Coarse-Graining Renormalization Using the Higher-Order Singular Value Decomposition

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Generalities

Tensor Networks

Tensor Network Diagrams:

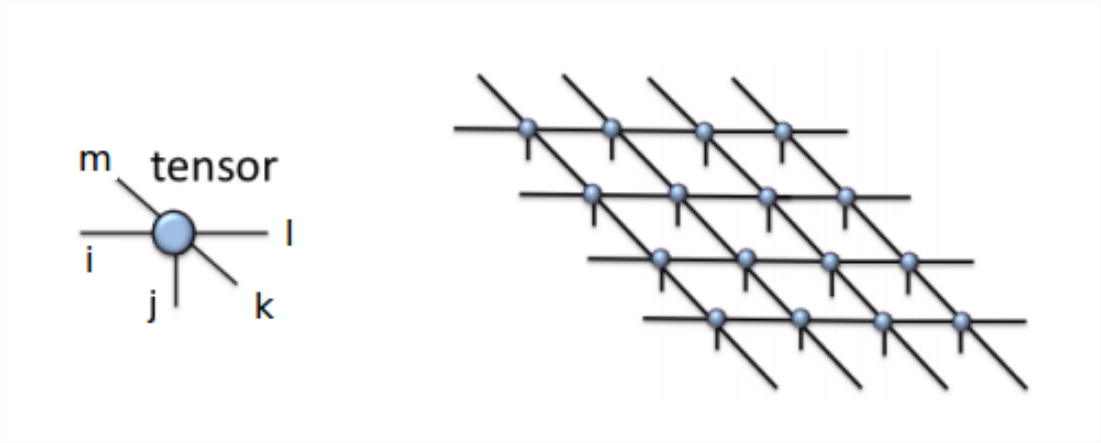


Figure 1: Taken from Orús (2014)

$$T_{ijklm}$$

Each tensor is represented by a node and each of its indices is represented by a leg.

Tensor Networks

Connected legs represent contracted indices between tensors

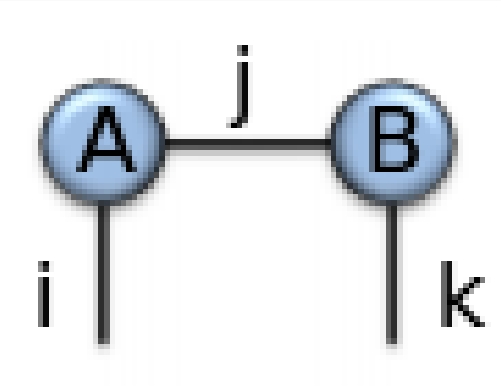


Figure 2: Taken from Orús (2014)

$$\sum_j A_{ij} B_{jk} = C_{ik}$$

Tensor Networks

States of physical systems can be decomposed into Tensor Networks in several ways. For example:

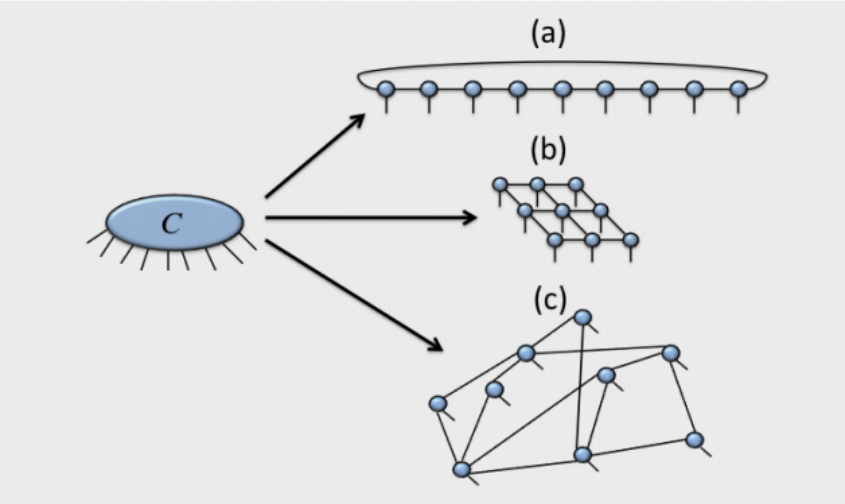


Figure 3: Decomposition of a state into (a) Matrix Product State. (b) Projected Entangled Pair State. (c) Arbitrary Tensor Network. Taken from Orús (2014)

Advantage: Non-physical bond dimensions can be truncated in order to reduce the dimension of the Hilbert Space!

Singular Value Decomposition

A way of reducing the dimension of a tensor index while making sure that the most relevant information is kept is by performing a Singular Value Decomposition **(SVD)** and keeping only the D dimensions related to the D biggest Singular Values.

SVD of a matrix:

$$M = U\Sigma V^{\dagger}$$

- M : n x m matrix
- U : n x n unitary matrix
- Σ : n x m pseudo-diagonal matrix of Singular Values in descending order
- $V^{\dagger}$: m x m unitary matrix

Ordering of Σ allows to truncate its dimension to some chosen value D so that the D biggest singular values are kept and the rest are discarded.

