Master Engineering Physics

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Master desertation

Thesis Tensor networks

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Contents

Todo list

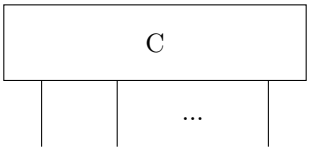


Figure 1: Caption

1 Introduction

write this

To deal with these strongly correlated systems, a class of methods called tensor networs were introced.

2 tensor networks

2.1 introduction

2.2 1D

2.2.1 MPS

A general quantum state with n sites can be described in a given basis $|i\rangle$ as

$$|\Psi\rangle = \sum_{i_1 i_2 \cdots i_n} C^{i_1 i_2 \cdots i_n} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle \tag{1}$$

This requires an exponential number d^n of coefficients C where d is the dimensions of basis $|i\rangle$.

In order to make the problem tractable, the following form is proposed as wavefunction:

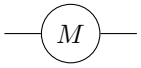
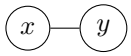
$$C^{i_1 i_2 \cdots i_n} = C^{1\,i_1}_{\ \ \alpha_1} C^{2\,i_2}_{\alpha_1 \alpha_2} \cdots C^{n\,i_n}_{\alpha_{n-1}} \tag{2}$$

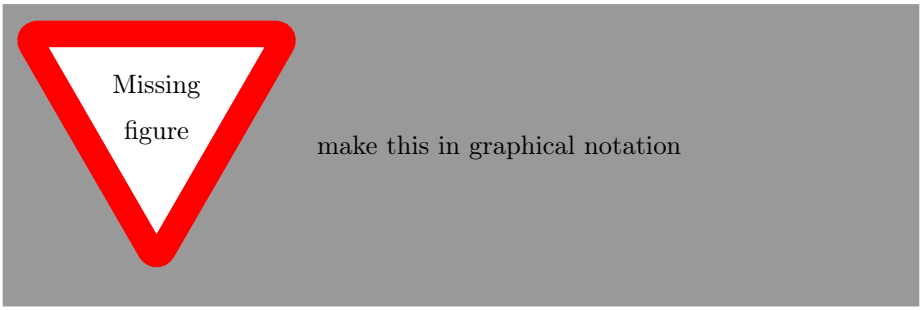
Where summation over shared indices is implied. It is always possible to find such an representation by means of matrix decomposition. The summation over α_i are called virtual bond and their dimension is denoted by χ.

Explicit translational invariance is given by tensor $C^i_{\alpha\beta}$ that don't depend on the location. The chain is closed by setting $\alpha_n = \alpha_0$. We can now write this as a Trace over matrix products:

$$|\Psi\rangle = \mathrm{Tr}\big(C^{i_1} C^{i_2} \cdots C^{i_n}\big) |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle \tag{3}$$

Table 1: Caption

conventional	Einstein	tensor notation
$\vec{x}$	x_α	
M	$M_{\alpha\beta}$	
$\vec{x}\cdot\vec{y}$	$x_\alpha y_\alpha$	



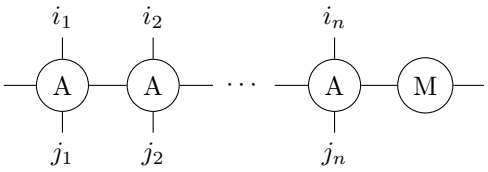
2.2.2 graphical notation

Tensor networks can be written in a graphical notation. The legs f a tensor denote the number of external indices. The upper Connected legs are summed. Some examples are shown in table 1

2.2.3 MPO

In a similar fashion, a Matrix Product Operator (MPO) is of the following form:

$$\begin{aligned}\hat{O} = \sum Tr(A^{i_1 j_1} A^{i_2 j_2} \cdots A^{i_n j_n} M) \\ \times |i_1\rangle\langle j_1| \otimes |i_2\rangle\langle j_2| \otimes \cdots \otimes |i_n\rangle\langle j_n|\end{aligned} \tag{4}$$



connect trace and hide legs at M

The matrix M contains the boundary conditions of the operator. Many Hamiltonians can be represented by an MPO. For ins

2.3 2D

2.3.1 PEPS

2.3.2 PEPO

3 Operator exponentials

3.1 Statistical mechanics

The physics of a system in thermodynamical equilibrium can be derived from it's partition function Z.

$$\begin{aligned} Z &= \sum e^{-\beta E_n} \\ &= \sum_n \left\langle n \left| e^{-\beta \hat{H}} \right| n \right\rangle \\ &= \mathrm{Tr}\left(e^{-\beta \hat{H}}\right) \end{aligned} \tag{5}$$

The first line is the partition function for clasical discrete systems. The index n runs of all possible microstates. It is know that the propability to find the system in a given microstates is given by:

$$p_i = \frac{\sum e^{-\beta E_i}}{Z} \tag{6}$$

An useful quantity is the density matrix ρ.

$$\begin{aligned} \rho &= \sum_j p_i \left|\Psi_j\right\rangle \left\langle\Psi_j\right| \\ &= \sum_j \frac{e^{-\beta \hat{H}}}{Z} \left|\Psi_j\right\rangle \left\langle\Psi_j\right| \end{aligned} \tag{7}$$

With this notation

$$\begin{aligned} Z &= \mathrm{Tr}(\rho) \\ \langle X \rangle &= \mathrm{Tr}\left(\rho \hat{X}\right) \end{aligned} \tag{8}$$

3.2 Time evolutions

3.3 Tensor network methods

3.3.1 Approximations to $\hat{U}(\delta)$

TEBD, MPO $W^{I,II}$

3.3.2 global Krylov method

3.3.3 MPS-local methods

local Krylov TDVP

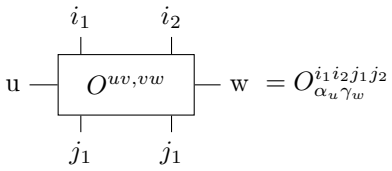
4 Tensor network manipulations

This section severs as an introduction of tensor network manipulations. The overview mainly focusses on MPS/MPO networks, but most of the oprations translate to the 2D case.

The manipulations of MPO's is done by manipulating the tensor into a matrix, performing some matrix calculations and casting it back into it's original form. This section gives some examples how these manipulations are done in practice:

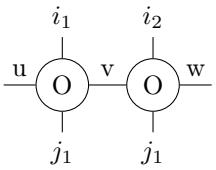
4.1 Basics

4.1.1 decomposition



$$
\begin{aligned}
&= O^{i_1 i_2 j_1 j_2}_{\alpha_u \gamma_w} \\
&\cong O^{uw}_{(\alpha_u i_1 j_1)(\gamma_w i_2 j_2)} \\
&= O^{uv}_{(\alpha_u i_1 j_1)\beta_v} O^{vw}_{\beta_v (\gamma_w i_2 j_2)}
\end{aligned}
\tag{9}
$$

$\cong$



Step 2 reshapes and groups the indices to one index. The dimension of this index is the sum of the seperate dimensions. Step 3 decomposes the matrix into a product of 2 matrices. The last step transforms the indices back to separate legs.

