Towards a New Algorithm for Quantum Many-Body Systems

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DECLARATION

Ich versichere, dass ich die Arbeit selbstständig verfasst und keine anderen als die angegebenen Quellen und Hilfsmittel benutzt sowie Zitate kenntlich gemacht habe.

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The aim of this thesis is to develop a new numerical algorithm for quantum many-body physics in the context of tensor networks (TNs) using continuous unitary transformations (CUT). At the heart of the CUT method lies the flow equation. Solving this equation for large systems requires truncation schemes. We present a new truncation scheme for CUT using entanglement-based methods from TNs. We call this method entanglement-CUT (eCUT). Amongst other things, it allows the computation of expectation values of local observables. The basic idea of the method can be applied to systems of any dimensionality by considering appropriate TNs. We show how to implement eCUT for a finite-sized one-dimensional system using matrix product operators (MPOs). An implementation is done for the transverse-field Ising model (TFIM) to study the viability of the truncation scheme using different generators. We present first benchmarking results that demonstrate the feasibility of the approximations in certain cases. In particular we are able to calculate the ground state energy of the TFIM for up to twenty sites.
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ACRONYMS

SVD singular value decomposition

rSVD randomized singular value decomposition

TN tensor network

MPS matrix product state

PEPS projected entangled pair state

DMRG density matrix renormalization group

TEBD time-evolving block decimation

iTEBD infinite time-evolving block decimation

OBC open boundary conditions

PBC periodic boundary conditions

MPO matrix product operator

PEPO projected entangled pair operator

CUT continuous unitary transformations

eCUT entanglement-CUT

TFIM transverse-field Ising model

ROD residual off-diagonality
Part I

INTRODUCTION AND THEORY
INTRODUCTION

A fascinating aspect of quantum many-body physics can be summarized by the words of Aristotle: *the whole is more than the sum of its parts*. The interplay of many simple elements often leads to new rich and complex phenomena, that the constituents of the many-body system themselves do not exhibit. This process is referred to as *emergence*. These emergent phenomena include effects such as superconductivity, superfluidity and magnetism. A lot of progress was made in this area and many new phases of matter were discovered, leading to the development of new materials and technological progress. A theoretical understanding of quantum many-body systems is therefore indispensable.

A fundamental problem of the physical description of quantum many-body systems is the *curse of dimensionality*: the number of parameters that is necessary to exactly describe a physical state of the system grows exponentially in the number of its subsystems \[1\]. In order to exemplify this, consider a 2-level system, e.g N spins \(1/2\). The dimension of the Hilbert space of such a system is \(2^N\), that is, exponentially large in the number of spins. If we insert a number of the order of the Avogadro number \(N \sim 10^{23}\), then the number of parameters to describe the system is \(\sim O\left(2^{10^{23}}\right)\). This is exponentially larger than the estimated number of atoms in the observable universe, which is of the order \(\sim 10^{80}\) \[2\].

An exact analytical solution is only possible for a limited number of models, so that we often have to rely on numerical simulations to solve a model. It is evident that, given the exponentially large requirements, this task is impracticable even with the computational resources available today. An efficient description of the underlying physics is indispensable.

In recent years, a new formalism for the description of quantum many-body systems was developed, called tensor networks (TNs). This new language is based on quantum entanglement, that is, the quantum correlations within a system. TNs can be regarded as the entanglement-representation of quantum states. It turns out that the physically interesting corner of the Hilbert spaces of a large class of quantum systems is populated by states with finite entanglement, hence these states can be efficiently represented by TNs.

A well-known type of TNs are matrix product states (MPS). MPS can be used to efficiently describe gapped one-dimensional quantum systems. It was shown that MPS are closely related to Steve White’s variational method called density matrix renormalization group (DMRG)
Many other methods were developed in the context of TNs, each having their advantages and disadvantages depending on the problem at hand. A *one size fits all* tool does not exist. For this reason, there is a constant demand for new tools that can extend our understanding of the *whole*.

The aim of this thesis is to develop a new algorithm for quantum many-body physics. We target to formulate an established method for deriving simpler effective models called CUT in the language of TNs. At the heart of CUT lies the so called *flow equation*, which is a coupled differential equation. Solving this equation for large systems requires *truncation schemes*. We aim to apply the entanglement based truncation methods from TNs to CUT, hence developing a new algorithm which we call eCUT.

The thesis is divided into three parts. The first part reviews some basis concepts of quantum many-body physics focusing on entanglement and introduces TNs and the CUT method. The second part examines some properties of our benchmarking model, the TFIM. In the third part we describe an implementation of eCUT for finite systems using the MPS formalism and show first benchmarking results.
We referred to TNs as the entanglement-representation of quantum states. Before we move to a more detailed description of the TN framework, we have to introduce the term entanglement in quantum physics. This chapter gives an overview of some basic concepts and is mainly based on Ref. [4].

2.1 ENTANGLEMENT

Entanglement is a non-local quantum correlation that has no classical analogue [4]. It describes the correlation of particles that are correlated in such a way that they cannot be described independently of each other. Instead, the quantum state of the whole system has to be regarded.

Consider two systems defined over the Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$:

$$|\psi_1\rangle \in \mathcal{H}_1, \quad |\psi_2\rangle \in \mathcal{H}_2. \quad (2.1)$$

A composite system is obtained by the tensor product of Hilbert spaces:

$$|\psi_3\rangle = |\psi_1\rangle \otimes |\psi_2\rangle, \quad |\psi_3\rangle \in \mathcal{H}_3 \quad (2.2)$$

In terms of basis states (e.g. qubits\(^1\)), we have

$$\{|0\rangle, |1\rangle\} \in \mathcal{H}_1 \quad \{|0\rangle, |1\rangle\} \in \mathcal{H}_2 \quad \rightarrow \quad \{|0\rangle \otimes |0\rangle, |0\rangle \otimes |1\rangle, |1\rangle \otimes |0\rangle, |1\rangle \otimes |1\rangle\} \in \mathcal{H}_3. \quad (2.3)$$

The dimension of the composite system is the product of the dimensions of the parts:

$$\dim(\mathcal{H}_1) = \dim(\mathcal{H}_2) = 2; \quad \dim(\mathcal{H}_3) = \dim(\mathcal{H}_1) \cdot \dim(\mathcal{H}_2) = 4. \quad (2.4)$$

Two possible states for the composite system are

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle) \equiv \frac{1}{\sqrt{2}} (|0\rangle |0\rangle + |0\rangle |1\rangle) \quad (2.5)$$

$$|\phi\rangle = \frac{1}{\sqrt{2}} (|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle) \equiv \frac{1}{\sqrt{2}} (|0\rangle |0\rangle + |1\rangle |1\rangle),$$

where we introduced a new notation on the right-hand side. The prefactors are normalization constants.

\(^1\)We use the common notation $\{|0\rangle, |1\rangle\}$ for the eigenstates of the Pauli operator $\sigma_z$ and $\{|+, -\rangle, |\pm\rangle \equiv \frac{1}{\sqrt{2}} (|0\rangle \pm |1\rangle)\}$ for the eigenstates of the Pauli operator $\sigma_x$.\hfill
We say a wave function $|\psi\rangle$ is entangled when it is not a product state of the wave functions of the subsystems:

$$|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2; \quad |\psi\rangle \text{entangled} \iff |\psi\rangle \neq |\psi_1\rangle \otimes |\psi_2\rangle.$$ (2.6)

Otherwise it is separable. Therefore, $|\psi\rangle$ in Eq. (2.5) is a product state and $|\psi\rangle$ is an entangled state:

$$\begin{align*}
\text{separable:} & \quad |\psi\rangle = \frac{1}{\sqrt{2}} (|0\rangle|0\rangle + |0\rangle|1\rangle) \\
\text{entangled:} & \quad |\psi\rangle = \frac{1}{\sqrt{2}} (|0\rangle|0\rangle + |1\rangle|1\rangle) \neq |\psi_1\rangle \otimes |\psi_2\rangle.
\end{align*}$$ (2.7) (2.8)

Entanglement is crucial to many quantum mechanical effects. Although its existence was doubted due to its non-locality, it was proven correct by many experiments [5] using Bell-inequalities [6]. Today, entanglements is regarded as a resource and lies at the heart of many applications like quantum computation, quantum teleportation and quantum cryptography.

### 2.1.1 Schmidt Decomposition

It is important to quantify entanglement. Here, we consider bipartite entanglement. We want to quantify the entanglement in a bipartite system. This can be done via the Schmidt Decomposition. Consider a bipartite state $|\psi_{AB}\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$, with $\dim(\mathcal{H}_A) = d_A$ and $\dim(\mathcal{H}_B) = d_B$. In general we can write

$$|\psi_{AB}\rangle = \sum_{ij} \psi_{ij} |i\rangle_A |j\rangle_B.$$ (2.9)

**Theorem 1** There is always a decomposition such that

$$|\psi_{AB}\rangle = \sum_{\alpha=1}^{\chi} \lambda_\alpha |\alpha\rangle_A |\alpha\rangle_B,$$ (2.10)

with $^A_{\alpha}\langle\alpha'|_A = ^B_{\alpha}\langle\alpha'|_B = \delta_{\alpha\alpha'}$, $\lambda_\alpha > 0$ and $\chi = \min(d_A, d_B)$.