Higher Order Singular Value Decomposition

Higher Order Singular Value Decomposition **(HOSVD)** is a generalization of SVD for tensors of rank higher than 2.

Unfolding of a tensor into a matrix:

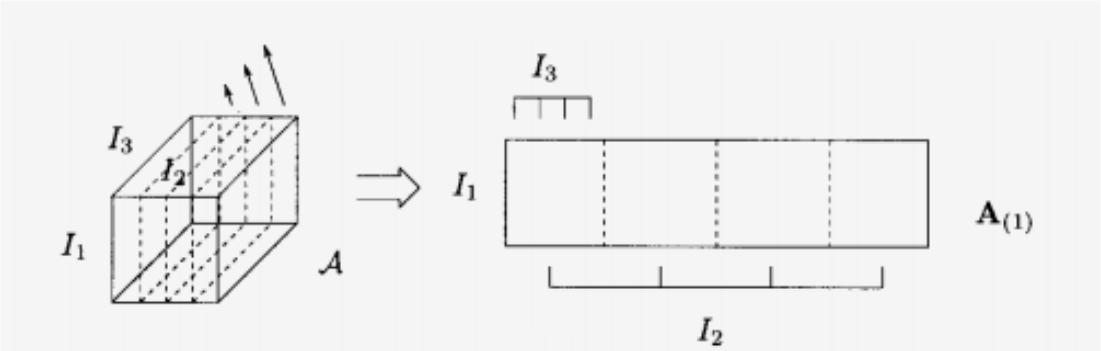


Figure 4: Unfolding of (I_1, I_2, I_3) tensor into $(I_1, I_2 I_3)$ matrix. Taken from de Lathauwer et al. (2000)

Higher Order Singular Value Decomposition

The HOSVD of a rank N tensor T of dimensions (I_1,I_2,...,I_N) is given by

$$T_{j_1,j_2,...,j_N} = S_{i_1,i_2,...,i_N} U^{(1)}_{i_1,j_1} U^{(2)}_{i_2,j_2} ... U^{(N)}_{i_N,j_N}$$

where

- S : rank N tensor of dimensions (I_1,I_2,...,I_N) with properties:
  - all-orthogonality: Two (N-1) rank sub-tensors $S_{i_n=\alpha}$ and $S_{i_n=\beta}$ are orthogonal for all values of n and $\alpha \neq \beta$.
  - ordering: $\|S_{i_n=1}\| \geq \|S_{i_n=2}\| \geq ... \geq \|S_{i_n=I_n}\| \geq 0$ for all values of n. $\|T\|$ is the Frobenius norm of a tensor.
- $U^{(n)}$: I_n x I_n unitary matrix

Higher Order Singular Value Decomposition

Theorem: The HOSVD of a tensor T is related to the SVD of its matrix unfoldings $A_{(n)}$ by

$$A_{(n)} = U^{(n)} S_{(n)} (U^{(n+1)} \otimes ... \otimes U^{(N)} \otimes U^{(1)} \otimes ... \otimes U^{(n-1)})^{\dagger}$$

Where $S_{(n)}$ is the n unfolding of the S tensor of the HOSVD of T. This can always be written as

$$A_{(n)} = U^{(n)} \Sigma^{(n)} V^{(n)\dagger}$$

Where it can be proven that the decomposition is in fact the SVD of $A_{(n)}$

Higher Order Tensor Renormalization Group

Tensor Renormalization Group (TRG)

- Devised by Levin and Nave in 2007 as a method for studying 2D classical models inspired by the success of Tensor Network based approaches for 1D quantum systems such as the Density Matrix Renormalization Group (DMRG).
- Coarse-graining of a lattice based on SVD of **matrices**.
- Difficult to extend to 3D due to the increase of order of local tensors and due to changes of lattice topology in the coarse graining process.

Higher Order Tensor Renormalization Group (HOTRG)

- Uses HOSVD of tensors instead of SVD of matrices, which results in a better truncation scheme.
- It is easily extended to 3D lattices.

HOTRG in the 2D Ising Model

2D Ising model in a square lattice Hamiltonian (no external field):

$$H = -\sum_{<i,j>} S^i S^j$$

First step is to convert the partition function

$$Z = \sum_{\{c\}} e^{-\beta H(c)}$$

Into a Tensor Network

HOTRG in the 2D Ising Model

To do this, consider the local interactions so that we can write $H^{loc}(S^i, S^j) = -S_i S_j$, which can be represented as the matrix

$$H^{loc} = \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}$$

and the Boltzmann factor can then be represented as

$$Q = \begin{bmatrix} exp(-\beta H_{11}^{loc}) & exp(-\beta H_{12}^{loc}) \\ exp(-\beta H_{21}^{loc}) & exp(-\beta H_{22}^{loc}) \end{bmatrix} = \begin{bmatrix} exp(\beta) & exp(-\beta) \\ exp(-\beta) & exp(\beta) \end{bmatrix}$$