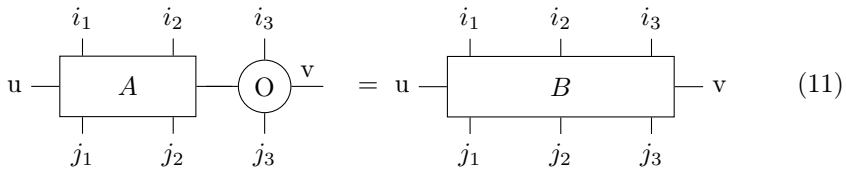
For an exact representation, the bond dimension of virtual level v is:

$$\dim v = \min(\dim u, \dim v) + 2 \dim i \tag{10}$$

Many different matrix decompositions exist. Some usefull examples here are svd decomposition and eigenvalue decomposition. The split in left and right matrix is not unique and differs per algoritm.

4.1.2 inverse

Suppose we want to find a MPO O for given tensors A and B such that the following holds:



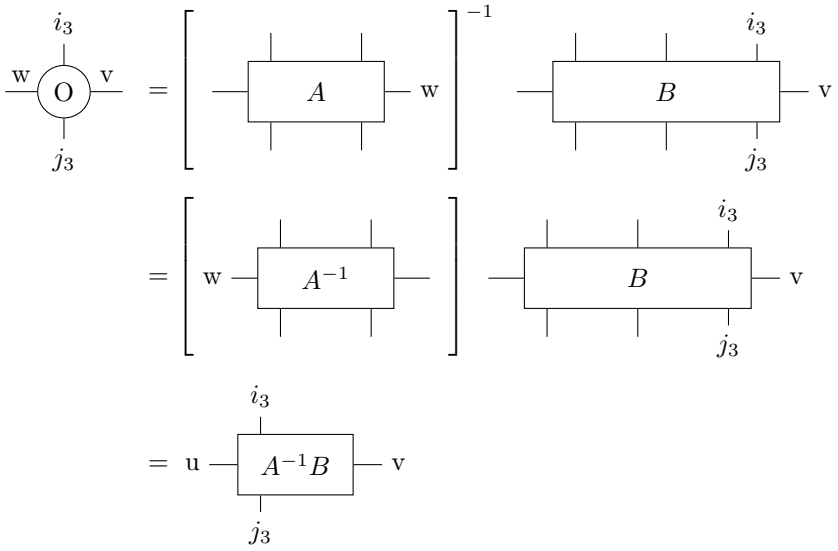
(11)

Again, the indices can be taken toghether in the following way: $\alpha = (ui_1j_1i_2j_2)$ and $\beta = (i_3j_3v)$:

$$A_{\alpha\gamma}O_{\gamma\beta} = B_{\alpha\beta} \tag{12}$$

This a a standard matrix equation and can hence be solved with linear algebra packages. Note that it is not necessary to calculate A^{-1} to obtain the solution. In matlab the procedures mldivide and lsqminnorm can be used, which give more robust solutions.

The solution will be denoted by



(13)

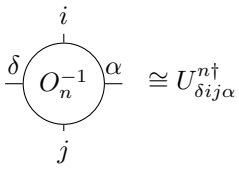
For the first equation the unmarked legs on the same positions need to be contracted with each other. The second line the mirrored positions are contracted.

If the tensor A is an MPO, the inverse can also be constructed as an mpo. This is espacially usefull if the MPO is created with decomposition for which the inverse can be computed easily, suchs as an svd decomposition.

Take has to be taken with the indices to apply the inverse.

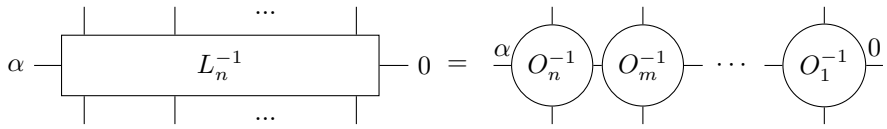
$$\begin{aligned} U^n_{(\alpha ij)\beta}A_{\beta\gamma} &= B_{\alpha ij\gamma} \\ A_{\delta\gamma} &= U^{n\dagger}_{\delta(\alpha ij)}B_{\alpha ij\gamma} \end{aligned} \tag{14}$$

If we now define the MPO O_n^{-1} equal to $U^{n\dagger}$ with the second index split and permuted:



$$\cong U^{n\dagger}_{\delta ij\alpha} \tag{15}$$

With the notation from eq. (13) we have:



(16)

The inverse can be applied sequentially.

PEPS inverse, fast version, bookkeeping

4.2 virtual levels and matrisation

From the construction with svd we can see that the dimension of virtual bond $\dim n = d^{2n}$ with d the dimension of $|i\rangle$. The virtual levels can be joined into a $\chi \times d \times d \times \chi$ dimensional tensor O. This tensor is given by a tridiagonal block matrix :

explain

$$O^{ij}_{\alpha\beta} = \begin{bmatrix} O^{00,ij} & O^{01,ij} & & \\ O^{10,ij} & O^{11,ij} & O^{12,ij} & \\ & O^{21,ij} & O^{22,ij} & \ddots \\ & & \ddots & \ddots \end{bmatrix} \tag{17}$$

The boundary conditions (leftmost and rightmost virtual level are zero) correspond to vectors:

$$\begin{aligned} l &= \begin{bmatrix} 1 & 0 & \cdots \end{bmatrix} \\ r &= l^T \end{aligned} \tag{18}$$

The total dimension is the sum of dimensions of the virtual level. In this case the

berken exact en maak tabletje voor de verschillende types

4.3 MPS algoritms

4.3.1 cononical form

schmidt decomp,

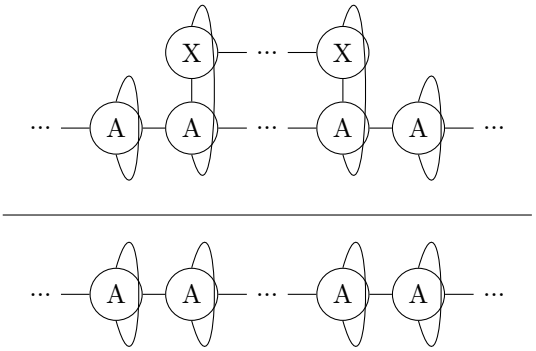
4.3.2 Expectation values

4.4 PEPS algorimts

4.5 compression

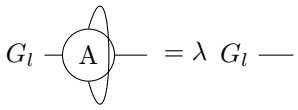
4.6 PEPS contraction

Suppose that the there is an MPO representation of $e^{-\beta \hat{H}}$ A and that the mpo represenation for X Y is localised over n sites, then the expactation value is given by:

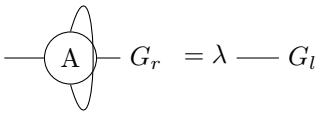
$\langle X \rangle =$ 

(19)

In the thermodynamic limit there are an infinity number of A to the left and the right. This can be simulated by taking the left and right fixed points of the traced MPO A corresponding to the largest eigenvector λ.

