PEPO cluster expansion of tensor exponential

David Devoogdt

Faculty of Engineering and Architecture
Ghent University

May 7, 2021

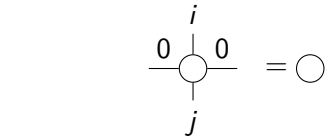
Intoduction

Statistical Quantum mechanics

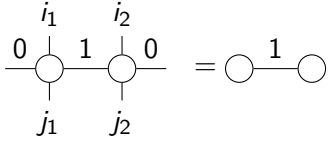
$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{Z} \tag{1}$$

$$\begin{aligned} Z &= \mathrm{Tr}\left(e^{-\beta \hat{H}}\right) \\ \langle X \rangle &= \mathrm{Tr}\left(\rho \hat{X}\right) \end{aligned} \tag{2}$$

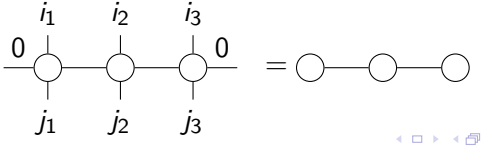
Graphical notation



(3)



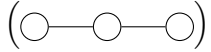
(4)



(5)

Graphical notation

$$\hat{H} = \left(\sum_{<ij>} H_2^i H_2^j + \sum_i H_1^i \right) \tag{6}$$

H 

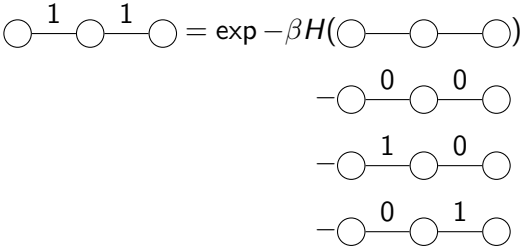
$$\begin{aligned} &= H_1 \otimes 1 \otimes 1 \\ &+ 1 \otimes H_1 \otimes 1 \\ &+ 1 \otimes 1 \otimes H_1 \\ &+ H_2 \otimes H_2 \otimes 1 \\ &+ 1 \otimes H_2 \otimes H_2 \end{aligned} \tag{7}$$

General idea

$$\bigcirc = \exp\left(-\beta H(\bigcirc)\right) \tag{8}$$

$$\overset{1}{\bigcirc\!\!-\!\!\bigcirc} = \exp -\beta H(\bigcirc\!\!-\!\!\bigcirc - \overset{0}{\bigcirc\!\!-\!\!\bigcirc}) \tag{9}$$

General idea



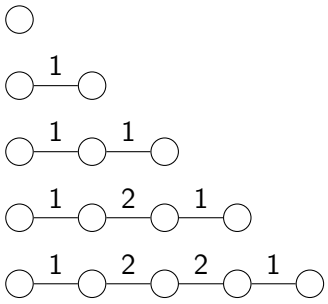
(10)

Advantages

- size extensive
- symmetry
- fast

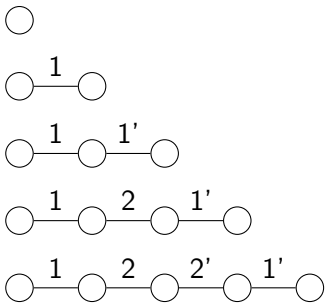
Construction 1D

Variant A



(11)

