# PEPO cluster expansion of tensor exponential

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# Intoduction

# Statistical Quantum mechanics

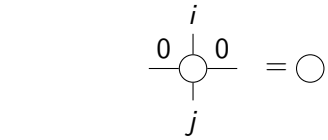


$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{Z} \tag{1}$$

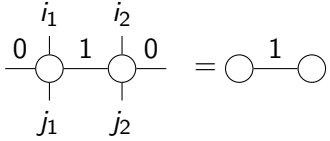
$$\begin{aligned} Z &= \mathrm{Tr}\left(e^{-\beta \hat{H}}\right) \\ \langle X \rangle &= \mathrm{Tr}\left(\rho \hat{X}\right) \end{aligned} \tag{2}$$

# Graphical notation






(3)

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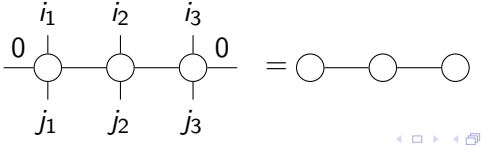
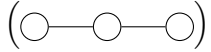



(5)

# 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

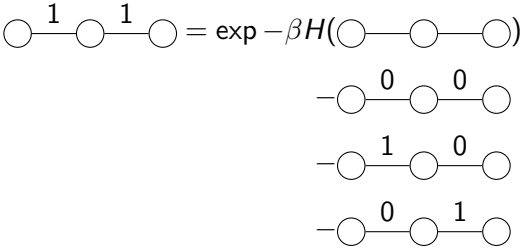


$$\bigcirc = \exp\left(-\beta H(\bigcirc)\right) \tag{8}$$

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

# General idea






(10)

# Advantages

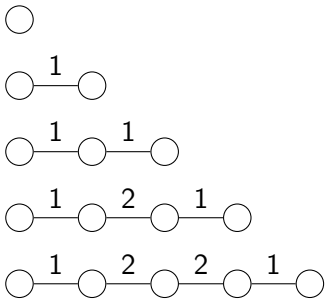


- size extensive
- symmetry
- fast

# Construction 1D

# Variant A

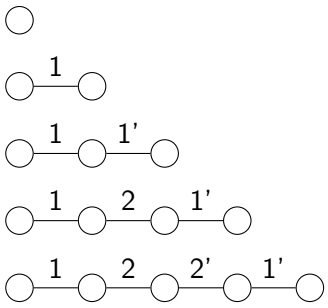





(11)

# Variant C



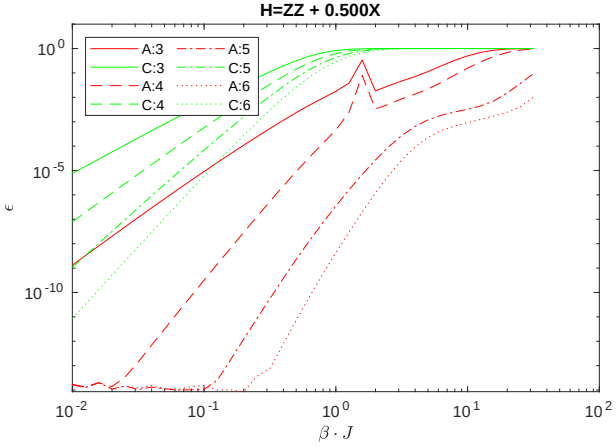


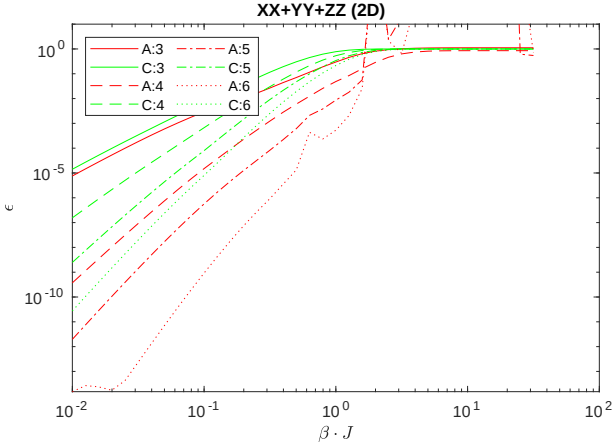

(12)

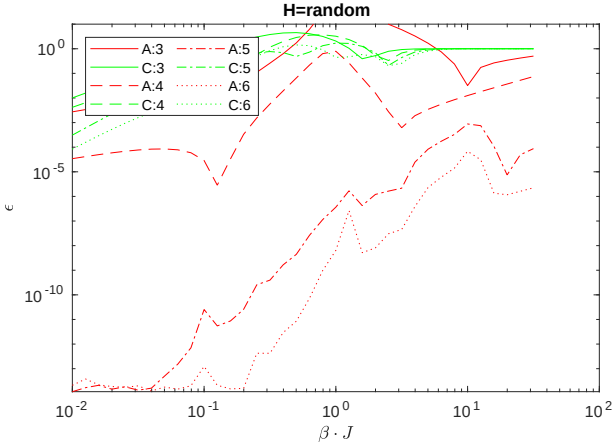
# Error measure



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



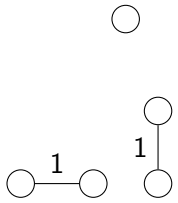




# Construction 2D

# Construction 2D: Linear blocks





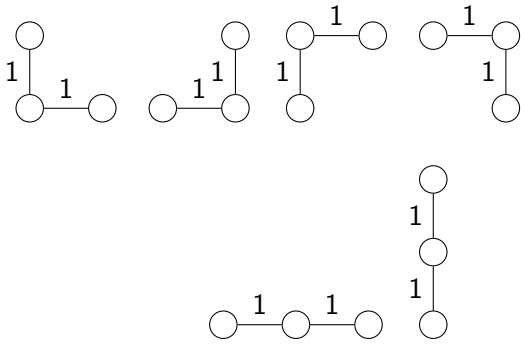
(14)