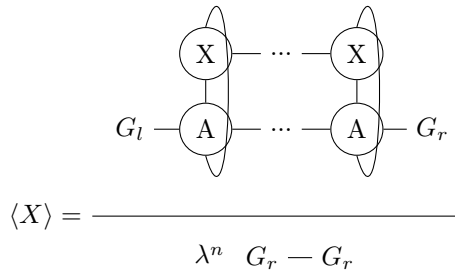


(20)



(21)

Equation eq. (19) can now be easily caclulated:



(22)

4.7 Vumps

4.8

5 contruction MPO

5.1 Time evolution methods

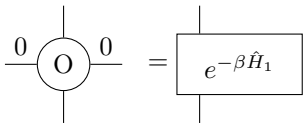
https://tensornetwork.org/

5.2 Cluster expansion

This thesis builds on the cluster expansions introduced in [1]. The idea is to create tensor network with a number of virtual levels. The representation is exact up to M connected sites, where M is the order. Different variations are possible. A Hamiltonian of the folowing form is assumed

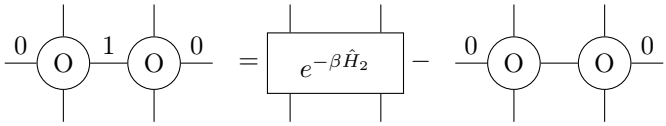
$$\hat{H}_n = \sum_{i=1}^{n-1} \hat{h}_{i,i+1} + \sum_{i=1}^{n} \hat{h'}_i \tag{23}$$

Virtual level zero is defined as follows:



(24)

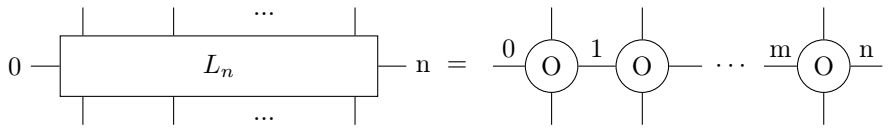
Similarly, the contraction of elements O_{01} and O_{10} are defined as follows:



(25)

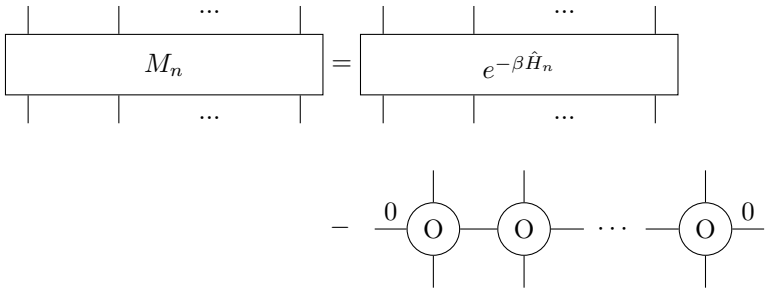
Some notation will be introduced that will be used later on. The rensor L_n is the contraction of n MPO's where the virtual index increases between each

bond. R_n is similar but the virtual bond starts from n and decreases. The tensor is defined in gra[hical notation by:



(26)

M_n is the difference between the exponentiated hamiltonian for n sites and the contraction of the MPO over all the currently assigned combinations of virtual levels.

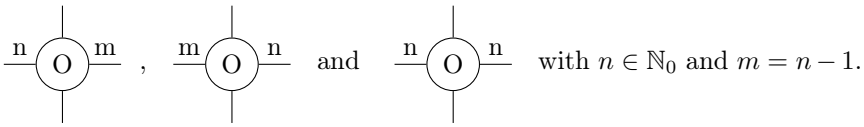


(27)

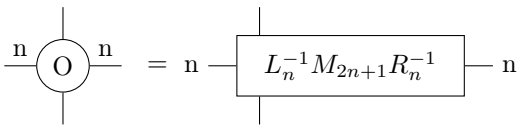
In what follows different constructions will detailed. Some notes on the practical implementation is given later in this section.

5.2.1 Type A

This type was originally proposed in [1]. The following types of blocks appear in the cluster expansion:



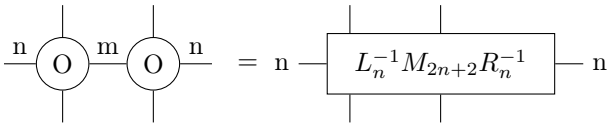
5.2.1.1 O^{nn} The O^{nn} block is defined by eq. (28)



(28)

The residual error M is calculated for a chain of size $2n + 1$. The left and right inverses L_n and R_n are applied to M to find the block O^{nn}.

5.2.1.2 O^{mn} **and** O^{nm} The contraction of O^{nm} and O^{mn} is defined by:



(29)

The individual elements O^{mn} and O^{nm} are obtained by doing an svd decoposition as explained in section 4.1.1. The square root of the singuar values is multiplied to the left and right of the decomposition. The operator L_{n+1} and R_{n+1} can be construdted directly.

implementeren en testen.

During the svd the bond dimension can be lowered by only keeping the rows and colums belonging to $\sigma_i > \sigma_0$. This also helps the invertibility. Increasing σ_0 reduces the precision of the MPO.

5.2.1.3 Truncation Intoduction of a new block can result in large fluctuating errors. This happens because the inverses are possible ill conditioned. Therefore the construction of the MPO should be stopped at a certain optimal order. Many different criteria can be tought of (and have been tried), but the most reliable method is as follows:

5.2.1.4 O^{nn} The O^{nn} blocks can form long chains. To test whether these chains improve accuracy, the norm (see section 9.1.1) of the residul error is calculated before and after the insertion of the block for a cyclic chain. A closed chain is used with the same number of sites. The closed chain resembles much better an infite chain than the open counterpart.

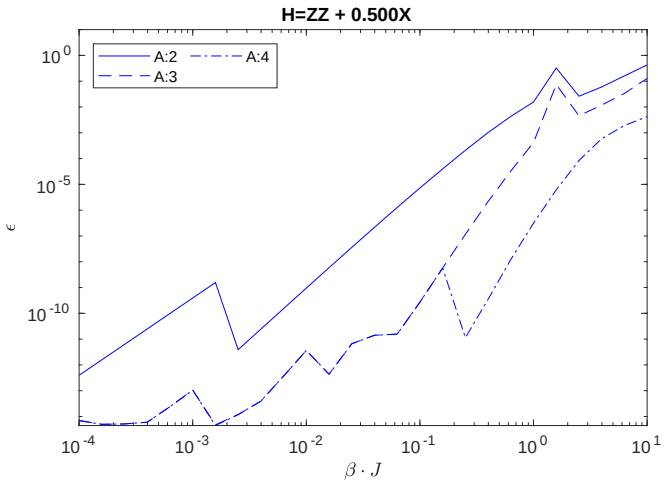
Only strict improvements are accepted, otherwise the MPO without the newly calculated blocks is returned.

5.2.1.5 O^{mn} **and** O^{nm} For these the same procedure holds.

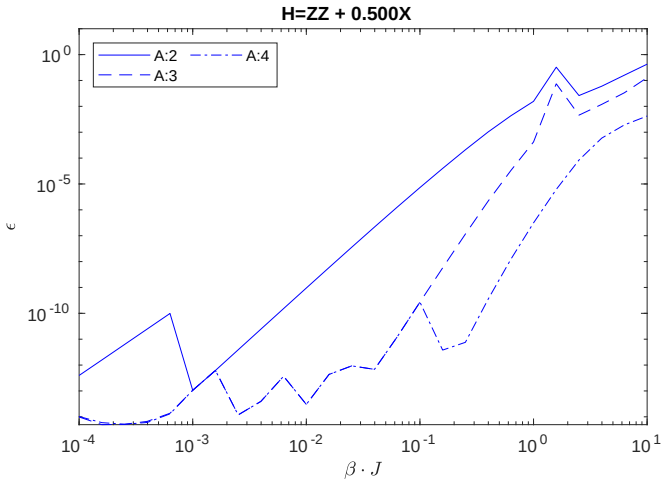
5.2.1.6 dimension From the construction is can be seen that the dimension of the new virtual level is at most d^2 times the dimension of the previous level. Depending on σ_0, the bond dimension is even lower.