This means there is an orthonormal basis for $\mathcal{H}_A$ and $\mathcal{H}_B$. The numbers $\lambda_\alpha$ are called Schmidt coefficients and the number of non-zero Schmidt coefficients $\chi$ is called Schmidt rank. The vectors $|\alpha\rangle_A, |\alpha\rangle_B$ are called Schmidt vectors. This theorem can be proven using singular value decomposition (SVD) [7].

For the states in Eq. (2.5) we find:

$$\begin{align*}
|\psi\rangle & : \quad \chi = 1, \quad \lambda_1 = 1 \\
|\phi\rangle & : \quad \chi = 2, \quad \lambda_1 = \lambda_2 = 1/\sqrt{2}
\end{align*}$$ (2.11)
For the product state we have $\chi = 1$. This is true in general:

$$\chi = 1 \iff |\psi_{AB}\rangle \text{ is separable.} \quad (2.12)$$

This means that, if we know the Schmidt decomposition of a state, we can decide if it is an entangled state by looking at its Schmidt rank. In fact, $\chi$ is a (discontinuous) measure of bipartite entanglement. The larger $\chi$, the more entangled is the state.

### 2.1.2 Von Neumann Entropy

Given a bipartite pure state $|\psi_{AB}\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ with the reduced density matrices

$$\rho_A = \text{tr}_B (|\psi_{AB}\rangle \langle \psi_{AB}|), \quad \rho_B = \text{tr}_A (|\psi_{AB}\rangle \langle \psi_{AB}|), \quad (2.13)$$

the Von Neumann entropy is given by:

$$S(\rho_A) \equiv - \text{tr} (\rho_A \ln \rho_A) = S(\rho_B) \quad (2.14)$$

In terms of the eigenvalues of the reduced density matrix $\rho_A$

$$\rho_A = \sum_{\alpha=1}^{\chi} \nu_\alpha |\alpha\rangle_A \langle \alpha|_A, \quad (2.15)$$

we find

$$S(\rho_A) = - \sum_{\alpha=1}^{\chi} \nu_\alpha \ln \nu_\alpha. \quad (2.16)$$

We can compute the reduced density matrices from the Schmidt decomposition:

$$|\psi_{AB}\rangle = \sum_{\alpha=1}^{\chi} \lambda_\alpha |\alpha\rangle_A \langle \alpha|_B \rightarrow \rho_A = \sum_{\alpha=1}^{\chi} \frac{\lambda_\alpha^2}{\nu_\alpha} |\alpha\rangle_A \langle \alpha|_A$$

$$\rho_B = \sum_{\alpha=1}^{\chi} \frac{\lambda_\alpha^2}{\nu_\alpha} |\alpha\rangle_B \langle \alpha|_B \quad (2.17)$$

Comparing Eq. (2.17) with Eq. (2.15), we see the relation between the Schmidt coefficients of $|\psi_{AB}\rangle$ and the eigenvalues of the reduced density matrices. $\rho_A$ and $\rho_B$ have the same rank and eigenvalue spectrum but different eigenvectors. The Von Neumann entropy takes the form:

$$S(\rho_A) = - \sum_\alpha \lambda_\alpha^2 \cdot \ln \lambda_\alpha^2. \quad (2.18)$$

An important property is that the Schmidt rank $\chi$ is an upper bound to $S(\rho_A)$:

$$S(\rho_A) \leq \ln \chi. \quad (2.19)$$
The Von Neumann entropy is also a measure of bipartite entanglement between two systems and also referred to as the entanglement entropy. It is the only measure of bipartite entanglement that satisfies the following properties:

- invariant under local unitary operations
- continuous (contrary to the Schmidt rank)
- additive, i.e. \( S(\ket{\psi_{AB}} \otimes \ket{\psi_{A'B'}}) = S(\ket{\psi_{AB}}) + S(\ket{\psi_{A'B'}}) \)

The von Neumann entropy yields \( S = 0 \) for a separable state and \( S = \ln \chi \) for a maximally entangled state.

### 2.2 Singular Value Decomposition

The singular value decomposition of a matrix is a useful theorem from linear algebra and is defined as follows [8]: Any matrix \( M \in \mathbb{C}^{m \times n} \), where \( n \) and \( m \) are arbitrary, can be factorized in the form

\[
M = U \Sigma V^\dagger
\]

where

- \( U \in \mathbb{C}^{m \times m} \) is unitary,
- \( V^\dagger \in \mathbb{C}^{n \times n} \) is the adjoint of a unitary matrix,
- \( \Sigma \in \mathbb{R}^{m \times n} \) is diagonal.

The matrices are represented schematically in Fig. 2.1. The diagonal entries \( \lambda_i \) of \( \Sigma \) are positive and real. They are called the singular values of the matrix \( M \) and are typically ordered in descending order, that is, \( \lambda_1 \geq \lambda_2 \geq \ldots \lambda_r \), where \( r = \min(m, n) \). Using this ordering, \( \Sigma \) is unique, whereas \( U \) and \( V^\dagger \) are not.

The computational complexity of algorithms for computing the SVD are of \( O(nm^2) \) for \( n < m \).

The SVD is used for example for data compression. It can be used for truncation schemes in tensor network algorithms, since the truncation of the singular values allows an approximation of the matrix \( M \). The SVD will be a crucial element of our truncation scheme as well.

![Figure 2.1: Schematic representation of a SVD for a \( m \times n \) matrix with \( m > n \).](image-url)
3

TENSOR NETWORKS

There is a large number of methods in the context of quantum many-body physics. The method of tensor networks is a fairly new approach for dealing with quantum many-body systems, both numerically and analytically. Tensor networks have become increasingly popular in recent years. They were applied to many different areas, even string theory [9].

Our review here is based on Ref. [2] which offers a good introduction into tensor networks and on Ref. [10]. For a more detailed review we refer to Refs. [11, 12].

3.1 WHY TENSOR NETWORKS?

The standard way of representing a quantum many-body wave function is by specifying its coefficients in a given basis. The number of these coefficients grows exponentially in the system size, hence this is a very inefficient representation. Furthermore this approach does not give any intuition about the structure of the entanglement between the constituents of the many-body system [2].

We will see that by representing the coefficients of the wave function in a network of tensors, the information about the quantum correlations is readily available, hence we speak of an entanglement representation of the quantum state.

Different types of states, e.g. 1d, 2d, critical, can be represented with different types of TNs, that suit them best [2]. The reason why TNs can be an efficient representation is that not all states in the exponentially large Hilbert space are equally relevant for us. Many Hamiltonians in nature tend to have only local interactions, that is, finite ranged interactions, e.g. nearest-neighbour, next-to-neighbour interactions, etc. One can show that the low-energy eigenstates of local gapped Hamiltonians obey the so-called area-law for the entanglement entropy [2]. This means that the entanglement entropy of a region scales with the area of its boundary and not with its volume (see Fig. 3.1). Instead of dealing with the full Hilbert space, we can target this corner directly with TN states, which by construction obey the area-law (see Fig. 3.8). These states can be efficiently represented by TN states, that is, only by a polynomial number of parameters.

In this chapter we will introduce a useful diagrammatic notation for TNs and explain how to break the exponentially large number of coefficients of the wave function into smaller pieces using MPS.
3.2 TENSOR NETWORK THEORY

We define a tensor as a multidimensional array of complex numbers. The rank of a tensor is the number of its indices. A rank-0 tensor is a scalar ($x$), a rank-1 tensor is a vector ($v_\alpha$) and a rank-2 tensor is a matrix ($A_{\alpha\beta}$).

We can introduce a diagrammatic notation which is a powerful tool for visualizing tensor networks. The tensors mentioned above are depicted in Fig. 3.2. A blob represents a tensor and its legs correspond to the indices of the tensor.

An index contraction is the sum over all possible values of the repeated indices of a set of tensors. A matrix product is written as

$$C_{\alpha\gamma} = \sum_{\beta=1}^{D} A_{\alpha\beta} B_{\beta\gamma}. \quad (3.1)$$

Another more complicated contraction is

$$F_{\gamma\rho\sigma} = \sum_{\alpha,\beta,\delta,\mu=1}^{D} A_{\alpha\beta\delta\sigma} B_{\beta\gamma\mu} C_{\delta\nu\mu\omega} E_{\nu\rho\alpha}, \quad (3.2)$$

where all indices can take $D$ different values for simplicity. Indices that are not contracted are called open indices. Contracting all indices leads again to a tensor where the legs correspond to the open indices.

In Fig. 3.3 the contractions in Eq. (3.1) and Eq. (3.2) are illustrated in diagrammatic notation.