Since the complete Hamiltonian is the sum over all lattice sites of the local interactions, the partition function can be written as

$$Z = \sum_{\{c\}} \prod_{<i,j>} Q_{S_i, S_j}$$

HOTRG in the 2D Ising Model

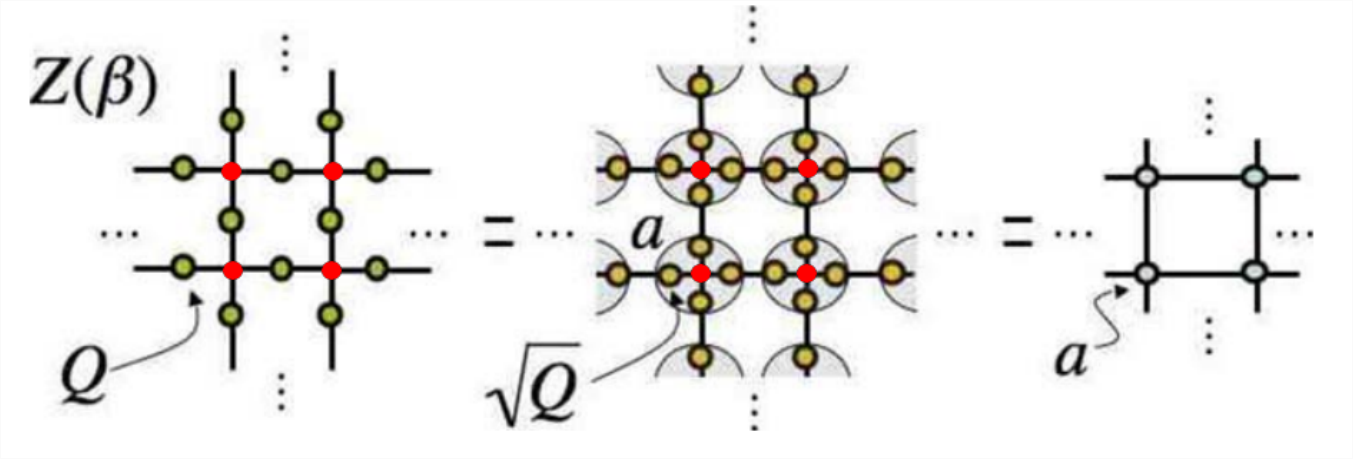


Figure 5: Taken from Orús and Vidal. (2008)

where the red dots are the generalized delta tensor: δ_{ijkl}. Because contraction means summing over all indices, this Tensor Network captures the sum over configurations that defines the partition function.

We take $\sqrt{Q}$ so we can write our Tensor Network as a periodic lattice with the same tensor **a** in each site.

$$a_{ijkl} = \sum_{s} (\sqrt{Q})_{is} (\sqrt{Q})_{js} (\sqrt{Q})_{ks} (\sqrt{Q})_{ls}$$

HOTRG in the 2D Ising Model

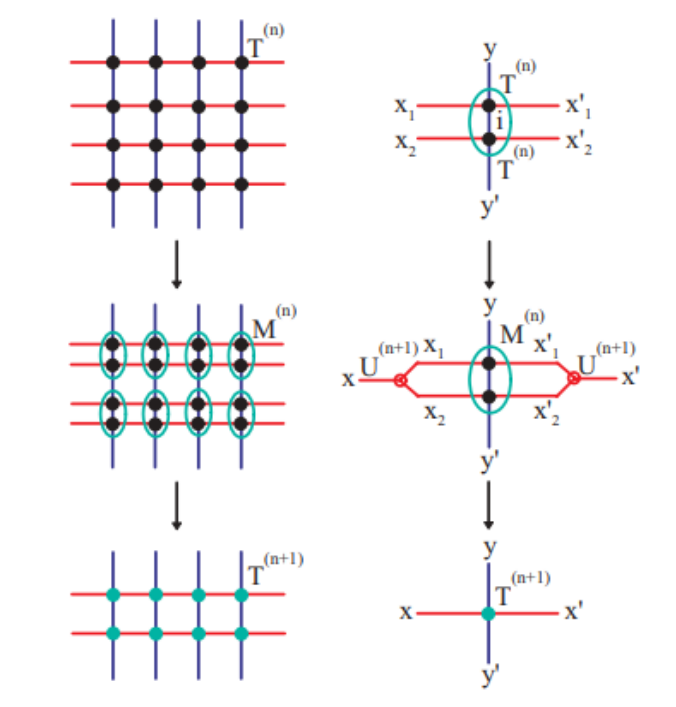


Figure 6: Coarse-graining step in the vertical direction. Taken from Xie et al. (2012)

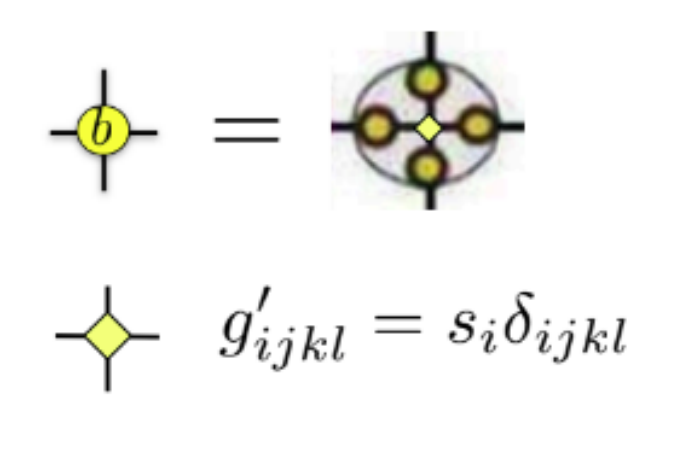
- U is obtained from the HOSVD of tensor M.
- U is truncated to the desired bond dimension D.
- Tensor **a** is updated as:

