

Introduction

Construction 1D

Construction 2D

Solvers

2D Transversal
Ising Model

Conclusion and
outlook

PEPO cluster expansion of Tensor Exponential

Subtitle

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Intoduction

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Intoduction

Statistical Quantum mechanics

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

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

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

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

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

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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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- represent as MPO/PEPO
- cluster by size, not in β

General idea

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

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

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

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

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

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

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Advantages

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- size extensive
- symmetry

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Variant C

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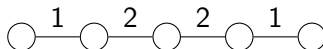
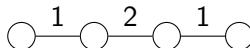
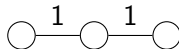
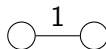
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Variant B

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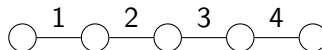
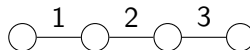
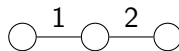
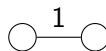
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Variant C

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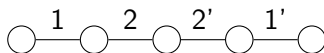
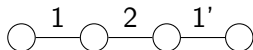
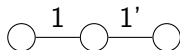
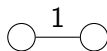
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- bond dimension
- "unwanted" chains

Error measure

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- cyclic
- relative
- 12 sites

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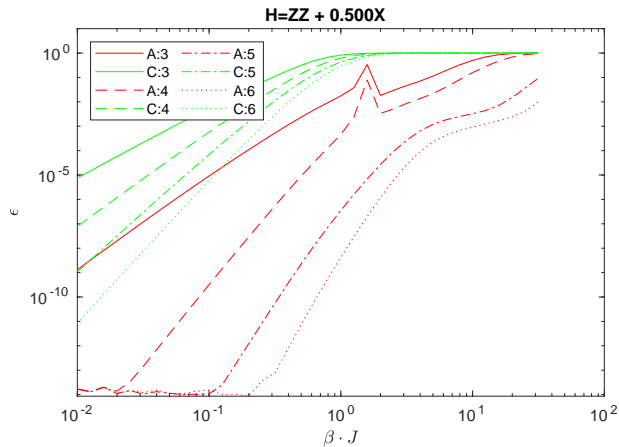
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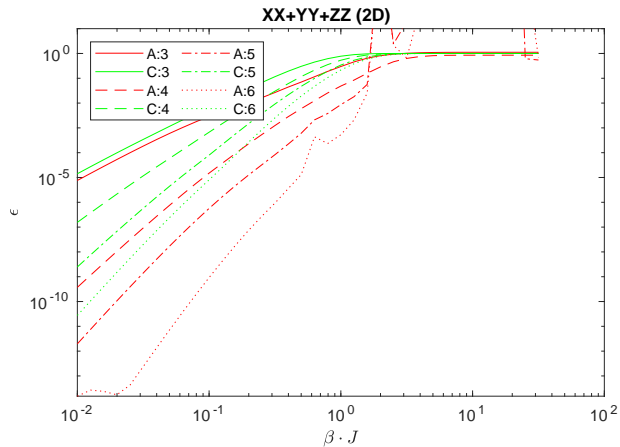
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Loops

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Construction 2D

Construction 2D: Linear blocks

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Construction 1D

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Linear blocks

Loops

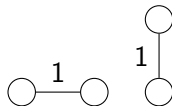
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Construction 2D: Linear blocks

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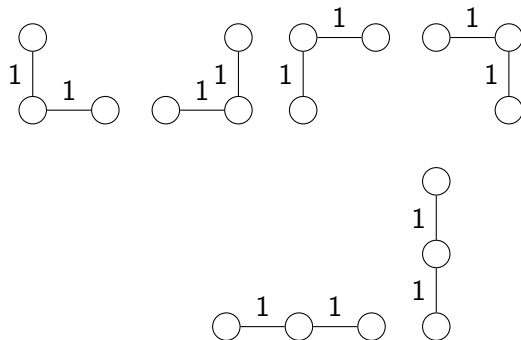
Linear blocks

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Construction 2D: Linear blocks

