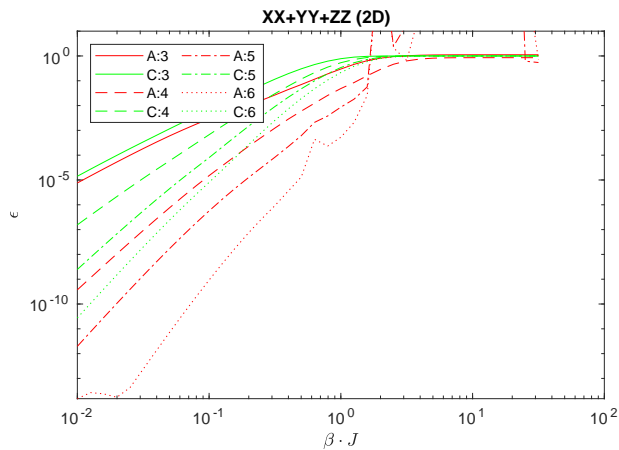
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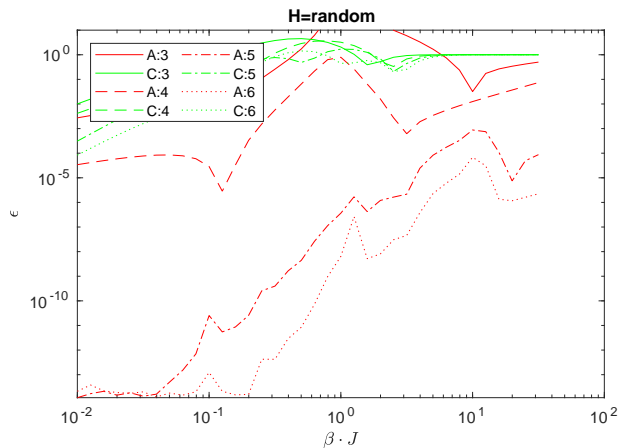
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Construction 2D: Linear blocks

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Construction 2D

Linear blocks

Loops

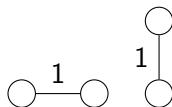
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Construction 2D: Linear blocks

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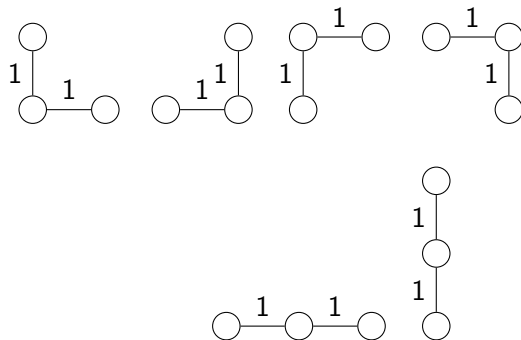
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Construction 2D: Linear blocks

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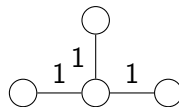
Linear blocks

Loops

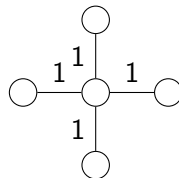
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Construction 2D: Linear blocks

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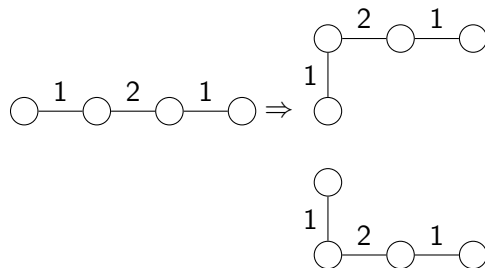
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And many more "linear" blocks

Loops

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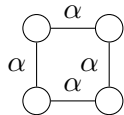
Linear blocks

Loops

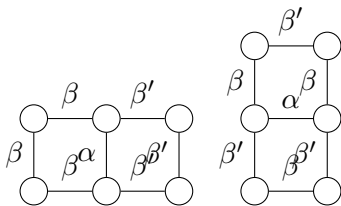
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- bond dim
- solver: see later

Unsolved

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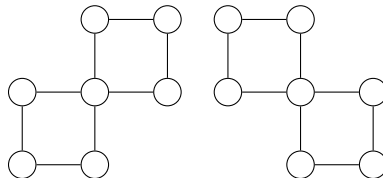
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Easy to solve on finite lattice, difficult in thermodynamic limit...