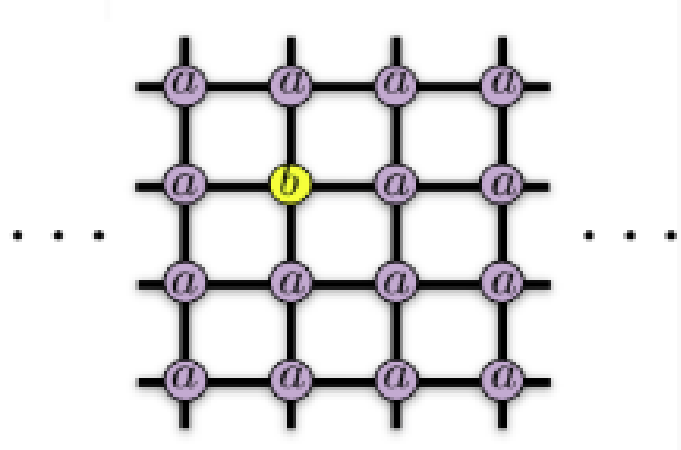
$$a^{(n+1)}_{xx'yy'} = \sum_{ijkl} U_{ijx} M_{ijklyy'} U_{klx'}$$

- A coarse-graining step consists of this being done once in the y direction and once in the x direction.

HOTRG in the 2D Ising Model

Measuring mean magnetization per site





$$b_{ijkl} = \sum_s s(\sqrt{Q})_{is}(\sqrt{Q})_{js}(\sqrt{Q})_{ks}(\sqrt{Q})_{ls}$$

$$m(\beta) =< s >= \frac{\sum_c s_r(c) e^{-\beta H(c)}}{Z}$$

HOTRG in the 3D Ising Model

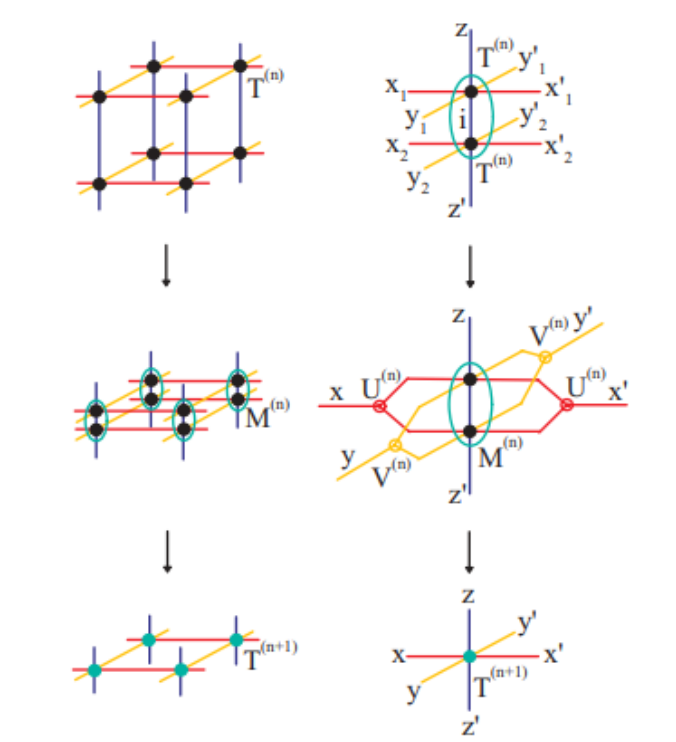


Figure 7: Coarse-graining step in the Z direction in 3D. Taken from Xie et al. (2012)

- Construct the partition function of the 3D model in an equivalent way, now with rank 6 tensors.
- Coarse-graining now must be done in X, Y and Z direction.
- When coarse-graining in the Z direction, we now need to truncate the bond dimensions in both the X and Y directions. Similar for the other two coarse-grainings.

Results

2D Ising Model

Magnetization

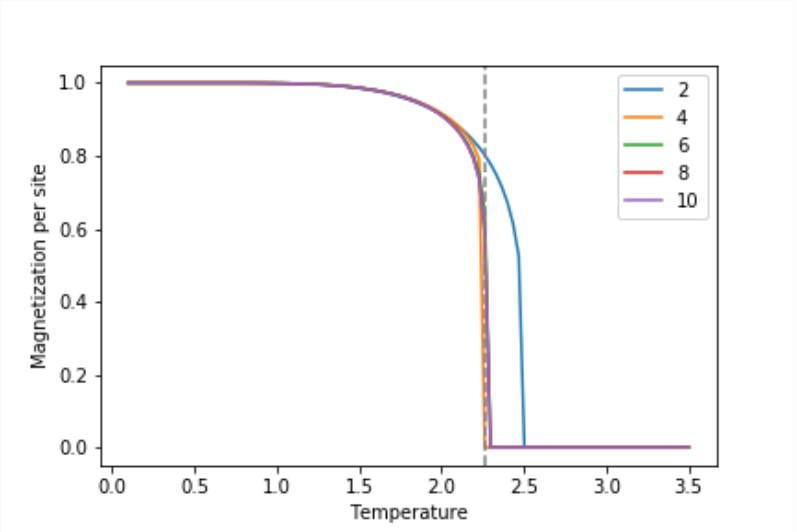


Figure 8: Magnetization per site obtained with HOTRG for 2D Ising model with no external field for different bond dimensions.