(15)

# Construction 2D: Linear blocks

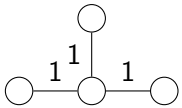




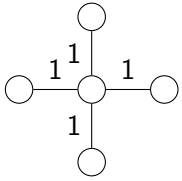

(16)

# Construction 2D: Linear blocks





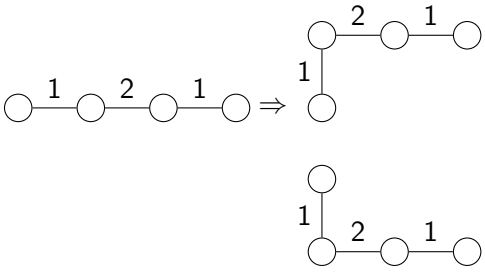

(17)




(18)

# Construction 2D: Linear blocks



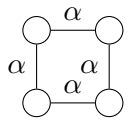



(19)

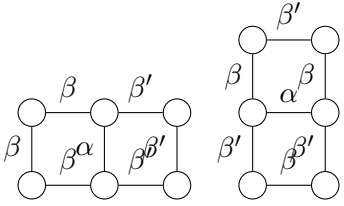
And many more "linear" blocks

# Loops






(20)

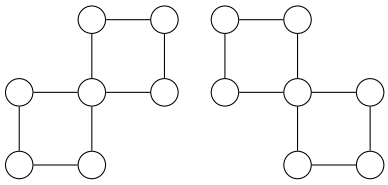



(21)

- bond dim
- solver: see later

# Unsolved





(22)

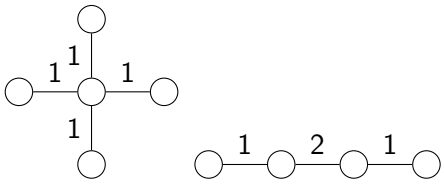
Easy to solve on finite lattice, difficult in thermodynamic limit...

# Solvers

# Linear solver

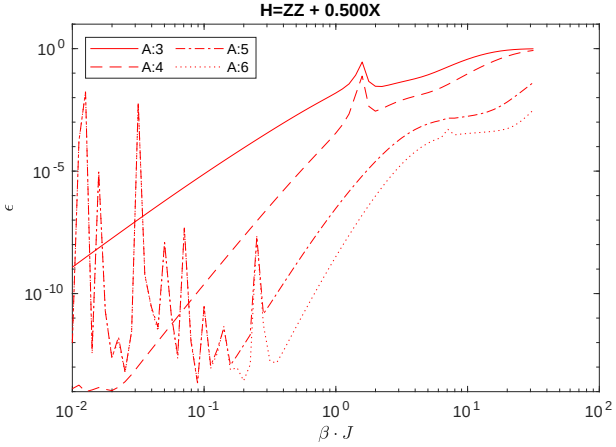


- pseudoinverse
- optimisation for tree graphs
- implemented for any shape




(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



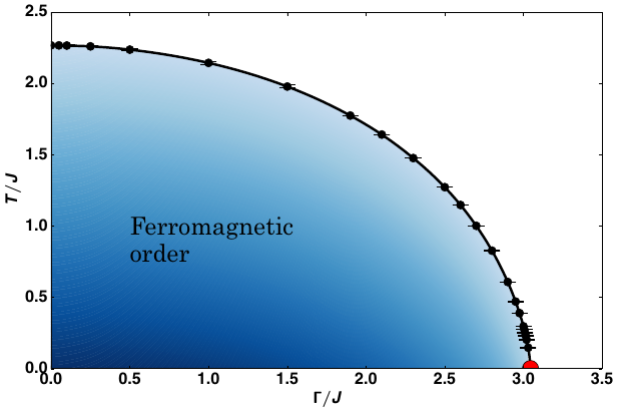
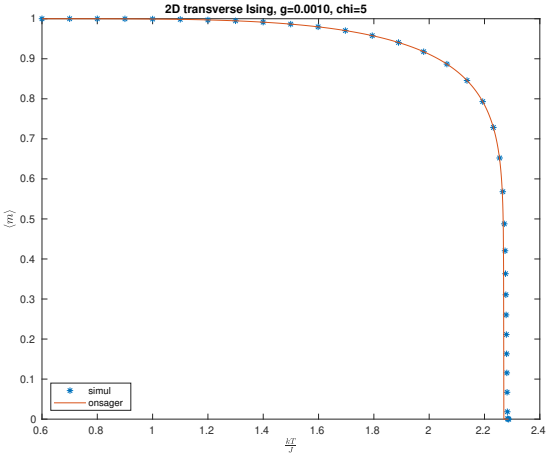



Figure: figure taken from [1]

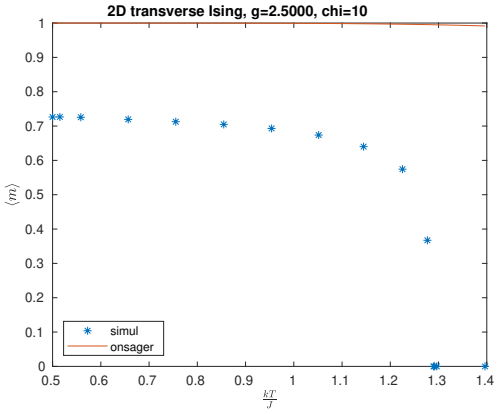
# First results





# 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