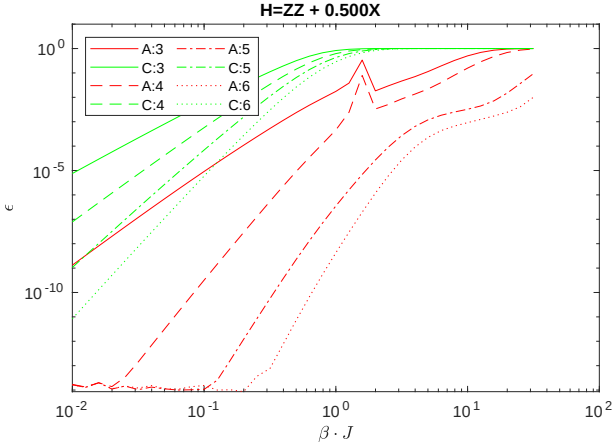
Variant C

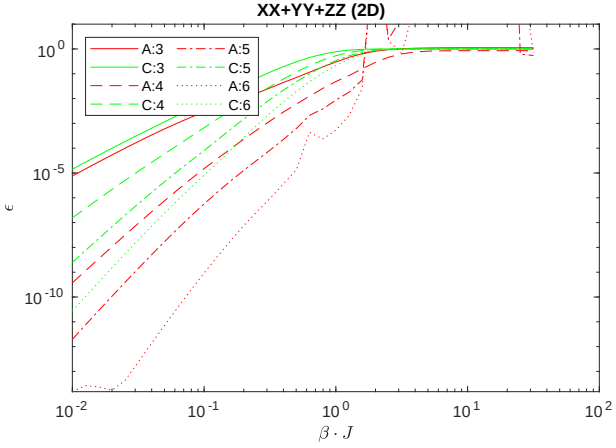


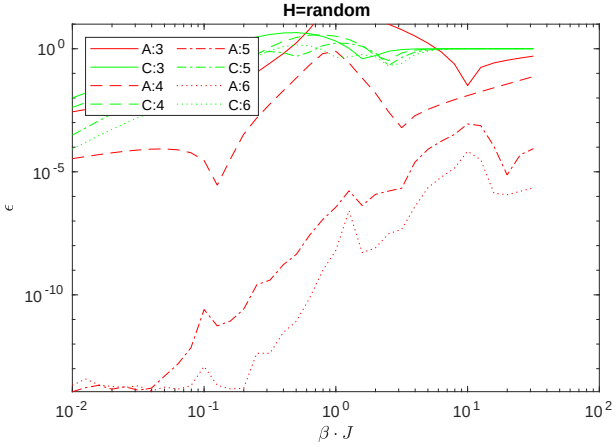
(12)

Error measure

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

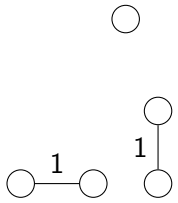






Construction 2D

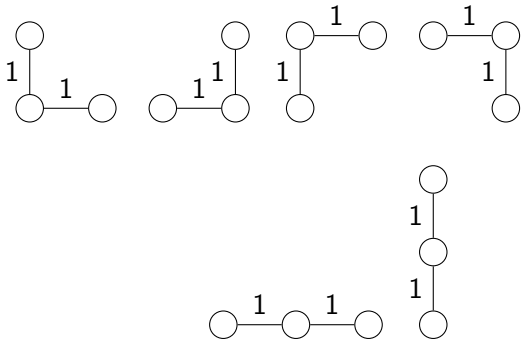
Construction 2D: Linear blocks



(14)

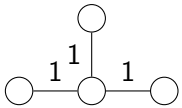
(15)

Construction 2D: Linear blocks

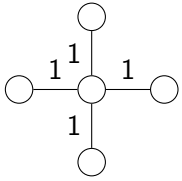


(16)

Construction 2D: Linear blocks

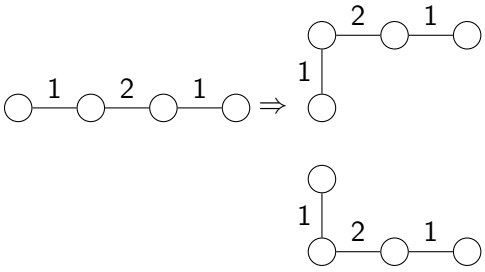


(17)



(18)

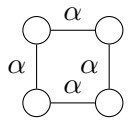
Construction 2D: Linear blocks



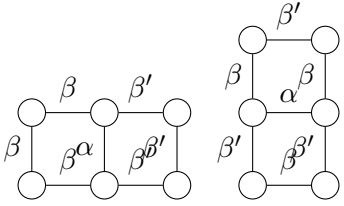
(19)

And many more "linear" blocks

Loops



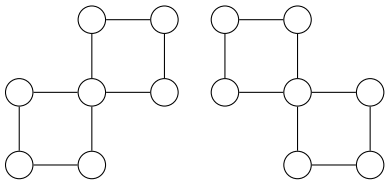
(20)