Exact solution:

- $T_c = \frac{2}{\ln(1+\sqrt{2})} \approx 2.2691853$
- $m(T) = (1 - (\sinh \frac{2}{T}^{-4}))^{1/8}$ for $T < T_c$
- $m(T) = 0$ for $T > T_c$

2D Ising Model

Magnetization

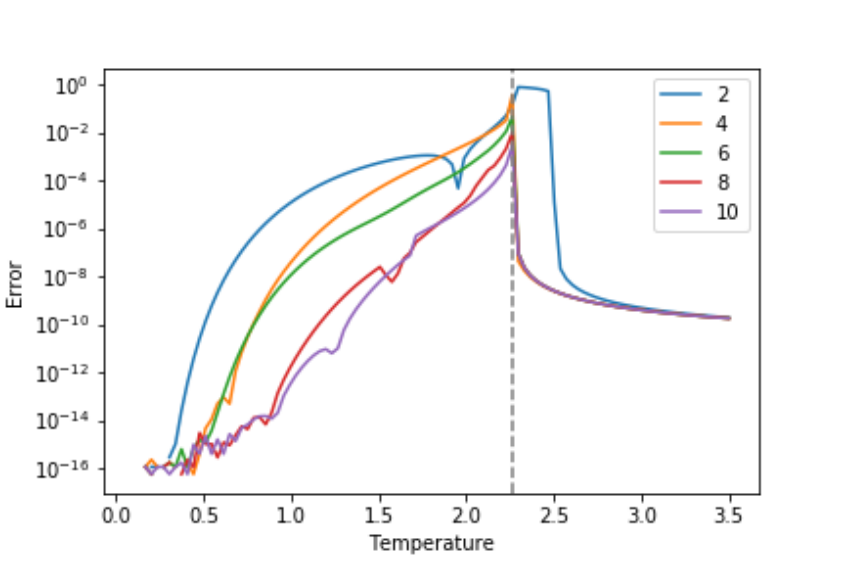


Figure 9: Relative error from analytic solution for different bond dimensions.

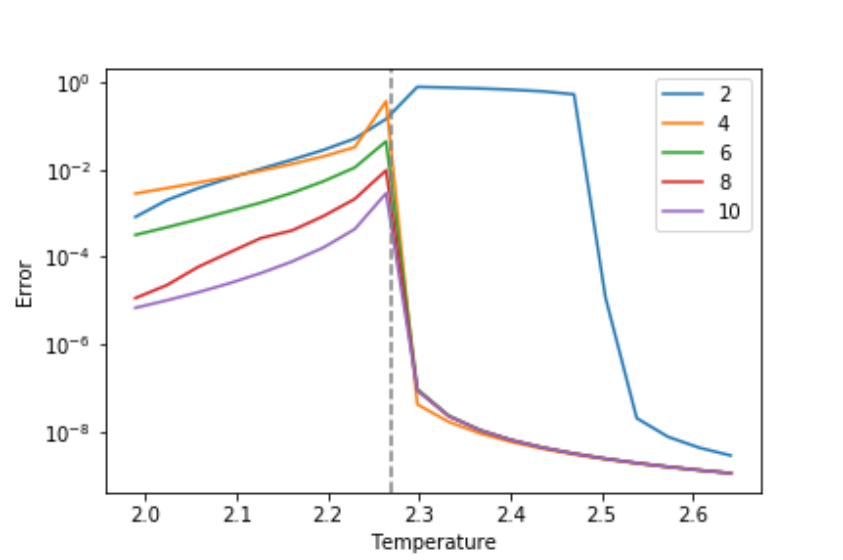


Figure 10: Detail of the error around T_c.

2D Ising Model

Free energy

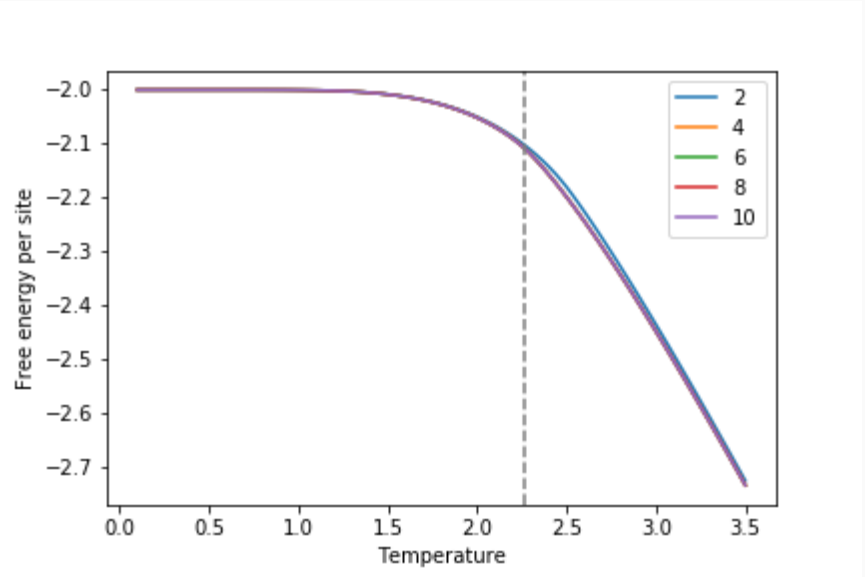


Figure 11: Free energy per site obtained with HOTRG for 2D Ising model with no external field for different bond dimensions.