A TN is a set of tensors where indices are contracted according to
3.3 Tensor Network Description of the Wave Function

We will explain the TN representation of a quantum many-body state. Consider a quantum many-body system of N particles where each particle is a p-level system. The wave function can be written as

\[ |\psi\rangle = \sum_{i_1 i_2 \ldots i_N=1}^{p} c_{i_1 i_2 \ldots i_N} |i_1\rangle \otimes |i_2\rangle \otimes \ldots \otimes |i_N\rangle \]

\[
\equiv \sum_{i_1 i_2 \ldots i_N=1}^{p} c_{i_1 i_2 \ldots i_N} |i_1, i_2 \ldots i_N\rangle,
\]

in the individual basis of the single particles \(|i_r\rangle (i_r = 1, \ldots, p)\). The coefficients \(c_{i_1 i_2 \ldots i_N}\) are \(p^N\) complex numbers which can be understood as the coefficients of a tensor \(C\) with \(N\) indices \(i_1 i_2 \ldots i_N\). Each of the indices can take up to \(p\) different values. Thus, \(C\) is a tensor of rank \(N\) with \(\mathcal{O}(p^N)\) coefficients. This means that the wave function is described by a number of parameters which is exponentially in the system size.

For computational purposes this is a very inefficient description of the quantum many-body system. The TN representation allows us to...
reduce the complexity by providing an accurate description of the entanglement properties of the state. The big tensor $C$ is decomposed into many tensors with smaller rank (see Fig. 3.5). The TN representation of the wave function typically depends on a polynomial number of parameters, hence it is a computationally efficient description. This new efficient description comes with a cost. We have to introduce new degrees of freedom which are represented by the connecting indices amongst the tensors in the TN. We call these new indices bond indices and the numbers of possible values are the bond dimensions. The maximum of these values is referred as the bond dimension of the tensor network. The bond indices have an important physical meaning. They represent the structure of the many-body entanglement in the quantum state $|\psi\rangle$ and the bond dimension is a quantitative measure of the amount of quantum correlations in the wave function.

A product state can be represented by a network of tensors each connected with a bond dimension $D = 1$. If there is entanglement present within the system, a larger bond dimension is necessary to accurately describe the physical system. Fig. 3.5 shows two prominent types of TN. The MPS family is used to simulate 1d quantum many-body systems which we will explain later in detail. PEPS is the natural generalization of MPS to higher spatial dimensions [2].

3.4 AREA-LAW IN TENSOR NETWORK STATES

We already mentioned an important property of TNs. They obey the so called area-law. We want to illustrate this using the example of PEPS. Consider a PEPS as depicted in Fig. 3.6 and divide it into an outer part.
and an inner part with block length \( L \). We want to estimate the entanglement entropy of the block. Therefore we combine all the indices (which have the dimension \( D \)) across the boundary of the block into one single index \( \tilde{\alpha} = \{\alpha_1 \alpha_2 \ldots \alpha_{4L}\} \) and write down the total wave function

\[
|\psi\rangle = \sum_{\tilde{\alpha}=1}^{D^{4L}} |\text{in}(\tilde{\alpha})\rangle \otimes |\text{out}(\tilde{\alpha})\rangle.
\]  

(3.4)

The reduced density matrix of the inner part is given by

\[
\rho_{\text{in}} = \sum_{\tilde{\alpha},\tilde{\alpha}'} X_{\tilde{\alpha}\tilde{\alpha}'} |\text{in}(\tilde{\alpha})\rangle \langle \text{in}(\tilde{\alpha}')|,
\]  

(3.5)

where \( X_{\tilde{\alpha}\tilde{\alpha}'} \equiv \langle \text{out}(\tilde{\alpha})|\text{out}(\tilde{\alpha}')\rangle \). The rank of the reduced density matrix is at most \( D^{4L} \). Note that the same result is obtained when considering the outer part. The entanglement entropy defined in Eq. (2.14) is then upper bounded by the rank of \( \rho_{\text{in}} \):

\[
S(L) \leq 4L \ln(D).
\]  

(3.6)

The size of the boundary is \( 4L \), hence this is an area-law for a two dimensional system and gives the upper limit of the amount of entanglement a certain bond dimension can encompass. That means also that entanglement in the TN depends on the bond dimension and the geometric pattern of the network [2].
The most prominent family of TNs are MPS, which we will focus on. MPS are used very successfully to simulate 1d quantum many-body systems with methods like DMRG and time-evolving block decimation (TEBD). MPS are TN states that correspond to an one-dimensional array of tensors as depicted in Fig. 3.7. There is one tensor per site in the many-body system. The connecting bond indices can take up to $D$ values. The open indices correspond to the physical degrees of freedom of the local Hilbert spaces which can take up to $p$ values. MPS can represent any quantum state of a many-body Hilbert space with a sufficiently large bond dimension [2]. But the bond dimension will grow exponentially large in the system size for arbitrary states. The key property of MPS is that they efficiently describe the corner of the large many-body Hilbert space where states with low entanglement live. This is exactly where the low-lying energy states of local and gapped Hamiltonians of 1d many-body systems lie. These states also obey the 1d area-law which is also true for MPS. Therefore, these states can be targeted directly with MPS and efficiently parametrized (see Fig. 3.8).

The Hamiltonian gap is the energy gap $\Delta E$ between the ground state and the first excited state. If in the thermodynamic limit $\Delta E \neq 0$, then a system is referred to as gapped. If $\Delta E = 0$, then the system is called gapless or critical [11]. MPS cannot efficiently describe critical or scale-invariant systems, where the correlation length is known to diverge. The correlation functions
Consider an arbitrary quantum many-body state like in Eq. (3.3). In order to decompose the state into an MPS representation, the tensor $C$ can be reshaped into a matrix. By performing successive SVDs, we can generate an MPS as depicted in Fig. 3.9. The coefficients can be written as

$$c_{i_1 i_2 \ldots i_N} = \sum_{\alpha_1, \ldots, \alpha_{N-1}=1}^D A^{[1]}_{\alpha_1} A^{[2]}_{\alpha_1 \alpha_2} \ldots A^{[N]}_{\alpha_{N-1}} = A_{i_1}^{[1]} A_{i_2}^{[2]} \ldots A_{i_N}^{[N]},$$

and in graphical notation as depicted in Fig. 3.10. An important feature of MPS is gauge freedom. We can introduce an invertible matrix between any pair of MPS tensors and obtain the same pure state [11] (see Fig. 3.11). It is

$$A_{i_k}^{(k)} A_{i_{k+1}}^{(k+1)} = A_{i_k}^{(k)} X X^{-1} A_{i_{k+1}}^{(k+1)},$$
for any $X \in \text{Gl}(D, C)$. By choosing such matrices for an entire MPS, we are choosing a so-called gauge. Given a quantum state $|\psi\rangle$ in terms of an MPS with OBC, there is a gauge called canonical form of the MPS, which is very convenient for analytical and numerical considerations. In the canonical form the coefficients of the wave function of a finite system of $N$ sites take the form

$$c_{i_1 i_2 \ldots i_N} = \gamma_1^{[1]} \lambda_1^{[1]} \gamma_2^{[1]} \lambda_2^{[1]} \gamma_3^{[1]} \lambda_3^{[1]} \cdots \lambda_{N-1}^{[1]} \gamma_{N-1}^{[1]} \gamma_N^{[1]} \lambda_N^{[1]} i_{i_1} \cdots i_{i_N} $$

(3.9)

where $A_{\alpha k-1}^{[k]} = \lambda_{\alpha k-1}^{[k]} i_{i_k}$ (for the bulk). The vectors $\lambda$ correspond to the Schmidt coefficients for each successive bipartition. The graphical representation of the canonical form can be seen in Fig. 3.12. The canonical form can be used for truncation as explained in Sec. 3.9.

### 3.7 Matrix Product Operators

The extension of the matrix product formalism to operators is straightforward. An operator in this formalism is called a matrix product operator (MPO). Any operator can be written as

$$\mathcal{O} = \sum_{i_1, \ldots, i_N, i'_1, \ldots, i'_N} c_{i_1, \ldots, i_N, i'_1, \ldots, i'_N} |i_1, i_2 \ldots i_N \rangle \langle i'_1, i'_2 \ldots i'_N|$$

$$= \sum_{i_1, \ldots, i_N, i'_1, \ldots, i'_N} c_{i_1, i'_1, \ldots, i_N, i'_N} |i_1, i_2 \ldots i_N \rangle \langle i'_1, i'_2 \ldots i'_N|. $$

(3.10)

The coefficients can be decomposed in the same manner as for MPS, where the double index $i_k i'_k$ is taking the role of the single index $i_k$ of an MPS:

$$c_{i_1, i'_1} \ldots (i_N, i'_N) = W_{i_1 i'_1}^{[1]} W_{i_2 i'_2}^{[2]} \ldots W_{i_N i'_N}^{[N]}. $$

(3.11)

Instead of one physical line, there are now two vertical lines: one for the incoming and one for the outgoing physical state, as shown in Fig. 3.13.
3.8 Operations of MPO and MPS