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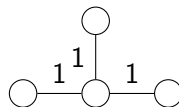
Linear blocks

Loops

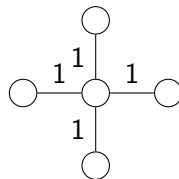
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Construction 2D: Linear blocks

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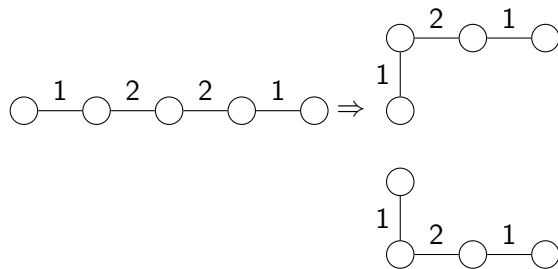
Linear blocks

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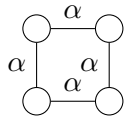
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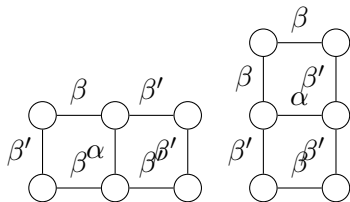
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And many more "linear" blocks

Loops



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- bond dim
- solver: see later

Unsolved

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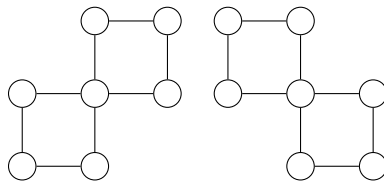
Linear blocks

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

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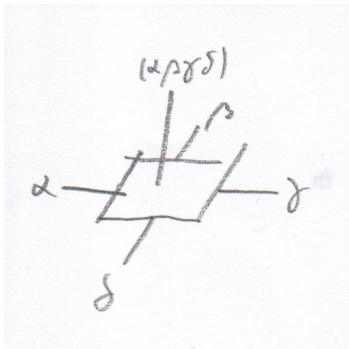
Normalisation: PEPS $O \rightarrow O/\alpha$

$$\frac{\exp A}{\alpha^N} = \exp(A - N \ln \alpha \cdot I) \quad (23)$$

Avoid large values in tensor

Fast cell contraction

- Bottleneck: find all possible contractions of virtual levels
- Solution: Construct sparse PEPO, contract geometry



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- "Linear" problems
- non-linear problems

Linear Solver

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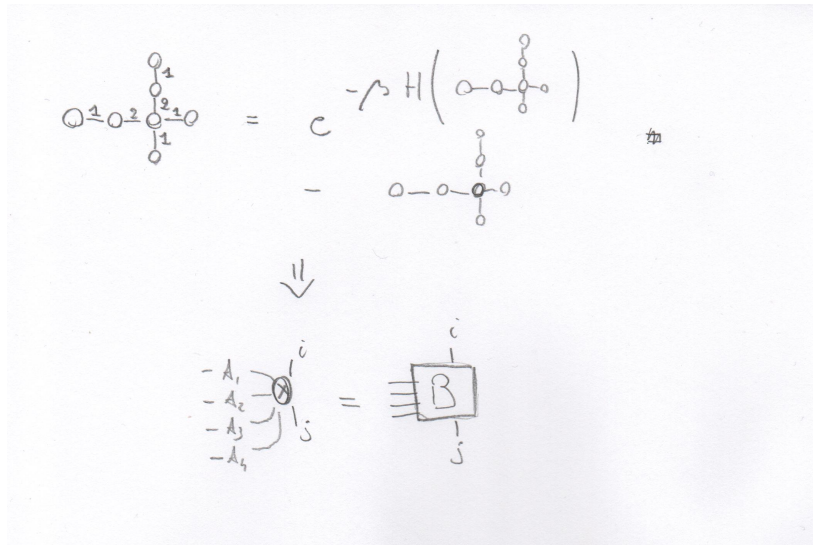
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Linear solver

