PEPO cluster expansion of Tensor Exponential

Subtitle

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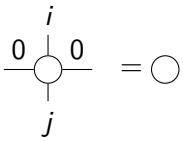
Intoduction

Statistical Quantum mechanics

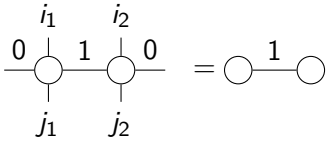
$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{Z} \tag{1}$$

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

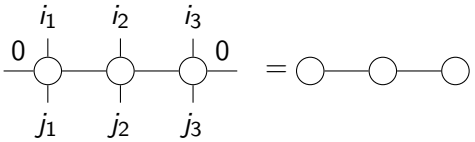
Graphical notation



$$= \quad (3)$$



$$= \quad (4)$$



$$= \quad (5)$$

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

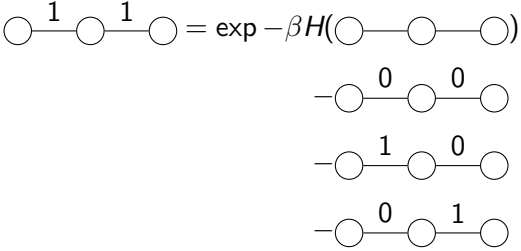
- represent as MPO/PEPO
- cluster by size, not in β

General idea

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

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

General idea



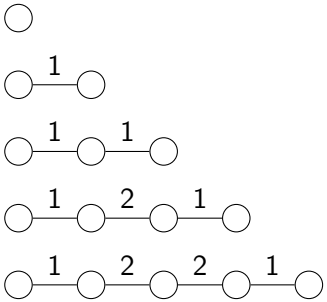
(10)

Advantages

- size extensive
- symmetry

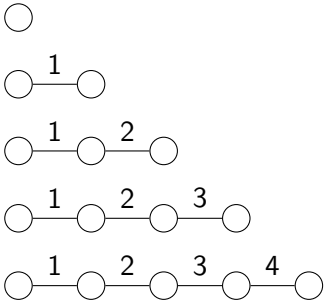
Construction 1D

Variant A



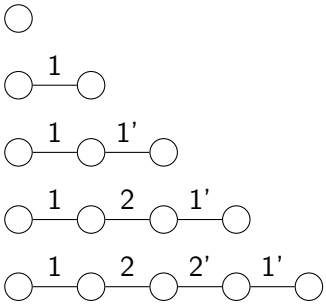
(11)

Variant B



(12)

Variant C

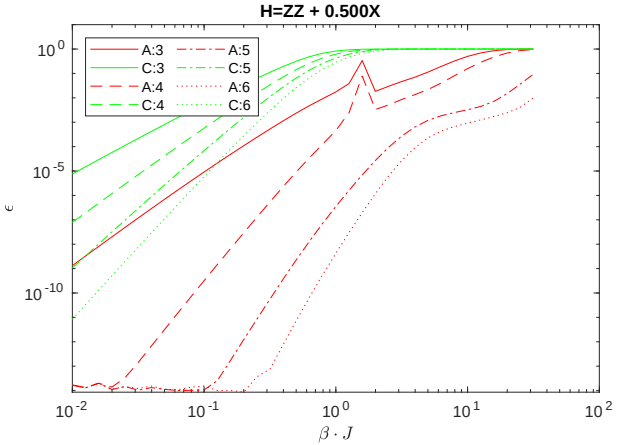


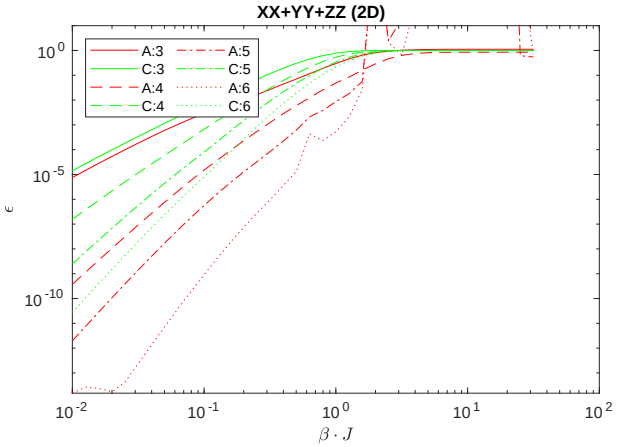
(13)