Applying an MPO to an MPS leaves the form of the MPS invariant. It is:

\[
\hat{O} |\psi\rangle = \sum_{i_1, \ldots, i_N, i'_1, \ldots, i'_N} \left( W^{[1]}_{i_{1}i'_1} W^{[2]}_{i_{2}i'_2} \cdots \right) \left( A^{[1]}_{i'_1} A^{[2]}_{i'_2} \cdots \right) |i_1, \ldots, i_N\rangle
\]

\[
= \sum_{i, i'} \sum_{a, b} \left( W^{[1]}_{b_{1}i} W^{[2]}_{b_{2}i} \cdots \right) \left( A^{[1]}_{a_{1}} A^{[2]}_{a_{2}} \cdots \right) |i\rangle
\]

\[
= \sum_{i, i'} \sum_{a, b} \left( W^{[1]}_{b_{1}i} A^{[1]}_{a_{1}} \right) \left( W^{[2]}_{b_{2}i} A^{[2]}_{a_{2}} \cdots \right) |i\rangle
\]

\[
= \sum_{i, i'} N^{[1]}_{i_1, i'_{1}} N^{[2]}_{i_2, i'_{2}} \cdots N^{[N]}_{i_N, i'_{N}} |i\rangle . \quad (3.12)
\]

The new MPS is built up by the matrices \(N^{[k]}_{i_k, i'_k}\) with

\[
N^{[k]}_{(b_{k-1}, a_{k-1}) (b_k, a_k)} = \sum_{i'_k} W^{[k]}_{b_{k-1}, b_k} A^{[k]}_{a_{k-1}, a_k}. \quad (3.13)
\]

The bond dimension of the new MPS is the product of the bond dimension of the original MPS with the bond dimension of the MPO. The operation can be written diagrammatically as in Fig. 3.14. The addition of two operators in their MPO representation with \(W^{[k]}_{i_k, i'_k} \tilde{W}^{[k]}_{i_k, i'_k}\). 

---

**Figure 3.13:** Graphical representation of an MPO.

**Figure 3.14:** An MPO acting on an MPS. The physical indices are contracted and a new MPS is obtained with a bond dimension that is the product of the original MPS and MPO.
is obtained by forming the direct sum $\mathcal{W}_i \oplus \mathcal{W}'_i$ for all sites $1 < k < N$. The resulting MPO has a bond dimension which is the sum of the bond dimensions of the original two MPOs. Other operations with MPS and MPOs are analogous to the given example and are shown in Fig. 3.15.

### 3.9 Truncation of MPS and MPO

From the previous section, it is evident that operations on MPOs and MPS come at the cost of a larger bond dimension. The bond dimensions are either summed or multiplied. Therefore, the MPS and MPOs need to be truncated, that is, approximated by MPS or MPOs with a lower bond dimension. This can be achieved in several ways, e.g. with a variational ansatz (like DMRG) or using the canonical form (like TEBD). In our approach we will be using the canonical form but there might be situations where a variational ansatz is necessary, e.g. when dealing with PBC.

We recall that, e.g. in the case for MPS, the coefficients can be written as is Eq. (3.9), where the vectors $\lambda$ correspond to the singular values between the bipartition at each site. The singular values are ordered decreasingly. Discarding all $\lambda_{\alpha > \alpha_0}$ leads to the truncation of the matrices $\Gamma^{[k]}$ and $\Gamma^{[k+1]}$ beyond the index $\alpha_0$.
One can set a maximum bond dimension $D_{\text{max}}$ and keep only the singular values up to this value or one can set a threshold and disregard all singular values smaller than this value. The former we call fixed bond dimension and the latter adapting bond dimension.

### 3.10 Time-Evolving Block Decimation

TEBD \([14, 15, 16]\) is an algorithm for simulating the time evolution of quantum lattice systems or for finding the ground state by using imaginary time evolution. Here, we briefly explain how the algorithm works.

For simplicity, consider a Hamiltonian for an open chain with short-range interactions, e.g. one with arbitrary single-body and two-body terms with nearest neighbour interactions:

$$H = \sum_{l=1}^{N} K_{1}^{[l]} + \sum_{l=1}^{N-1} K_{2}^{[l,l+1]}.$$  \hfill (3.14)

The aim is to simulate the evolution of a system initially in the state $|\psi_{0}\rangle$ for a time $T$ according to the Hamiltonian $H$. This is achieved by applying an evolution operator to the MPS representation of the state for each discretized time step.

(i) **Initialization**: Initialize a state $|\psi_{0}\rangle$ that has a non-zero overlap with the ground state of the Hamiltonian in canonical form.

(ii) **Evolution**: Assuming the Hamiltonian does not depend on time, the evolved state reads:

$$|\psi_{T}\rangle = \exp(-iHT)|\psi_{0}\rangle$$  \hfill (3.15)

The Hamiltonian can be decomposed into an even and odd part, $H = F + G$, with

$$F = \sum_{\text{event}} F^{[l]} = \sum_{\text{event}} \left( K_{1}^{[l]} + K_{2}^{[l,l+1]} \right),$$  \hfill (3.16)

$$G = \sum_{\text{odd l}} G^{[l]} = \sum_{\text{odd l}} \left( K_{1}^{[l]} + K_{2}^{[l,l+1]} \right),$$  \hfill (3.17)

so that any two-body terms commute: $[F^{[l]}, F^{[l']}]=0$, $[G^{[l]}, G^{[l']}]=0$. This allows for a Suzuki-Trotter expansion of $\exp(-iHT) = \exp(-i(F+G)T)$, where the first order leads to

$$U_{F\delta} \equiv e^{-iF\delta}, \quad U_{G\delta} \equiv e^{-iG\delta}.$$  \hfill (3.18)

$U_{F\delta}$ and $U_{G\delta}$ can be expressed as a product of two-body gates $V_{2}^{[l]}$ and $W_{2}^{[l]}$,

$$U_{F\delta} = \prod_{\text{event}} V_{2}^{[l]}, \quad V_{2}^{[l]} \equiv e^{-iF^{[l]}\delta} \quad \text{even } l,$$  \hfill (3.19)

$$U_{G\delta} = \prod_{\text{odd } l} W_{2}^{[l]}, \quad W_{2}^{[l]} \equiv e^{-iG^{[l]}\delta} \quad \text{odd } l.$$  \hfill (3.20)
Figure 3.16: The MPS evolves by applying unitary gates successively at odd and even sites [16].

Figure 3.17: After the application of a unitary gate the tensors are contracted and decomposed again using SVD [16].

At each time step $\delta$, the gates $U_{F\delta}$ and $U_{G\delta}$ are applied iteratively to either even or odd sites respectively, as sketched in Fig. 3.16. At each step the MPS is updated. This is done a number $O(T/\delta)$ of times. The necessary steps are depicted in Fig. 3.17.

The same procedure can be used to obtain the ground state using imaginary time evolution,

$$
|\psi_{gs}\rangle = \lim_{\tau \to \infty} \frac{\exp(-H\tau)|\psi_0\rangle}{\|\exp(-H\tau)|\psi_0\rangle\|}
$$

(3.21)

provided $\langle \psi_0 | \psi_{gs} \rangle \neq 0$. Simulations of infinite-sized systems are also possible by assuming a translational invariant chain. The algorithm is called infinite time-evolving block decimation (iTEBD) and explained in detail in Ref. [16].
CONTINUOUS UNITARY TRANSFORMATIONS

In the previous chapter we introduced TNs as a new language for quantum many-body systems. In this chapter we turn to a method that was initially developed outside of the context of TNs. Later, we will formulate this method using the TN language.

The method of CUT or also called the flow equation method was proposed by Wegner [17] in 1994 in the context of condensed matter theory. Independently a similar idea was developed by Glazek and Wilson [18, 19] in the context of high-energy physics under the name similarity renormalization scheme. Here, Wegner’s approach is introduced. A detailed description of the method and its applications can be found in the textbook of Stefan Kehrein [20]. The overview given here is based on Refs. [21, 22] and [23].

Often one is interested in effective Hamiltonians which contain the same information as the original ones but allow for easier calculations of physical properties. This is usually achieved by unitary transformations. CUT is a systematical way to obtain these transformations, which is otherwise a difficult task.

4.1 THE FLOW EQUATION

In general a Hamiltonian is transformed by a finite number of unitary transformations

\[ H_{\text{eff}} = U^\dagger H U \]  

with

\[ U := U_1 U_2 \ldots U_N. \]  

The idea of CUT is to replace the finite number of unitary transformations by infinitely many

\[ U := \prod_{n=1}^{M} U_k, \quad M \to \infty, \]  

where \( U_k \) is constructed from \( H_k \) so that \( \lim_{M \to \infty} H_M \) has a diagonal form. This leads to a unitary transformation which changes continuously as a function of an auxiliary flow parameter \( \ell \) parametrizing the continuous transformation

\[ H(\ell) = U^{\dagger}(\ell)H(0)U(\ell). \]  

21
The initial Hamiltonian for $\ell = 0$ flows into a diagonal form for $\ell \to \infty$. The flow can be expressed in terms of a generator $\eta(\ell)$ by taking the derivative of Eq. (4.4)

$$\frac{\partial H(\ell)}{\partial \ell} = \left( \frac{\partial U(\ell)}{\partial \ell} \right) H(0) U(\ell) + U(\ell) H(0) \left( \frac{\partial U(\ell)}{\partial \ell} \right)$$

$$+ U(\ell) H(0) \left[ \frac{\partial U(\ell)}{\partial \ell} \right] U(\ell) + H(\ell) \left[ \frac{\partial U(\ell)}{\partial \ell} \right].$$

(4.5)

Defining the anti-hermitian generator

$$\eta(\ell) = -U(\ell) \left( \frac{\partial U(\ell)}{\partial \ell} \right)$$

(4.6)

and using

$$\frac{\partial}{\partial \ell} U(\ell) U(\ell) = \left( \frac{\partial U(\ell)}{\partial \ell} \right) U(\ell) + U(\ell) \left( \frac{\partial U(\ell)}{\partial \ell} \right) = 0$$

(4.7)

we can write the flow equation as

$$\frac{\partial H(\ell)}{\partial \ell} = [\eta(\ell), H(\ell)].$$

(4.8)

The flow equation (4.8) defines the change of the Hamiltonian and is crucial to the CUT-approach. The unitary $U(\ell)$ can be obtained from the generator by multiplying Eq. (4.6) from left by $U(\ell)$:

$$\frac{\partial U(\ell)}{\partial \ell} = -U(\ell) \eta(\ell).$$

(4.9)

This yields a differential equation which can be formally solved by

$$U(\ell) = \mathcal{L} \exp \left( -\int_{\ell}^{0} \eta(\ell') \, d\ell' \right),$$

(4.10)

where $\mathcal{L}$ is the $\ell$-ordering operator that orders the terms from left to right in increasing order of $\ell$.