$$f = \frac{-T \ln Z}{N}$$

Onsager's exact solution:

$$\beta f(T) = \ln 2 + \frac{1}{2\pi^2} \int_0^\pi \int_0^\pi \ln\left[\cosh^2 2\beta - \sinh^2 2\beta(cos\theta_1 + cos\theta_2)\right] d\theta_1 d\theta_2$$

Free energy

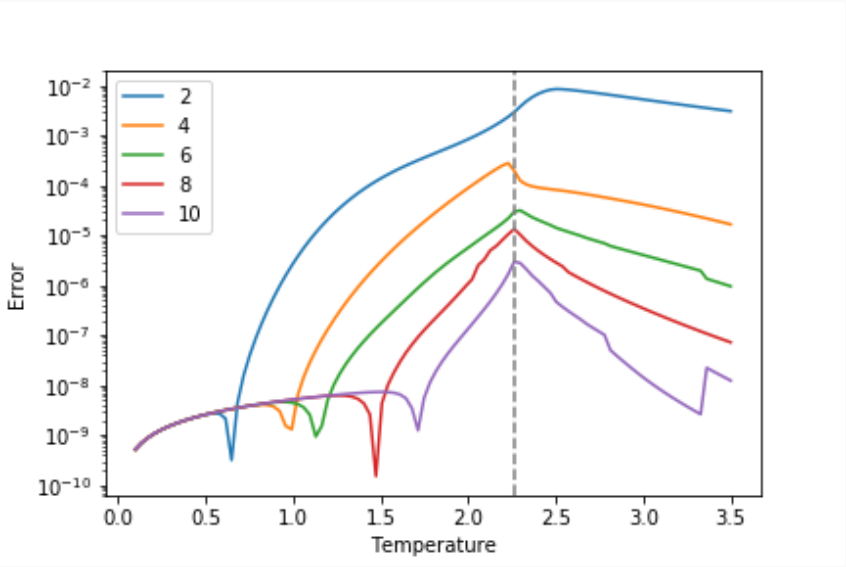


Figure 12: Relative error from Onsager's solution for different bond dimensions.

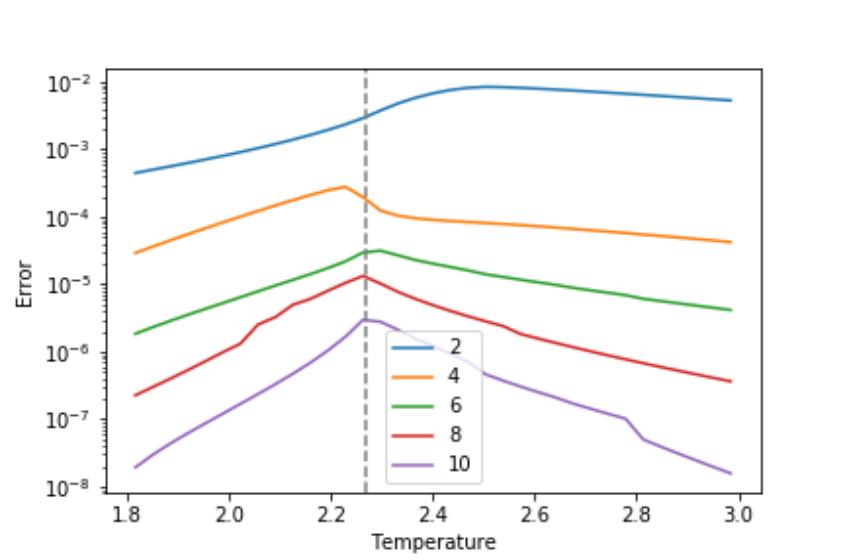


Figure 13: Detail of the error around T_c.