- bond dimension
- "unwanted" chains

Error measure

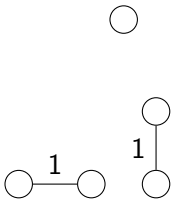
- cyclic
- relative
- 12 sites





Construction 2D

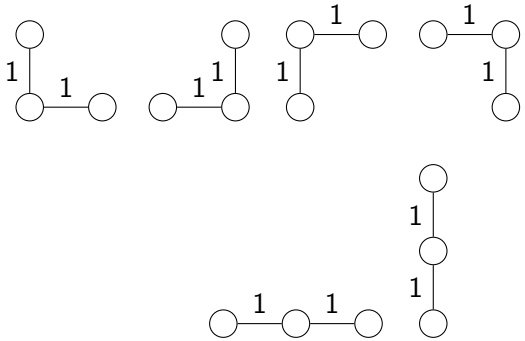
Construction 2D: Linear blocks



(14)

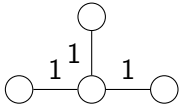
(15)

Construction 2D: Linear blocks

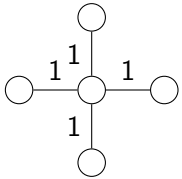


(16)

Construction 2D: Linear blocks

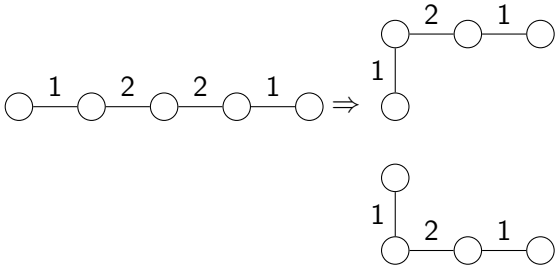


(17)



(18)

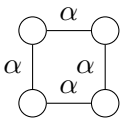
Construction 2D: Linear blocks



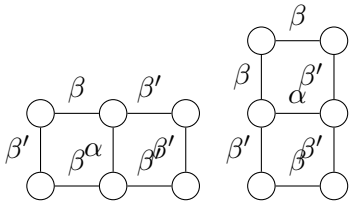
(19)

And many more "linear" blocks

Loops



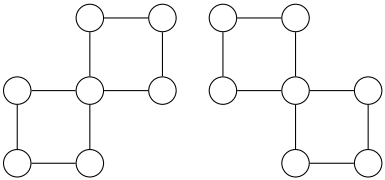
(20)



(21)

- bond dim
- solver: see later

Unsolved



(22)

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

Solvers

Numerical considerations

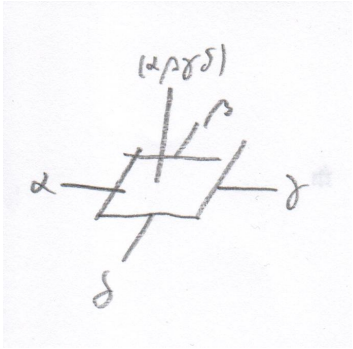
Normalisation: PEPS $O \to O/\alpha$

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

Avoid large values in tensor

Fast cell contraction

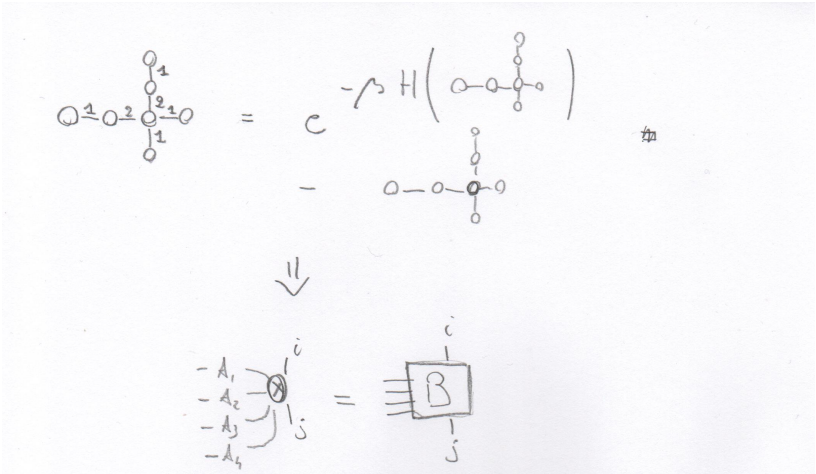
- Bottleneck: find all possible contractions of virtual levels
- Solution: Construct sparse PEPO, contract geometry