### 4.2 Transformation of Observables

Observables $O$ are transformed in the same way as the Hamiltonian. They obey the flow equation

$$\frac{\partial O(\ell)}{\partial \ell} = [\eta(\ell), O(\ell)]$$

(4.11)

with the initial condition $O(0) = O$. During the flow the structure of $O(\ell)$ becomes in general more and more complicated. For $\ell \to \infty$ we obtain an easier structure for the Hamiltonian but this will not be the case for observables using the same transformation.
4.3 Generators

Besides solving the flow equation (4.8) one has to choose an appropriate generator for the flow. Over the last 20 years several generators were developed. All generators have their advantages and disadvantages depending on the properties one wants to study.

4.3.1 Wegner’s Generator

Wegner proposed [17] to split the Hamiltonian into a diagonal part \( H_d \) and a non-diagonal part \( H_{nd} \) and defined the generator

\[
\eta^w(\ell) = [H_d(\ell), H_{nd}(\ell)] = [H_d(\ell), H(\ell)].
\] (4.12)

The second equality is valid because the diagonal part commutes with itself. We can show that this choice yields a (block)-diagonal Hamiltonian. We use the notation \( \langle i | H | j \rangle = h_{ij} \) for the matrix elements of the Hamiltonian and \( h_{ii} = \epsilon_i \) for the diagonal elements. We omit writing the \( \ell \)-dependence for the sake of clarity.

The Hamiltonian is explicitly given as

\[
H = \begin{pmatrix}
\epsilon_0 & h_{01} & h_{02} & \cdots & h_{0N} \\
h_{10} & \epsilon_1 & h_{12} & \cdots & h_{1N} \\
h_{20} & h_{21} & \epsilon_2 & \cdots & h_{2N} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
h_{N0} & h_{N1} & h_{N2} & \cdots & \epsilon_N
\end{pmatrix}.
\] (4.13)

The matrix elements of the generator are

\[
\eta^w_{ij} = h_{ij}(\epsilon_i - \epsilon_j).
\] (4.14)

The derivative of the matrix elements of the Hamiltonian are

\[
\frac{\partial h_{ij}}{\partial \ell} = \sum_k \eta^w_{ik} h_{kj} - \sum_k h_{ik} \eta^w_{kj} = \sum_k (\epsilon_i + \epsilon_j - 2\epsilon_k) h_{ik} h_{kj}.
\] (4.15)

For the diagonal elements this yields

\[
\frac{\partial \epsilon_i}{\partial \ell} = \frac{\partial h_{ii}}{\partial \ell} = 2 \sum_k (\epsilon_i - \epsilon_k) h_{ik} h_{ki}.
\] (4.16)

To see that the off-diagonal elements decrease during the flow, we inspect the trace of \( H^2(\ell) \) which is invariant under unitary transformations:

\[
\text{const.} = \text{Tr}\{H^2\} = \sum_{i,k} h_{ik} h_{kl} = \sum_i \epsilon_i^2 + \sum_{i,k \neq i} h_{ik} h_{kl}.
\] (4.17)
Using $\partial / \partial \ell \text{Tr}\{H^2\} = 0$, we get

$$\sum_i \frac{\partial \varepsilon_i^2}{\partial \ell} = - \sum_{i,k \neq i} \frac{\partial}{\partial \ell} (h_{ik} h_{ki})$$

(4.19)

and further

$$\sum_i \frac{\partial \varepsilon_i^2}{\partial \ell} = 2 \sum_i \varepsilon_i \frac{\partial \varepsilon_i}{\partial \ell}$$

$$= 2 \sum_i \left( \varepsilon_i \cdot 2 \sum_k (\varepsilon_i - \varepsilon_k) h_{ik} h_{ki} \right),$$

(4.20)

where we used Eq. (4.17). By reordering the double sum and using Eq. (4.19) we get the expression

$$\sum_{i,k \neq i} \frac{\partial}{\partial \ell} |h_{ik}|^2 = -2 \sum_{i,k} (\varepsilon_i - \varepsilon_k)^2 |h_{ik}|^2.$$  \hspace{1cm} (4.21)

The hermiticity of the Hamiltonian implies that $h_{ki} = h_{ik}^*$ and so we have

$$\sum_{i,k \neq i} \frac{\partial}{\partial \ell} |h_{ik}|^2 = -2 \sum_{i,k} (\varepsilon_i - \varepsilon_k)^2 |h_{ik}|^2 \leq 0.$$  \hspace{1cm} (4.22)

This means that the sum over all squared off-diagonal elements is a monotonically decreasing function. During the flow, the off-diagonal elements will decrease. The right hand side of Eq. (4.22) shows that the flow stops for degeneracies, so for $\ell \to \infty$ the Hamiltonian will converge to a block-diagonal form. Another disadvantage of Wegner’s generator is that it does not preserve band structure. An initial band-diagonal Hamiltonian will lose its structure during the flow. The structure of the Hamiltonian during the flow is depicted in Fig. 4.1.

Figure 4.1: Structure of the Hamiltonian for Wegner’s generator. The initial band structure is not preserved during the flow. For $\ell \to \infty$ the matrix is diagonal up to degenerate subspaces.
4.3.2 Mielke’s Generator

To overcome the aforementioned disadvantage, Mielke [24] proposed another generator that preserves the band structure. The generator is defined as

$$\eta_{ij}^M(\ell) = \text{sgn}(i - j)h_{ij}(\ell),$$

(4.23)

where we introduced the sign function that depends on the row and columns indices. The generator given explicitly takes the form

$$\eta^M = \begin{pmatrix}
0 & -h_{01} & -h_{02} & \cdots & -h_{0N} \\
h_{10} & 0 & -h_{12} & \cdots & -h_{1N} \\
h_{20} & h_{21} & 0 & \cdots & -h_{2N} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
h_{N0} & h_{N1} & h_{N2} & \cdots & 0
\end{pmatrix}.$$  

(4.24)

The flow of the matrix elements is

$$\frac{\partial h_{ij}}{\partial \ell} = \sum_k (\eta_{ik}^M h_{kj} - h_{ik} \eta_{kj}^M)$$

$$= \sum_k (\text{sgn}(i - k)h_{ik}h_{kj} - \text{sgn}(k - j)h_{ij}h_{kj}).$$

(4.25)

For the off-diagonal elements we get

$$\frac{\partial h_{ij}}{\partial \ell} = -\text{sgn}(i - j)(h_{ii} - h_{jj})h_{ij}$$

$$+ \sum_{k \neq \{i,j\}} (\text{sgn}(i - k) - \text{sgn}(k - j))h_{ik}h_{kj},$$

(4.26)

and for the diagonal elements we have

$$\frac{\partial \epsilon_i}{\partial \ell} = \frac{\partial h_{ii}}{\partial \ell} = 2 \sum_{k \neq i} \text{sgn}(i - k)|h_{ik}|^2.$$  

(4.27)

The sum of the first $r + 1$ diagonal elements is a monotonically decreasing function

$$\frac{\partial}{\partial \ell} \sum_{n=0}^r \epsilon_n = -2 \sum_{n=0}^r \sum_{k > r} |h_{nk}|^2 \leq 0.$$  

(4.28)

If we assume that the system is bounded from below, $\sum_{n=0}^r \epsilon_n$ has a lower limit and therefore

$$\lim_{\ell \to \infty} |h_{nk}|^2 = 0 \quad \forall n, k : n \neq k,$$

(4.29)

since $r$ is arbitrary. The off-diagonal elements vanish and we obtain a diagonal Hamiltonian. This generator has some interesting properties. An important feature is that the diagonal elements are ordered
for large $\ell$. Since the off-diagonal elements vanish in this limit, we see that the second term in Eq. (4.26) becomes negligible because it is quadratic in the off-diagonal elements. Since the off-diagonal elements must decrease, we have

$$\text{sgn}(i-j)(\varepsilon_i - \varepsilon_j) > 0. \quad (4.30)$$

That means that the diagonal elements are ordered so that $i < j \Rightarrow \varepsilon_i < \varepsilon_j$. Notice also that the off-diagonal element decrease exponentially for large $\ell$. Away from this limit, they can even increase, so that the Hamiltonian can be less diagonal during the flow than for $\ell = 0$. As already mentioned, the band structure is conserved. Consider a band diagonal Hamiltonian:

$$h_{ij}(\ell = 0) = 0 \quad \text{if} \quad |i-j| > M. \quad (4.31)$$

Then, the first term in Eq. (4.26) is zero and the second term vanishes because of the sum of the sign functions, so that the band is conserved.