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Linear solver

Non-linear solvers

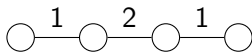
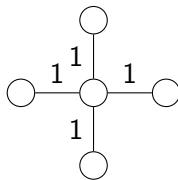
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Solvers

Linear solver

- pseudoinverse
- optimisation for tree graphs
- implemented for any shape



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```
[map, ~] = create_map([0, 0, 5, 0;  
                      0, 0, 6, 0;  
                      1, 2, 3, 4;  
                      0, 0, 7, 0], obj.numopts);  
pattern = {[2, 2, 1, 1]};  
[obj, ~, ~, ln_prefact, ~] = solve_lin_and_assign(obj, map, pattern, ln_prefact);  
o_
```


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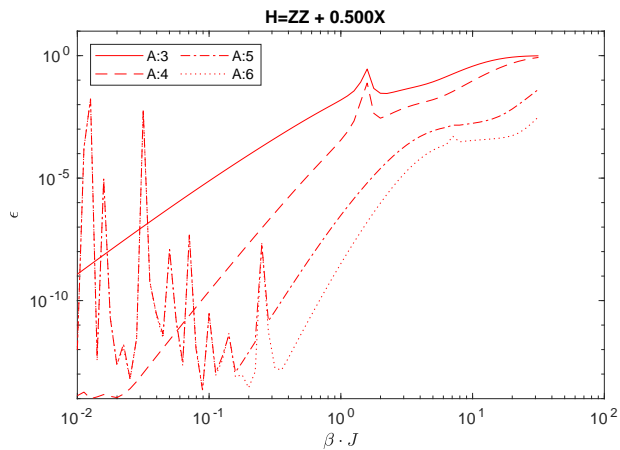
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sequential linear

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- initialize randomly
- use linear solver for 1 tensor
- fast

true non-linear solver

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- Matlab fsolve
- exact jacobian
- multiple patterns
- multiple maps

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**2D Transversal
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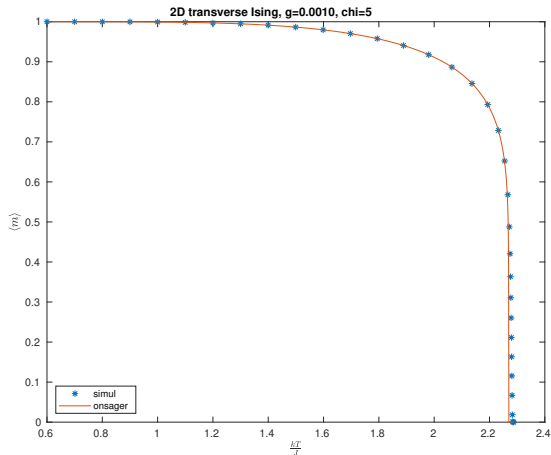
First results

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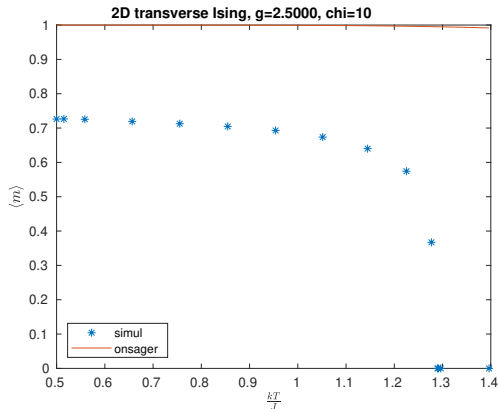
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First results

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First results



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Conclusion and outlook

Conclusion

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- Working code for 1D and 2D
- General solvers
- Promising first results in 2D

Outlook: short term

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- Accurate estimate transversal Ising quantum critical point
- Improve blocks for loops
- continuous improvements framework

Outlook: long term

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- Incorporate symmetries of Hamiltonians
- Look at other (types of) Hamiltonians
- Generalize for other lattice geometries
- Generalize to 3D

References I

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