5.2.1.7 discussion The only parameter in the construction is σ_0 As can be seen in **??**, mainly the construction for small values of β get affected by the choice of σ_0.This can be seen in fig. 2. A good tradeoff seems to be $\sigma_0 = 10^{-12}$. There is almost no precision loss vor small β, while for intermediate it performs optimal for intermediate β.

In practice, the truncation criterium is not completely optimal in some specific cases.

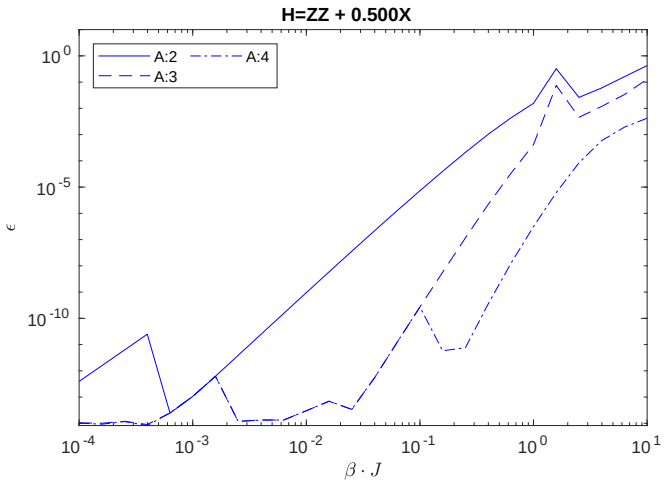


(a) 10^{-10}

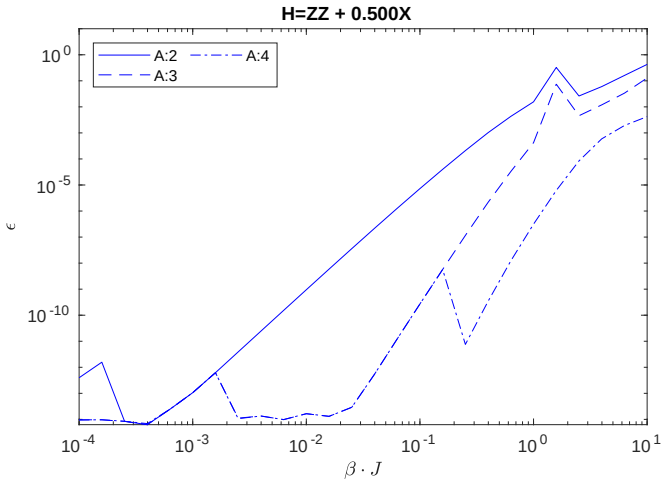


(b) 10^{-11}

Figure 2: A figure with two subfigures

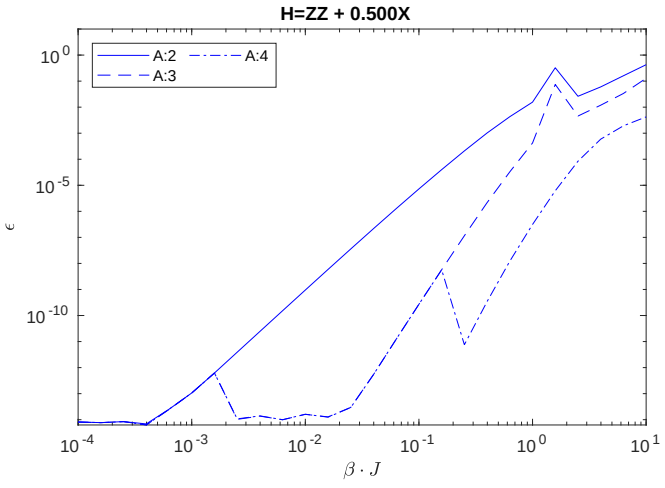


(c) 10^{-12}



(d) 10^{-13}

Figure 2: A figure with two subfigures

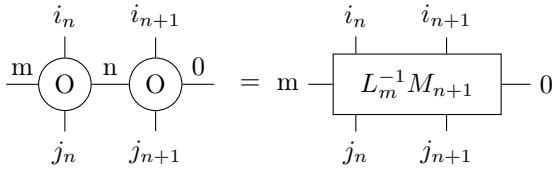


(e) 10^{-14}

Figure 2: A figure with two subfigures

5.2.2 Type B

Type B only contains blocks of the following form; O^{mn} and O^{n0}



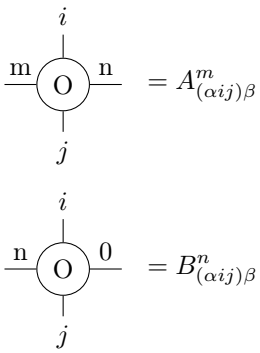
$$\cong X_{(\alpha_m i_n j_n)(i_{n+1} j_{n+1})} \tag{30}$$
$$= U^n \Sigma V^\dagger$$

The following split is made: $O^{mn} \cong U^n$ and $O^{n0} \cong \Sigma V^\dagger$. In this way the inverse exists and doesn't need any calculation: $O^{mn} = U^\dagger$.

implement this!

5.2.2.1 dimension From the construction the bond dimension grows from the left to the right. For the last step, there are only d^2 non zero singular values. Each steps adds d^2 to the dimension. For the last step, only d^2 non zero singular

values need to be keeped. With the following natation:



(31)

The bond dimension of lower virtual levels can be reduced if we can solve the following equations simultaneously:

Then the MPO doesn't change if there are matrices A'^n, A'^{n+1} and B'^n such that

$$\begin{aligned} S &= A^m A^n = A'^m A'^n \\ T &= A^m B^n = A'^m B'^n \end{aligned} \tag{32}$$

Such matrices with optimal bond dimension can be found with generalised SVD. Generalised SVD decomposes 2 matrices as follows:

$$\begin{aligned} S^\dagger &= (U\Sigma_1)Q^\dagger \\ T^\dagger &= (V\Sigma_2)Q^\dagger \end{aligned} \tag{33}$$

The new bond dimension is the $\dim n' = d^2 \cdot \min(\dim n - 1, \dim(n+1))$. The dimension is higher than type A.

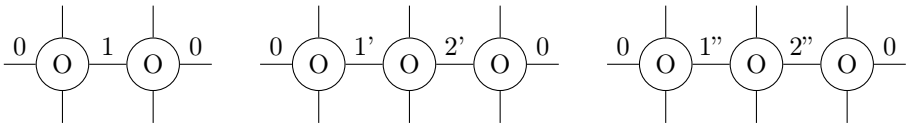
meer uitleg gsvd https://nl.mathworks.com/

5.2.2.2 discussion This type has no parameters to fine tune. The only blocks appearing in this series expansion are explicitly calculated to lower the remaining error. The inverse is well defined. It is expected that the error increases strictly with increasing temperature and keeps decreasing for higher orders.