### 4.3.3 Variational Generator

In general, diagonalizing the whole Hamiltonian is computationally too expensive and often we are only interested the ground state properties and low lying energies. Dawson et al. $[25]$ used a variational calculation to propose a generator that decouples the ground state from the rest. Following the derivation in Ref. $[21]$, we require that the matrix element $\varepsilon_0$ decreases as fast as possible and minimize the expression

$$\frac{\partial \varepsilon_0(\ell)}{\partial \ell} = \frac{\partial \langle 0|H(\ell)|0 \rangle}{\partial \ell}, \quad (4.32)$$

where $|0\rangle = (1,0,\ldots,0)^\top$ is chosen as a reference state. This leads to the matrix elements for the generator $\eta^{deo}$

$$\eta^{deo}_{ij}(\ell) = h_{i0}(\ell)\delta_{0j} - \delta_{i0}h_{0j}(\ell), \quad (4.33)$$

and explicitly:

$$\eta^{deo} = \begin{pmatrix}
0 & -h_{01} & -h_{02} & \cdots & -h_{0N} \\
h_{10} & 0 & 0 & \cdots & 0 \\
h_{20} & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
h_{N0} & 0 & 0 & \cdots & 0
\end{pmatrix}. \quad (4.34)$$
The flow of the matrix element \( \varepsilon_0 \) is given by

\[
\frac{\partial \varepsilon_0}{\partial \ell} = \sum_k \eta_0^\text{deo} h_{k0} - \sum_k h_{0k} \eta_0^\text{deo} \\
= \sum_k [(h_{00} \delta_{0k} - \delta_{00} h_{0k}) h_{k0} - h_{0k} (h_{k0} \delta_{00} - \delta_{k0} h_{00})] \\
= 2|h_{00}|^2 - 2 \sum_k |h_{0k}|^2
\]

\[
\frac{\partial \varepsilon_0}{\partial \ell} = -2 \sum_{k=1}^{N} |h_{0k}|^2 \leq 0, \quad (4.35)
\]

where we used Eq. (4.15) and Eq. (4.33). This means that \( \varepsilon_0(\ell) \) is a monotonically decreasing function. If we assume that \( H \) is bounded from below it is:

\[
\lim_{\ell \to \infty} |h_{0k}(\ell)|^2 = 0 \quad \forall k : k > 0, \quad (4.36)
\]

and \( \varepsilon_0(\ell) \) converges to an eigenvalue of the Hamiltonian. In Sec. 4.3.5 we show that the eigenvalue is the ground state energy.

### 4.3.4 Block Generator

Similar to the extension of the ground state generator for Hamiltonians in second quantization to include one-particle subspaces [21], we can extend the variational generator to block-diagonalize the Hamiltonian with a block containing the low lying energies. We define the generator as

\[
\eta_{ij}^b(\ell) = \sum_{n=0}^{r} (h_{in}(\ell) \delta_{nj} - \delta_{in} h_{nj}(\ell)). \quad (4.37)
\]

For \( r = 0 \) we obtain \( \eta^\text{deo} \). The idea is that for \( r > 0 \) the Hamiltonian will flow into a block diagonal form with a block \( r + 1 \times r + 1 \) that is the subspace of the lowest \( r + 1 \) energies and a block with the rest. The structure of the generator is schematically depicted in Fig. 4.2 and Fig. 4.3 shows the expected form of the Hamiltonian.

We have to prove that this generator yields the desired flow. The flow is

\[
\frac{\partial h_{ij}}{\partial \ell} = \sum_k \eta_{ik}^b h_{kj} - h_{ik} \eta_{kj}^b \\
= \sum_k \sum_{n=0}^{r} (h_{in} \delta_{nk} - \delta_{in} h_{nk}) h_{kj} - h_{ik} (h_{kn} \delta_{nj} - \delta_{kn} h_{nj}) \quad (4.38)
\]
For the diagonal elements for $i \leq r$ we obtain
\[
\frac{\partial \varepsilon_i}{\partial \ell} = 2 \sum_{n=0}^{r} |h_{in}|^2 - 2 \sum_{k} |h_{ik}|^2 \\
= -2 \sum_{k>r} |h_{ik}|^2.
\] (4.39)

This is a monotonically decreasing function and assuming that the system is bounded from below, it follows that
\[
\lim_{\ell \to \infty} |h_{ik}|^2 = 0 \quad \forall i, k : i \leq r, k > r.
\] (4.40)

That means we obtain a $r + 1 \times r + 1$ block for $\ell \to \infty$ as desired.

The remaining task is to show that the eigenvalues of the block are the lowest $r + 1$ eigenvalues of the Hamiltonian as done in the following section.

### 4.3.5 Identical Transformation of Subspaces

We want to show that the block generator transforms the subspace of the block in the same way as Mielke’s generator. We start with the special case $\tau = 0$, where $\eta^b = \eta^{\text{deo}}$ and follow the derivation in Ref. [21]. We denote the vacuum state with $|0\rangle = (1, 0, \ldots, 0)^T$. Instead
of transforming the Hamiltonian with $H(\ell) := U(\ell)^\dagger H(\ell = 0)U(\ell)$ we transform the state by $|0(\ell)\rangle = U(\ell)|0(\ell = 0)\rangle$. This is analogous to passing from the Heisenberg picture to the Schrödinger picture. The flow of the vacuum state is

$$\frac{\partial |0(\ell)\rangle}{\partial \ell} = \frac{\partial U(\ell)}{\partial \ell} |0\rangle$$

which yields

$$= U(\ell) U(\ell)^\dagger \frac{\partial U(\ell)}{\partial \ell} |0\rangle$$

$$= -\eta(\ell) |0\rangle.$$  \hspace{1cm} (4.42)

We can introduce a basis $\{|n\rangle\}$ and obtain

$$\frac{\partial |0(\ell)\rangle}{\partial \ell} = -\sum_n U(\ell) |n\rangle \langle n| \eta(\ell)|0\rangle.$$  \hspace{1cm} (4.44)

The definition of the matrix elements $\eta_{n0}$ are the same for $\eta^M$, $\eta^b$ and $\eta^\text{deo}$ respectively:

$$\eta_{n0}(\ell) = \begin{cases} h_{n0}(\ell) & \text{for } n > 0 \\ 0 & \text{for } n = 0 \end{cases}.$$  \hspace{1cm} (4.45)

Applying to Eq. (4.44) yields

$$\frac{\partial |0(\ell)\rangle}{\partial \ell} = -\sum_{n \neq 0} U(\ell) |n\rangle \langle n| H(\ell)|0\rangle$$

$$= -\left(\sum_n U(\ell) |n\rangle \langle n| H(\ell)|0\rangle\right) + U(\ell) |0\rangle \langle 0| H(\ell)|0\rangle.$$  \hspace{1cm} (4.46)

We shift the $\ell$-dependency to the vacuum state and obtain

$$\frac{\partial |0(\ell)\rangle}{\partial \ell} = -H |0(\ell)\rangle + |0(\ell)\rangle \langle 0(\ell)| H|0(\ell)\rangle$$

$$= [P_0(\ell), H] |0(\ell)\rangle.$$  \hspace{1cm} (4.48)

where we defined the $\ell$-dependent projector $P_0(\ell) := |0(\ell)\rangle\langle 0(\ell)|$. Since the flow depends only on $|0(\ell)\rangle$ itself and the initial Hamiltonian $H$, the considered generators transform the vacuum state $|0(\ell)\rangle$ in the same way. This statement is valid for the exact flow without truncations. The key point of the proof is that the matrix elements $\eta_{n0}$ are defined identically for the considered generators. We want to generalize this proof for $r > 0$. We denote the states
with \( |n\rangle, n = 0, \ldots, N, \) e.g \( |0\rangle = (1, 0, \ldots, 0)^T \) and \( |1\rangle = (0, 1, \ldots, 0)^T \).