(21)

- bond dim
- solver: see later

Unsolved



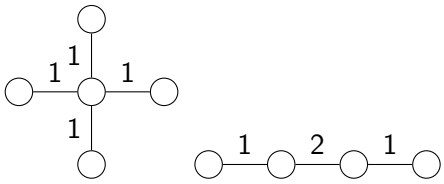
(22)

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

Solvers

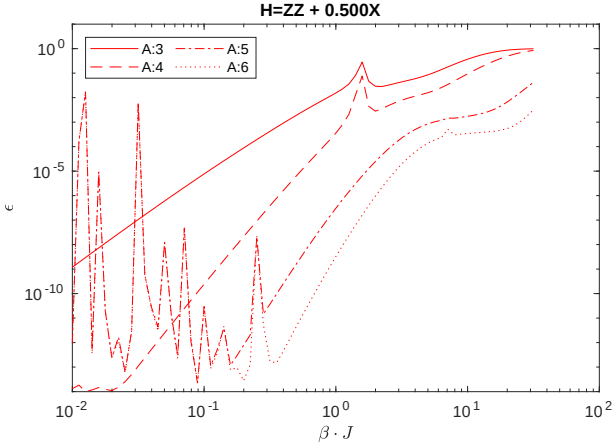
Linear solver

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



(23)

```
[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);
```



sequential linear

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

true non-linear solver

- Matlab fsolve
- exact jocobian
- multiple patterns
- multiple maps

2D Transversal Ising Model

Overview

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

Overview

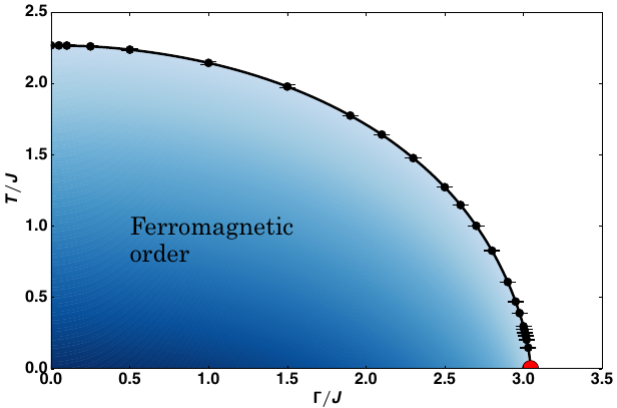
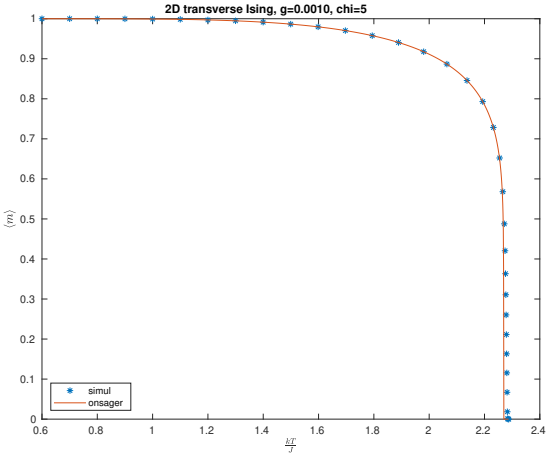
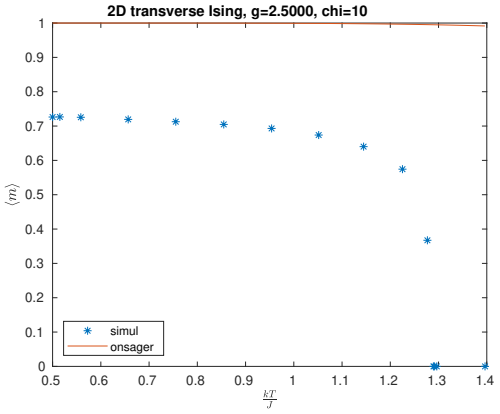


Figure: figure taken from [1]

First results



First results



Conclusion and outlook

Conclusion

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

Outlook: short term

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

Outlook: long term

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

References I


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