Solver

- "Linear" problems
- non-linear problems

Linear Solver



Linear solver

- 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);
```

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

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

Overview

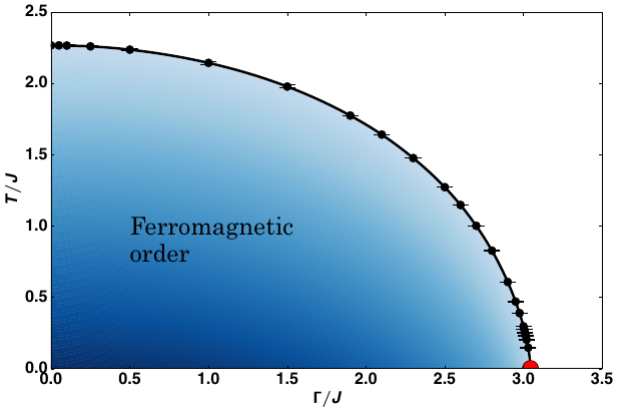
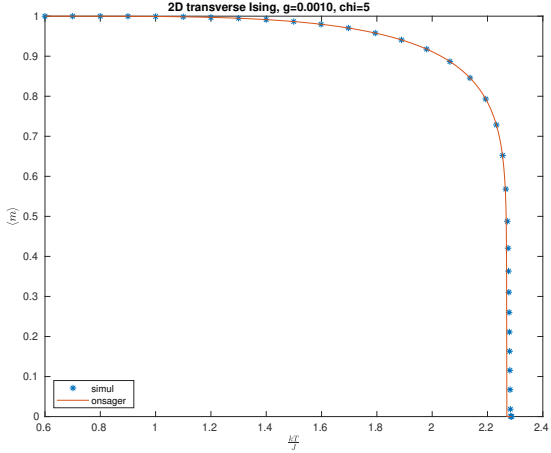
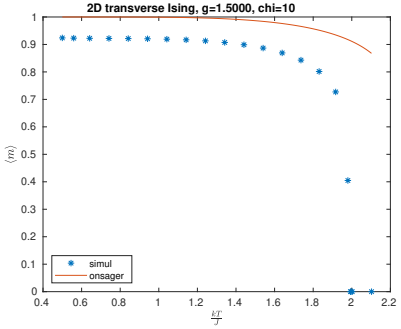


Figure: figure taken from [1]

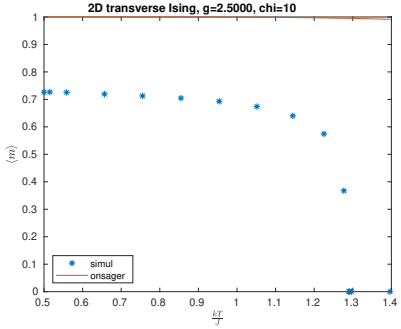
First results



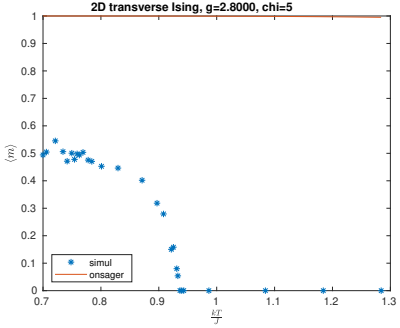
First results



First results



First results



Conclusion and outlook

Conclusion

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

Short term

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

Short term

- Incorporate symmetries Hamiltonian
- Look at other models
- 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