Consider the flow of any state \( n < r \)

\[
\frac{\partial}{\partial \ell} |n(\ell)\rangle = \frac{\partial U(\ell)}{\partial \ell} |n\rangle \\
= U(\ell) \eta(\ell) |n\rangle \\
= -\sum_m U(\ell) |m\rangle \langle m| \eta(\ell) |n\rangle.
\]

The matrix elements \( \eta_{mn}(\ell) \) for Mielke’s generator are given by

\[
\eta_{mn}(\ell) = \text{sgn}(m - n) h_{mn}(\ell)
\]

and for the block generator

\[
\eta_{mn}(\ell) = \begin{cases} 
\text{sgn}(m - n) h_{mn}(\ell) & \text{for } n \leq r, m > r \text{ and } m \leq r, n > r \\
0 & \text{for } n, m \leq r \text{ and } n, m > r
\end{cases}
\]

Hence we have for Mielke’s generator

\[
\frac{\partial}{\partial \ell} |n(\ell)\rangle = -\sum_m \text{sgn}(m - n) U(\ell) |m\rangle \langle m| H(\ell) |n\rangle \\
= -\sum_{m > r} U(\ell) |m\rangle \langle m| H(\ell) |n\rangle \\
- \sum_{m \leq r} \text{sgn}(m - n) U(\ell) |m\rangle \langle m| H(\ell) |n\rangle.
\]

By adding and subtracting terms we obtain

\[
\frac{\partial}{\partial \ell} |n(\ell)\rangle = -U(\ell) H(\ell) |n\rangle \\
+ \sum_{m \leq r} U(\ell) |m\rangle \langle m| H(\ell) |n\rangle \\
- \sum_{m \leq r} \text{sgn}(m - n) U(\ell) |m\rangle \langle m| H(\ell) |n\rangle.
\]

Shifting the \( \ell \)-dependence to the states yields

\[
\frac{\partial}{\partial \ell} |n(\ell)\rangle = -H |n(\ell)\rangle \\
+ \sum_{m \leq r} |m(\ell)\rangle \langle m| H |n(\ell)\rangle \\
- \sum_{m \leq r} \text{sgn}(m - n) |m(\ell)\rangle \langle m| H |n(\ell)\rangle.
\]
For the block-generator we get
\[
\frac{\partial}{\partial \ell} |n(\ell)\rangle = -\sum_{m > r} \text{sgn}(m - n) U(\ell) |m\rangle \langle m| H(\ell)|n\rangle \\
= -\sum_{m} U(\ell) |m\rangle \langle m| H(\ell)|n\rangle \\
+ \sum_{m \leq r} U(\ell) |m\rangle \langle m| H(\ell)|n\rangle \\
= -U(\ell) H(\ell) |n\rangle \\
+ \sum_{m \leq r} U(\ell) |m\rangle \langle m| H(\ell)|n\rangle ,
\] (4.59)

and shifting \(\ell\)-dependence to the states yields
\[
\frac{\partial}{\partial \ell} |n(\ell)\rangle = -H |n(\ell)\rangle \\
+ \sum_{m \leq r} |m(\ell)\rangle \langle m(\ell)| H|n(\ell)\rangle .
\] (4.60)

Notice that the transformation of the subspace with \(|n\rangle\) with \(n \leq r\) for both generators is independent from all other states with \(n > r\) and only depends on the initial Hamiltonian and the states \(n \leq r\) themselves. The generators only differ in the last term of Eq. (4.58). But this term only includes the off-diagonal elements in the \(r + 1 \times r + 1\)-block, which vanish for Mielke’s generator but do not transform for the block generator. That means both generators transform the considered subspace in the same way but Mielke’s generator additionally diagonalizes the block. In fact we could have chosen a generator which transforms exactly like Mielke’s generator by including the off-diagonal elements of the block, but diagonalizing the residual small block after the flow should be more efficient with conventional methods.

4.4 Truncation schemes

Up to this point we have introduced the flow equation and several generators but we have not given a prescription of how to solve the flow equation. From Eq. (4.16) one can see that we have to deal with coupled differential equations which become more and more complicated during the flow, so that we have to introduce approximations at some point. Several systematic ways to obtain sensible approximations \[26\], so called truncation schemes, were developed which we only want to mention here and refer the reader to the references. Wegner’s own approach was self-similar CUT which is also used in Ref. [21]. Here only terms which are considered to be important to the physical problem are regarded and other terms are neglected. The more terms are included the more reliable the calculation gets. The
challenge is to determine which terms are important and which are not [27].

There is perturbative scheme called \textit{perturbative CUT} [28] and \textit{enhanced perturbative CUT}. In the perturbative approach the non-diagonal part $H_{nd}$ is considered as a small perturbation to the diagonal part $H_d$ of the bare Hamiltonian [27]. The flow expansion is then expanded accordingly. An overview over the mentioned schemes and more is given in Ref. [26].

Our aim in this thesis is to test a new truncation scheme based on the entanglement content of operators along the flow. This is achieved by translating the flow equation approach into the tensor network language and expressing operators as e.g. MPOs. We present this new scheme in detail in chapter 6.
Part II

TRANSVERSE FIELD ISING MODEL AND TEBD
The one-dimensional Ising model in a transverse field (TFIM) with nearest neighbour interactions is a well-studied model and will serve as our benchmarking model.

The Hamiltonian is gapped, hence useful in the context of MPS. It shows no phase transition at finite temperature but exhibits a quantum phase transition at zero temperature. It can be shown that the TFIM can be mapped to the 2d classical Ising model [29], which was solved by Onsager in 1944 [30]. The TFIM was solved by Pfeuty in 1970 [31] based on the works of Lieb, Schultz and Mattis [32]. The spin-correlation functions are computed in Refs. [33, 34]. A list of systems on which the TFIM is applicable can be found in Ref. [35].

The Hamiltonian for the one-dimensional ferromagnetic transverse field Ising model with open boundary conditions is given by

$$H = -h_0 \sum_{j=1}^{N} S_j^z - J_0 \sum_{j=1}^{N-1} S_j^x S_{j+1}^x \quad h_0, J_0 > 0,$$

(5.1)

where the local spin operators are defined as

$$S_j^{x,z} = \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes S_j^{x,z} \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes \mathbb{1},$$

(5.2)

$S^x$ and $S^z$ are components of the standard spin-$\frac{1}{2}$ operators. This model describes a spin-$1/2$ chain with $N$ sites and nearest-neighbour interaction, coupling strength $J_0$ in the x-direction and an external magnetic field $h_0$ along the z-axis.

The Ising interaction $J$ tends to order the spins along the x-axis and the magnetic field destroys the order by flipping the spins. In the absence of a magnetic field the system is completely ordered. All spins are aligned in parallel. For an infinite magnetic field the system becomes completely disordered. The order parameter is the magnetization $M_x = \langle gs | S^x | gs \rangle$.

In the thermodynamic limit the system undergoes a second order phase transition at the critical point $h_0 = J_0/2$. Due to the $Z_2$-symmetry of the Hamiltonian $S^x \rightarrow -S^x$ for $h_0 = 0$, the ground state is twofold degenerate. All spins are either pointing upwards or downwards, that means the symmetry in the Hamiltonian is spontaneously broken. The magnetic field destroys the symmetry in the Hamiltonian, hence we have a unique ground state in the disordered phase.
5.1 Exact Diagonalization of the Hamiltonian

We solve the TFIM Hamiltonian for a finite size $N$ and with open boundary conditions and proceed as in Ref. [36]. We perform a set of canonical transformations that will map the problem of diagonalizing a $2^N \times 2^N$ Hamiltonian to an eigenvalue problem of an $N \times N$ matrix. In the end we will obtain a system of noninteracting fermions.

We begin by expressing the spin operators in terms of the Pauli matrices

\[ S^x = \frac{h}{2} \sigma^x, \quad S^z = \frac{h}{2} \sigma^z, \quad h = 1, \] (5.3)

and we find

\[ H = -h \sum_{j=1}^{N} \sigma^z_j - J \sum_{j=1}^{N-1} \sigma^x_j \sigma^x_{j+1}, \] (5.4)

with $J = J_0/4$ and $h = h_0/2$. The Pauli matrices can be expressed in terms of ladder operators

\[ \sigma^x_j = \sigma^+_j + \sigma^-_j, \quad \sigma^z_j = 2\sigma^+_j \sigma^-_j - 1, \] (5.5)

which commute on different sites $i \neq j$. The Hamiltonian is then:

\[ H = N h - 2h \sum_{j=1}^{N} \sigma^+_j \sigma^-_j - J \sum_{j=1}^{N-1} (\sigma^+_j \sigma^+_{j+1} \sigma^-_j \sigma^-_{j+1} + \sigma^+_j \sigma^+_{j+1} \sigma^-_j \sigma^-_{j+1}). \] (5.6)

In order to obtain the correct fermionic anticommutation relations, we perform the Jordan-Wigner transformation

\[ \sigma^+_j = a^\dagger_j (-1)^{\sum_{k<j} a^\dagger_k a_k}, \quad \sigma^-_j = (-1)^{\sum_{k<j} a^\dagger_k a_k} a_j, \] (5.7)

which maps the commuting ladder operator to anticommuting fermionic operators $a_j$ and $a^\dagger_j$:

\[ \{ a^\dagger_i, a_j \} = \delta_{ij}, \quad \{ a_i, a_j \} = 0. \] (5.8)

The Hamiltonian reads

\[ H = N h - 2h \sum_{j=1}^{N} a^\dagger_j a_j - J \sum_{j=1}^{N-1} (a^\dagger_j a_{j+1} + a^\dagger_{j+1} a_j + h.c.), \] (5.9)

and describes an interacting fermion model. It is convenient to perform another transformation in a way that we only have to deal with
real matrices. We write the fermionic operators in terms of Majorana fermions:

\[ a_j = \frac{1}{2} (c_j + i d_j), \quad a_j^\dagger = \frac{1}{2} (c_j - i d_j). \]  