2D Ising Model

Internal Energy and Heat Capacity

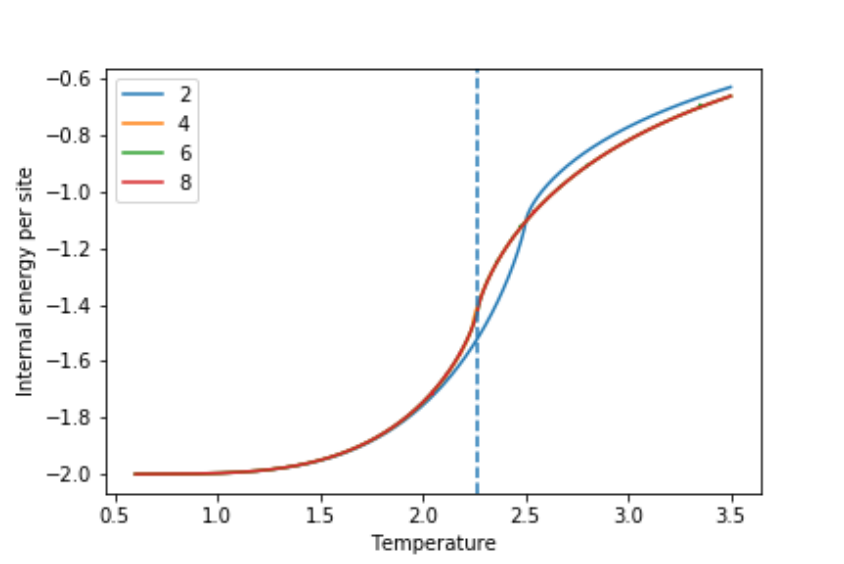


Figure 14: Internal energy per site obtained with HOTRG for 2D Ising model with no external field for different bond dimensions.

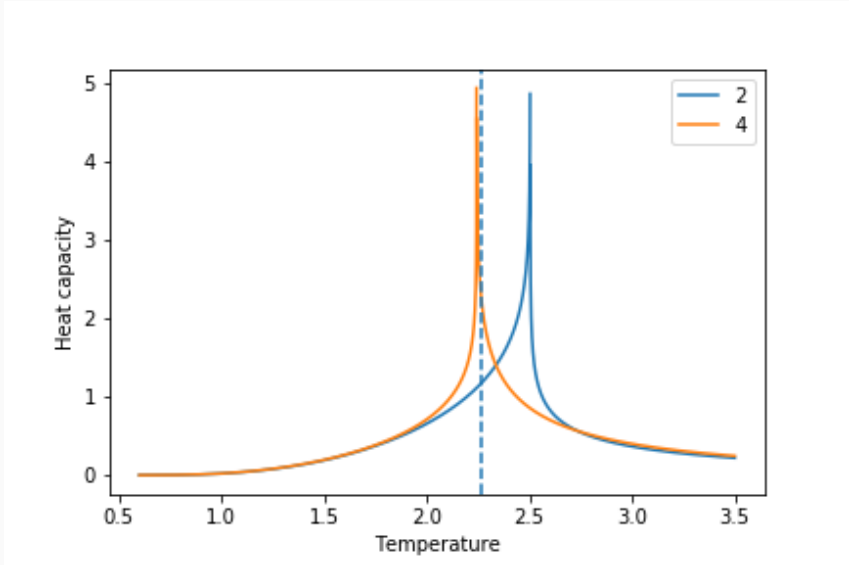


Figure 15: Heat capacity per site obtained with HOTRG for 2D Ising model with no external field for different bond dimensions.

$$u = -\frac{1}{N}\frac{\partial \ln(Z)}{\partial \beta}$$

$$c_H = \left(\frac{\partial u}{\partial T}\right)_H$$

3D Ising Model

Magnetization

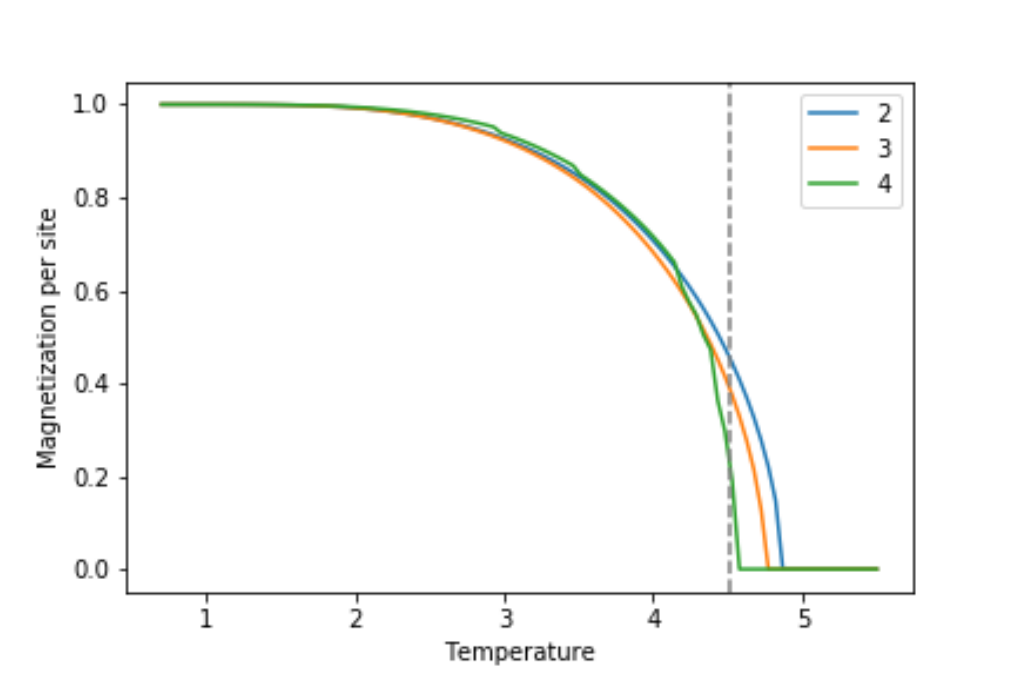


Figure 16: Magnetization per site obtained with HOTRG for 3D Ising model with no external field for different bond dimensions. Grey line shows the best value found by Xie et al. for the critical temperature: $T_c = 4.511544$

According to Xie et al., results converge for $D \geq 13$!