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- types of inversion
- numerical stability
- implemented for any shape
- if connected -> split with SVD

```
[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.
```

sequential linear

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

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true non-linear solver

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

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$$\hat{H} = -J \left(\sum_{\langle ij \rangle} \sigma_i^x \sigma_j^x + \Gamma \sum_i \sigma_i^z \right) \quad (24)$$

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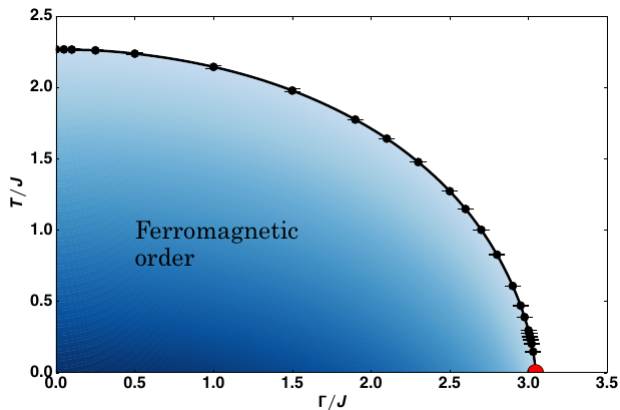


Figure: figure taken from [1]

First results

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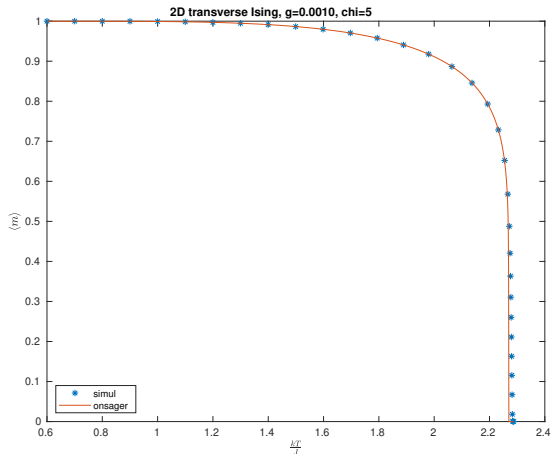
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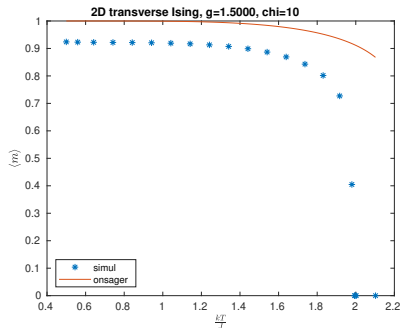
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First results

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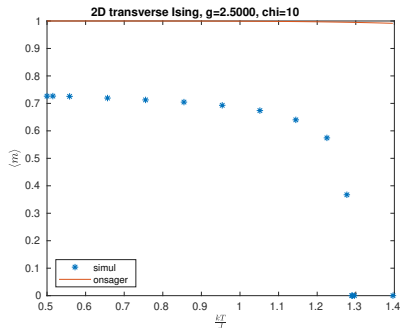
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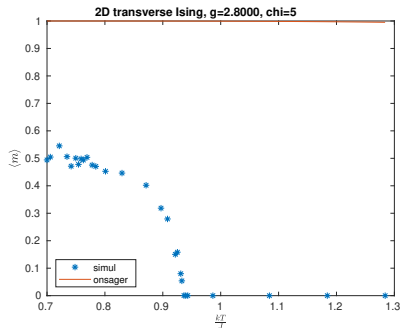
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Conclusion

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

Short term

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- Accurate estimate Transversal using quantum critical point
- Improve blocks for loops
-

Short term

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- Incorporate symmetries Hamiltonian
- Look at other models
- Generalize for other lattice geometries
- Generalize to 3D

References I

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S. Hesselmann, S. Wessel, Thermal ising transitions in the vicinity of two-dimensional quantum critical points, Phys. Rev. B 93 (2016) 155157.

doi:10.1103/PhysRevB.93.155157.

URL <https://link.aps.org/doi/10.1103/PhysRevB.93.155157>