5.2.3 Type C

primed virtual levels

This type implements the same strict type as Type B, blubut in a different way. No calculation is involved, except the calculation of the the exponentiated hamiltonian to certain order. The following kind of MPO strings are allowed:



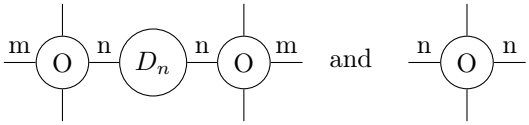
and so forth. All but one MPO elements are chosen to be the identity matrix. The middle one is the exponentiated hamiltonian with reshaped legs.

Primed levels are in fact just non overlapping virtual levels. They can be mapped to normal virtual levels.

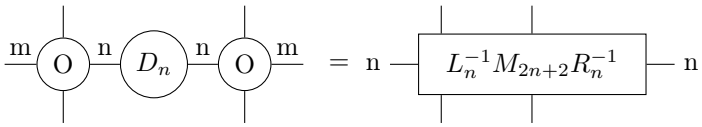
5.2.3.1 discussion As can be expected from the construction, the bond dimension grows very fast. This type is just as precise as Type B.

5.2.4 Type D

This type uses a differemt setup which tries to capture the best of both Type A and B. Type could handle long range correlation better because of the introuction of O^{nn}, but the inverse was not necesarily well defined. Type B had well conditioned inverses, but performed in most of the cases worse. The block appearing in type D are as follows:



Similar to type A,



(34)

$$= U \Sigma V^\dagger$$

Matrix D_n is the singular value diagonal matrix devided by a normalisation factor ϕ. Both U and V are multiplied by $\sqrt{\phi}$.

5.2.4.1 discussion It's not completely clear what the values of ϕ should be. If ϕ is to large, large chains are not surpressed. If phi is to small, the O^{nn} blocks will become large and hence the chain will diverge again. A reasonable value is the sum of the singular values.

other things could be tried here, WIP

5.2.4.2 matrisation The cost of this type lies in the fact that it has no compact way of casting it to a matrix. The following works, but has quite a large dimension:

O_{00} O_{01} O_{10} O_{12} O_{21}	$-2O_{01}$ $-2O_{12}$	O_{01} O_{12}	$O_{01}D_1^{1/2}$
O_{10} O_{21}			
O_{10} O_{21}		O_{11} O_{22}	
$D_1^{1/2}O_{10}$			$D_1^{-1/2}O_{12}D_2^{1/2}$ $D_2^{1/2}O_{21}D_1^{-1/2}$

fix this

5.3 Implementation details

All of the above types are implemented for arbitrary order in Matlab.

5.3.1 Source code structure

The source code for this project can be found on github. The implementation of these types can be found under `src/generateMPO.m`. In this class the different types of MPO can be constructed. It bundles some helper functions such as contracting a chain or cycle of MPO's or construction of an exponentiated hamiltonian for the given input hamiltonian. Other examples are making L_n^{-1} by sequential invers MPO contractions,...

`src/test.m` contains the code to create the plots to compare different types and orders. The other files in the folder are self-explanatory.

5.3.2 internal representation

Two main inernal representations are used to construct the given MPO. Either, the MPO is stored as a cell of matrices, or as one big matrix where the blocks are added to during the construction. The output type can be chosen. For some types, sparse matrices are used during the construction. Given that matlab does't support multidimensional matrices by default, this library is used.

5.3.3 normalisation factor

An overal normalisation factor κ per site is used to keep the numbers in matric within a reasonable range. In practice, $e^{\beta H_n}$ is divided by by κ^n. Otherwise nothing has to be changed to the algorithms. κ can be changed during the construction by absorbing the factor in the matrices.

5.3.4 buffering results

The matrix exponential for different number of sites is called on many different places. The results for chain and cycle are stored in the class to save computing time the next time.

5.3.5 Optimalisations

The construction is not yet fully optimised for speed. The arrays can be cast to Matlab gpuArray's to offload the calculations.

6 contruction PEPO framework

7 Models

7.1 Ising model

7.1.1 Classical Ising

The classical ising model is given by the following hamiltonian:

$$H = -J\left(\sum_{<ij>}\sigma_i\sigma_j + g\sum_i \sigma_i\right) \tag{35}$$

where $< ij >$ runs over all neighbouring lattice sites. Classical refers to the fact that all the operators in the hamiltonian commute with each other. The values of σ depends on the spin dimension. For spin 1/2 lattices $\sigma \in -1, +1$.

7.1.1.1 1D Phase Diagram

7.1.1.2 2D Phase Diagram

7.1.2 Quantum Ising

In the quantum Ising model, the operators no longer commute with each other. An example is the transversal ising model given by:

$$\hat{H} = -J\left(\sum_{<ij>}\sigma_i^x\sigma_j^x + g\sum_i \sigma_i^z\right) \tag{36}$$

7.1.2.1 1D Phase Diagram

7.1.2.2 2D Phase Diagram

7.2 Heisenberg

The heisenberg model is given by:

$$\hat{H} = -\left(\sum_{<ij>} J_x\sigma_i^z\sigma_j^z + J_y\sigma_i^y\sigma_j^y + J_z\sigma_i^z\sigma_j^z + h\sum_i \sigma_i^z\right) \tag{37}$$

These models have different names depending on the values of J_α with $\alpha = x, y, z$. $J_x = J_y \neq J_z = \Delta$ is called the XXZ model.

7.3 Random

It's also possible to construct random hamiltonians.

in basis: hermitian H

8 Criticality

(

scale invariancem, critical points, universality,critical exponents)

9 Benchmarking

9.1 dioganalsation

The performance of the MPO construction can be compared with the exact diagonalisation of the hamiltonian for a given number of sites. To obtain a faithful results, the number of sites should be as high as possible. In practice, diagonalisation of large matrices becomes slow and memory consuming. The size grows exponentially in the number of sites: $d^n \times d^n$. A double takes 8 bytes of memory.A Rough estimated of the amount of RAM R needed to store this complex array is:

$$R = d^{2n} \times 16bytes \tag{38}$$

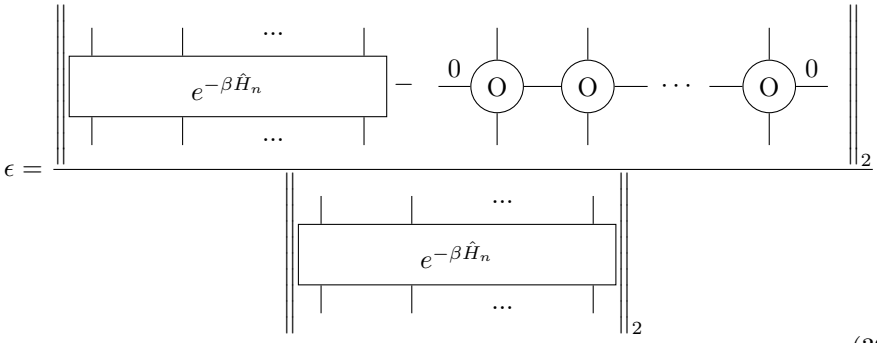
Which means a 14 site chain already takes up GB of RAM.

time complexity algoritms

9.1.1 norms

The schatten 2 norm is used in the following analysis, dentoted by $\|\cdot\|_2$. In the figures the relative error ϵ is reported.

trace norm, schatten p norm, ...