3D Ising Model

Free energy

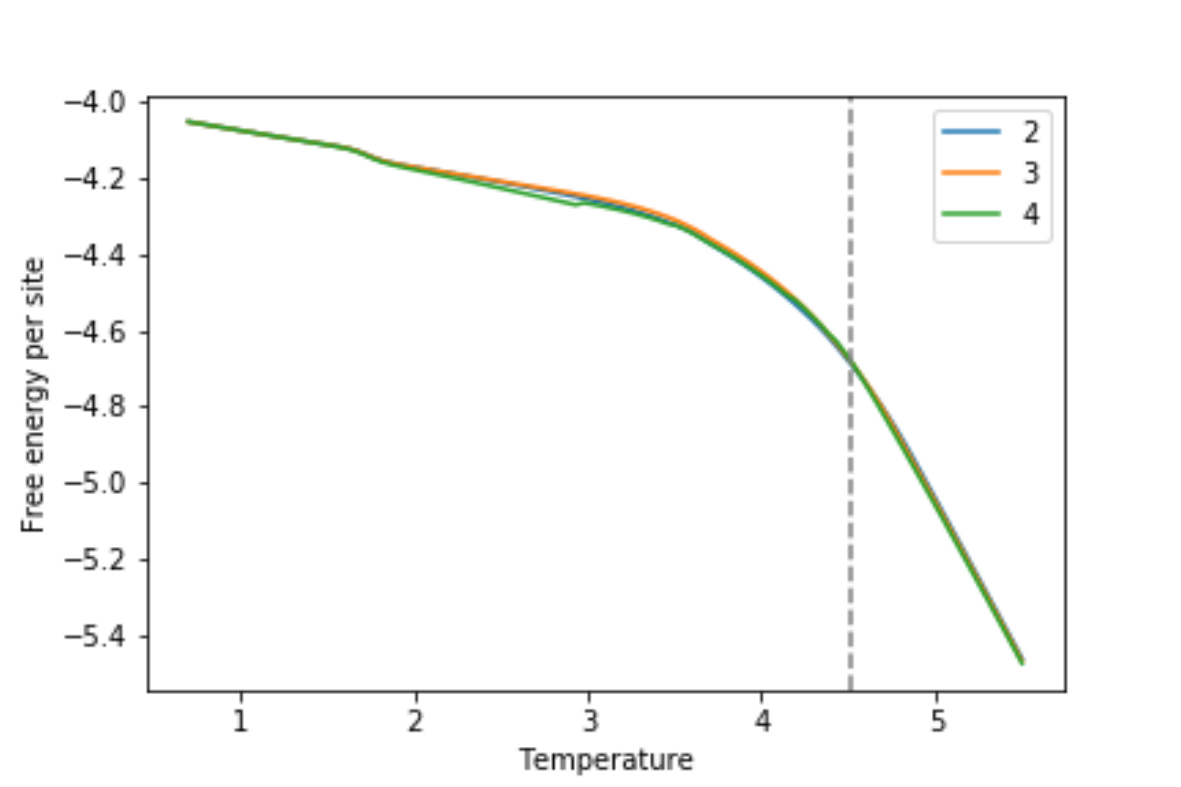


Figure 17: Free energy per site obtained with HOTRG for 3D Ising model with no external field for different bond dimensions. Grey line shows the best value found by Xie et al. for the critical temperature: $T_c = 4.511544$

Conclusion

Conclusions

The method works!

Conclusions

How could it be improved:

- Finding a more efficient way of implementing the methods in order to be able to compute for higher values of D (specially in the 3D case).
- Find a better computer.
- Construct a tensor network that allows to find the Internal Energy per site using HOSVD instead of obtaining it via numerical derivation of the partition function.

Conclusions

What else can be done?

- **Higher Order Second Renormalization Group (HOSRG):** Extends HOTRG from a local optimization method to a global one by taking in account the renormalization effect of the environment in each coarse-graining step.
- **Application to quantum lattice models:** Use Trotter-Suzuki decomposition to exploit the equivalence between a d-dimensional quantum lattice model with a (d+1)-dimensional classical model and use the methods discussed here.

Questions?

References i

- Z. Y. Xie, J. Chen, M. P. Qin, J. W. Zhu, L. P. Yang, and T. Xiang, Phys. Rev. B 86, 045139 (2012).
- R. Orús and G. Vidal, Phys. Rev. B 80, 094403 (2009)
- M. Levin and C.P. Nave, Phys. Rev. Lett 99, 12061 (2007)
- L. de Lathauwer, B. de Moor, and J. Vandewalle, SIAM J. Matrix Anal. Appl. 21, 1253 (2000)
- R. Orús, cond-mat.str-el arXiv:1306.2164v3 (2014)