(39)

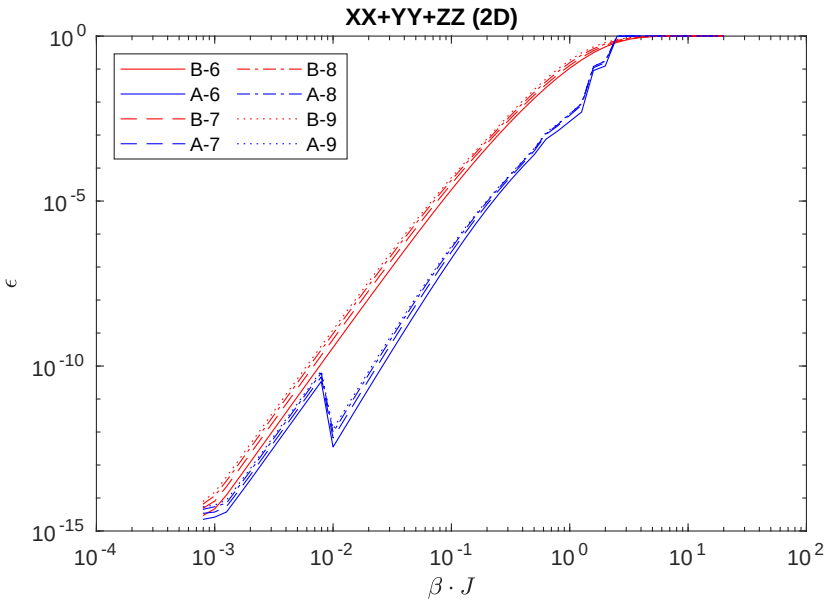
make version for cyclic

9.1.1.1 system size and cyclicity This norm can only be calculated for a finite number of sites. The influence of the number of sites for a linear and cyclic fig. 3 . As expected, the cyclic norm represents large systems better for the same number of sites. The linear norm keeps increasing with every added site.

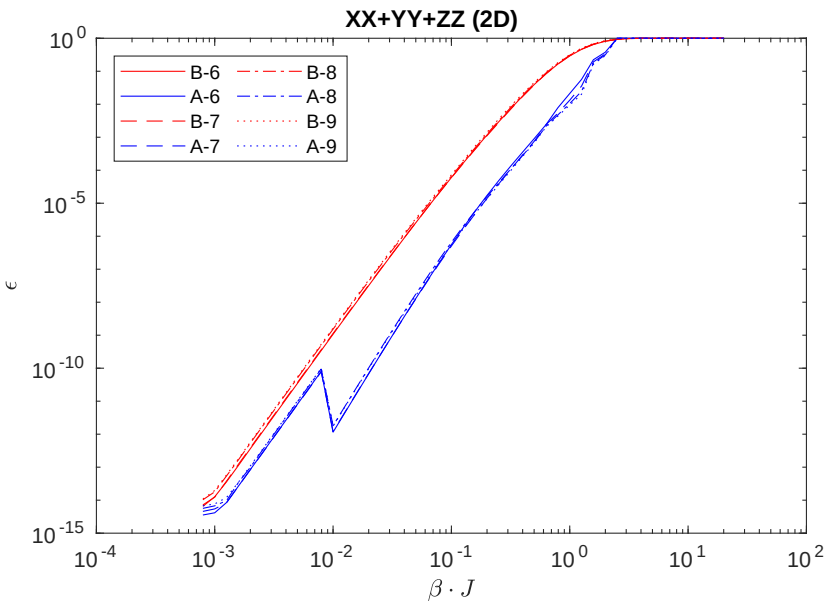
Calculating the cyclic norm comes at the extra cost of contracting a cyclic tensor network.

calculate complexity

In this chapter, the cyclic norm will be given for M=8 sites.



(a) test



(b) test

Figure 3: test

9.1.2 Ising

The first model used to benchmark the different types of MPO's is the transversal ising model. For type A the ϵ increases with β. As expected, the relative error decreases with increasing order.

The behaviour of type B is more chaotic. The error increases no longer monotonously. For small values of β, the order is truncated.

For type 5 fig. 5, there is a consitent improvement over type B.

larger orders need reimplementation (non matrix based)

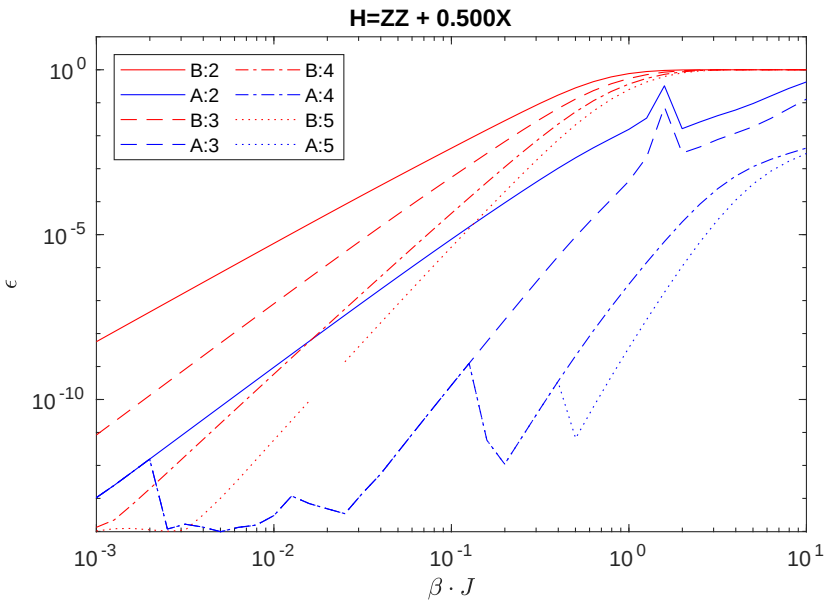


Figure 4: Comparison type A and B for Transversal Ising

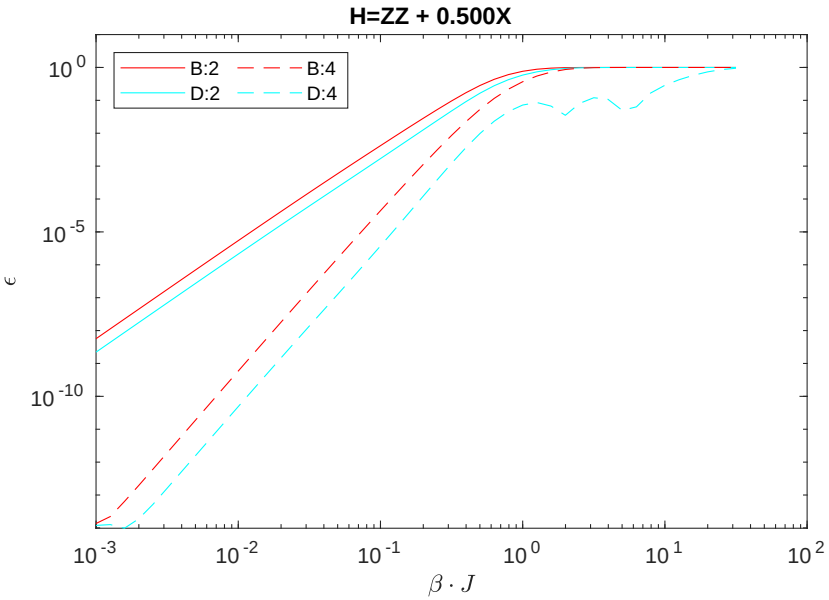


Figure 5: Comparison type C and B for Transversal Ising

9.1.3 Heisenberg

For the Heisenberg model, type A is also an improvement over type B. For large values of β, increasing the order does not help. Type 5 fig. 7 is more promising, but higher orders require to much memory to simulate.

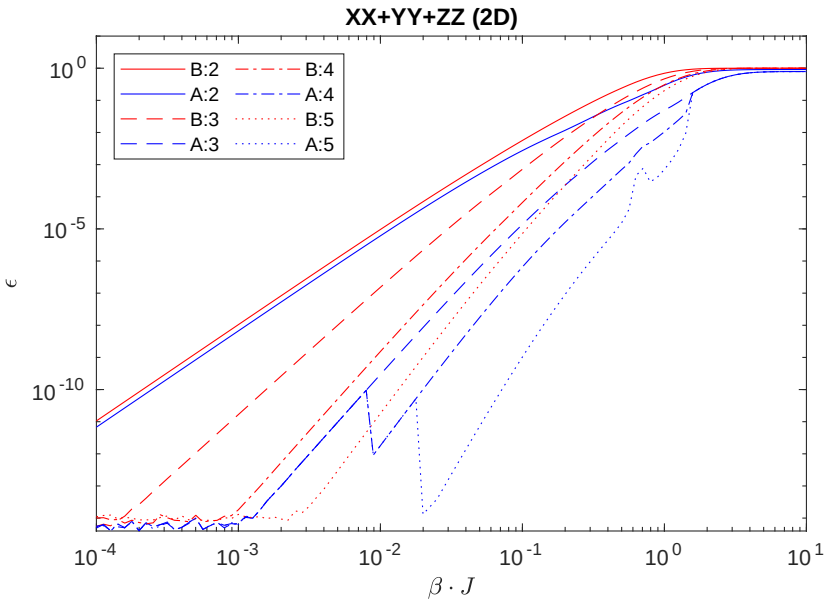


Figure 6: Comparison type A and B for Heisenberg

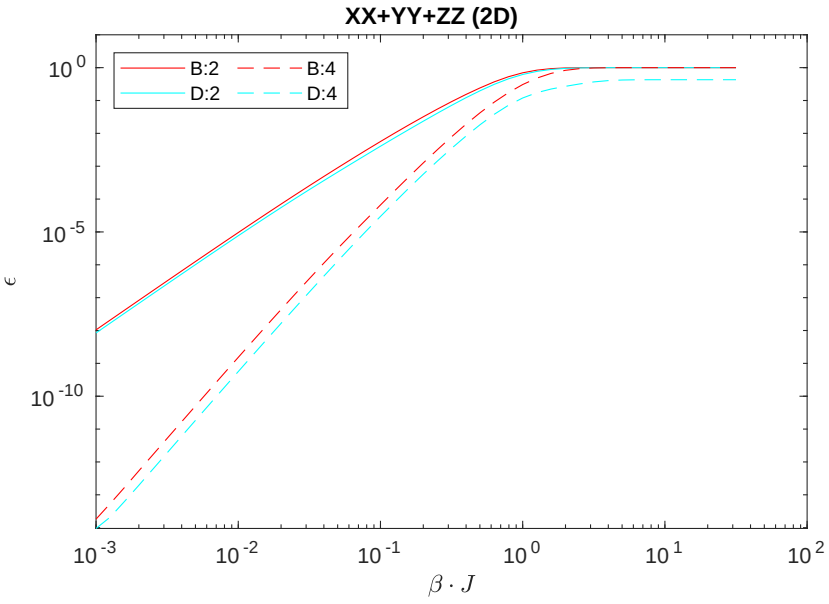


Figure 7: Comparison type C and B for Heisenberg

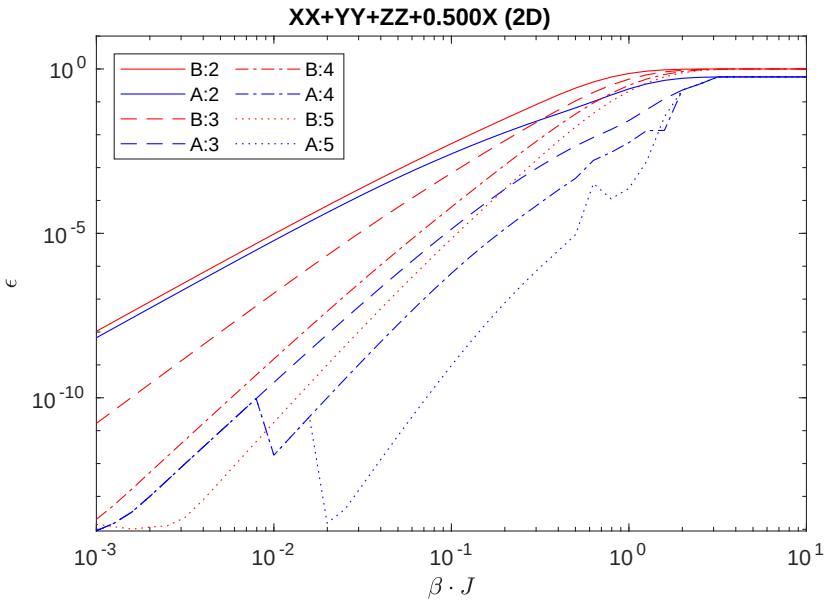


Figure 8: transversal XXX

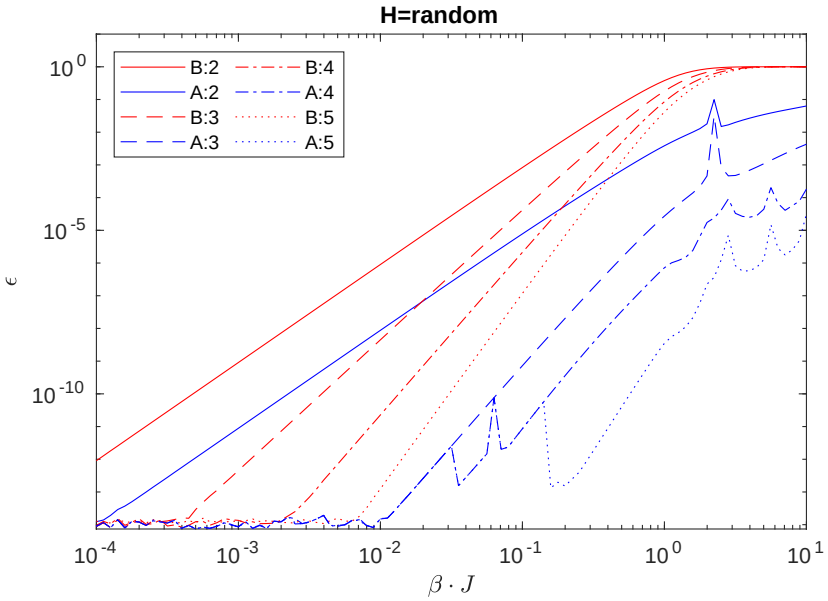
run with M=11

9.1.4 Random

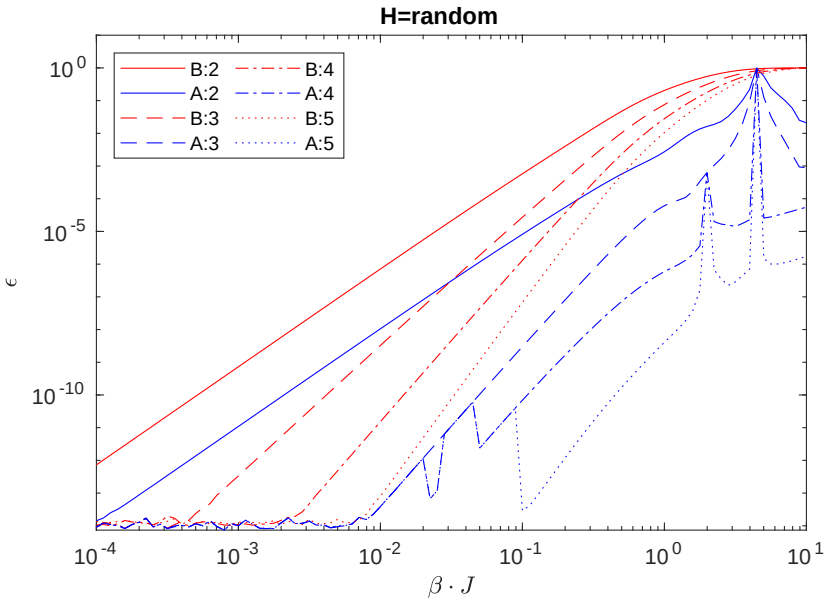
To give a representative overview for random hamiltonians, several simulations were run. The single site and nearest neighbourgh hamiltonians are generated by making hermitian matrices with random real and complex numbers between -1 and 1. In order to compare the different graphs, the engergy scale is set such that the norm of the 2 site hamiltonian is 1.

Clearly, the performance of type B is almost independent on the chosen random variables. For type A there is more variation. Still, A performs almost always better than B. For some random models, such as fig. 9b, the order is truncated at low order for high temperatures (see peak at $\beta J \approxeq 4$). It6s unclear why this behaviour emerges. Manually overinding the sefagaurd machanism

blabla

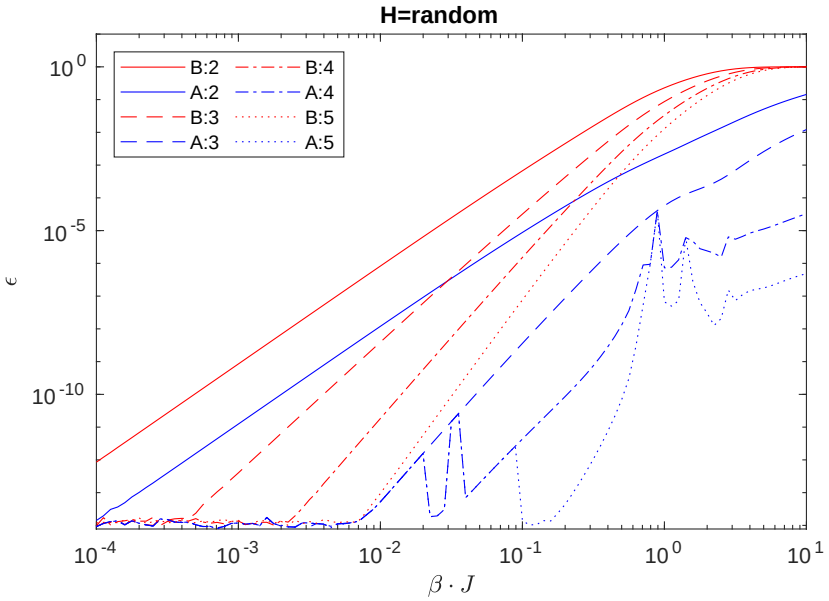


(a) test

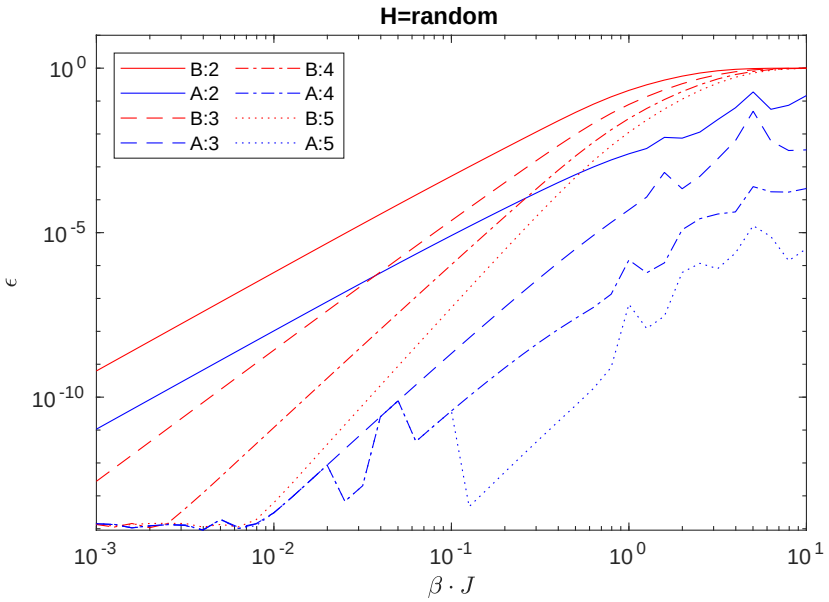


(b) test

Figure 9: test



(c) test



(d) test

Figure 9: test (cont.)

Also here type D improve the results of type B. For high β truncation seems

necessary.

nog niet klaar

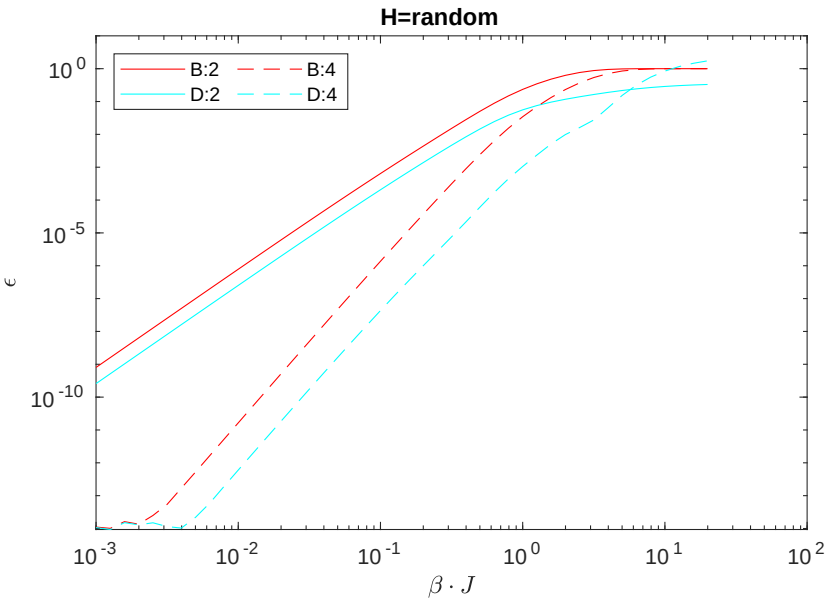


Figure 10: Comparison type C and B for random Hamiltonian

9.2 analytical results

References

[1] B. Vanhecke, M. Damme, L. Vanderstraeten, F. Verstraete, Symmetric cluster expansions with tensor networks (12 2019).