(5.10)

The Majorana operators \( c_j \) and \( d_j \) are self-adjoint and satisfy the anticommutation relations:

\[ \{ c_i, c_j \} = \{ d_i, d_j \} = 2 \delta_{ij}, \quad \{ c_i, d_j \} = 0 \]  

(5.11)

\[ c_j^\dagger = c_j, \quad d_j^\dagger = d_j, \quad c_j^2 = d_j^2 = 1. \]  

(5.12)

The new Hamiltonian is

\[ H = -i \hbar \sum_{j=1}^{N} c_j d_j - i J \sum_{j=1}^{N-1} c_{j+1} d_j. \]  

(5.13)

Using the notation \( \vec{c} = (c_1, c_2, \ldots, c_N)^T \) we can write this equation in a compact form

\[ H = \frac{i}{4} (\vec{c}^\dagger \vec{d}) \begin{pmatrix} 0 & B \\ -B^T & 0 \end{pmatrix} M (\vec{c} \vec{d}), \]  

(5.14)

where \( B \) is a \( N \times N \) Toeplitz matrix of the form

\[ B = 2 \begin{pmatrix} -h & 0 & 0 & \cdots & \cdots & \cdots & 0 \\ -J & -h & 0 & 0 & \vdots \\ 0 & -J & -h & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -J & -h & 0 & 0 \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -J & -h & 0 \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -J & -h \\ \end{pmatrix}. \]  

(5.15)

The remaining task is to diagonalize the \( 2N \times 2N \) matrix \( M \). Since \( B \) is real, \( M \) is a real and skew-symmetric matrix. The eigenvalues of such a matrix always come in pairs \( \pm \epsilon \). The spectral theorem states that any real skew-symmetric matrix can be block-diagonalized by a special orthogonal matrix:

\[ M = O M' O^T, \]  

(5.16)

1 A Toeplitz matrix is a matrix which has constant values along the negative-sloping diagonals.
with

\[ M' = \begin{pmatrix}
0 & \epsilon_1 & 0 & \cdots & \cdots & \cdots & 0 \\
-\epsilon_1 & 0 & 0 & 0 & \cdots & \cdots & \cdots \\
0 & 0 & 0 & \epsilon_2 & \cdots & \cdots & \cdots \\
o \cdots & -\epsilon_2 & \cdots & \cdots & \cdots & \cdots & \cdots \\
\vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \ddots \\
0 & 0 & 0 & 0 & \cdots & -\epsilon_{N-1} & 0 \\
0 & \cdots & \cdots & \cdots & \cdots & \cdots & \epsilon_N \\
0 & \cdots & \cdots & \cdots & \cdots & 0 & -\epsilon_N \\
\end{pmatrix}, \quad (5.17) \]

This can be brought into the form

\[ M' = \begin{pmatrix}
0 & E \\
- E & 0 \\
\end{pmatrix}, \quad (5.18) \]

with \( E = \text{diag}(\epsilon_1, \epsilon_2, \ldots, \epsilon_N) \). We can define a new set of Majorana operators through a canonical transformation:

\[ \begin{pmatrix}
\vec{e} \\
\vec{f}
\end{pmatrix} = O^T \begin{pmatrix}
\vec{c} \\
\vec{d}
\end{pmatrix}, \quad (5.19) \]

and rewrite the Hamiltonian as

\[ H = \frac{i}{4} N \sum_{j=1}^{N} \epsilon_j (e_j f_k - f_k e_j) = \frac{i}{2} \sum_{k=1}^{N} \epsilon_k e_k f_k. \quad (5.20) \]

The Majorana operators can then again be expressed as another set of fermionic operators:

\[ \eta_j = \frac{1}{2} (e_j + i f_j), \quad \eta^\dagger_k = \frac{1}{2} (e_k - i f_k), \quad (5.21) \]

and the Hamiltonian becomes

\[ H = \sum_{k=1}^{N} \epsilon_k \left( \eta^\dagger_k \eta_k - \frac{1}{2} \right). \quad (5.22) \]

This is a model of non-interacting fermions. The \( \epsilon_k \) are the energies of the modes and can be calculated just by diagonalizing the matrix B. This can be done analytically but we restrict ourself to a numerical calculation, which can be done easily for a \( N \times N \) matrix.

When no excitations are present, we get the ground state energy

\[ E_0 = -\frac{1}{2} \sum_{k=1}^{N} \epsilon_k, \quad (5.23) \]
and by exciting the modes we can build up the whole spectrum:

\[
H = \sum_{k=1}^{N} \epsilon_k \eta_k^\dagger \eta_k + E_0. \tag{5.24}
\]

Fig. 5.1 shows the ground state energy per site for 8 and 20 sites and for the thermodynamic limit as calculated by Pfeuty. The lowest three energy eigenvalues for 20 sites are depicted in Fig. 5.2. We denote them with \(E_0\), \(E_1\) and \(E_2\), where \(E_0 \leq E_1 \leq E_2\), and \(E_0\) being the ground state energy. For future considerations the energy gaps between these energies play an important role. We define two gaps as

\[
\Delta E_{01} = E_0 - E_1, \quad \Delta E_{02} = E_0 - E_2. \tag{5.25}
\]

In the thermodynamic limit the ground state is twofold degenerate in the ordered phase. The degeneracy gets lifted at the critical point. On
the other hand, the gap to the first excited state closes at the critical point, hence we have $E_{02} = 0$ at $J = h$.

For a finite number of sites this is not the case as we can see in Fig. 5.3, where both gaps are plotted for several system sizes. We can see that $\Delta E_{02}$ has a minimum (but does not vanish) at a point shifted to the left for smaller system sizes. The gap $\Delta E_{01}$ is exponentially small for low magnetic fields and increases octically close to the point where $\Delta E_{01}$ has a minimum. Compare this also to the lowest mode energies for 20 sites which are depicted in Fig. 5.4. For low magnetic fields the smallest mode energy is exponentially small and so is the gap $\Delta E_{01}$.

Figure 5.4: Energies of the smallest five modes for 20 sites.
5.2 Benchmarking TFIM with TEBD

The TEBD algorithm was introduced in Sec. 3.10 and will be used for a numerical calculation of some properties of the model which can serve as a benchmark for our algorithm in the next chapter. TEBD allows us to calculate the ground state energy for an arbitrary number of sites and other observables like the magnetization. We run our simulations for different bond dimensions and system sizes. The relative deviation of the ground state energy compared to the exact results is plotted in Fig. 5.5 (lower panel). The results for iTEBD, that is, for a translational invariant infinite chain, show a peak exactly at the critical point $h/J = 1$. This is expected since MPS cannot describe critical systems with a finite bond dimension. Comparing the lower panel with the upper panel, where the order parameter $M_x$ is plotted, we find that the magnetization drops to zero at the critical point as predicted.

We find a similar behaviour for the two finite size calculations, although there is no critical point in finite systems. The deviations peak as the order parameter goes to zero. The peaks are shifted to the left as the system size decreases, which is also in accordance with our discussion in Sec. 5.1.

The influence of the bond dimension can be seen in Fig. 5.6, where the relative deviation is plotted for two bond dimensions for 20 sites. Increasing the bond dimension reduces the error, since an MPS with a larger bond dimension can encompass a larger amount of entanglement in the system.
Figure 5.6: The relative deviation of the ground state energy compared to the exact results for $N = 20$. 

\[
\begin{align*}
\text{Relative Deviation} & \quad h/J \\
10^{-15} & \quad 10^{-13} & \quad 10^{-11} & \quad 10^{-9} & \quad 10^{-7} & \quad 10^{-5} & \quad 10^{-3}
\end{align*}
\]
Part III

NEW TRUNCATION SCHEME FOR CUT
In chapter 4 we presented the general framework of CUT and the necessity of truncation schemes became clear. Tensor networks offer a canonical truncation scheme, which is based on entanglement. It is for that reason we can efficiently approximate states with finite entanglement using tensor networks, e.g. MPS and PEPS. DMRG and TEBD are algorithms based on this property.

It seems reasonable to apply this approach to CUT by formulating the flow equation in the tensor network language. For this to work efficiently the limitation is the same as in other tensor network algorithms: the amount and structure of entanglement. In contrast to e.g. TEBD where the quantum states are truncated, we have to approximate operators in the CUT method. Since the structure in the tensor network language is the same for states and operators, this is done analogously. We call this new method entanglement-CUT (eCUT). It is important to note that entanglement in this sense is understood as the quantum correlations in the description of operators instead of states.

In this chapter we present how eCUT can be implemented for one-dimensional finite-size systems using MPOs. Later, we will present first benchmarks of the algorithm by applying it to the TFIM. Of course, this concept can be generalized to other systems, e.g. 2d systems by using projected entangled pair operators (PEPOs).

### 6.1 The Algorithm

The idea is to discretize the expression for the continuous unitary transformation in Eq. (4.10). We break the $\ell$-ordered integral into $M$ smaller steps of size $\delta \ell$:

\[
U(\ell) \approx u_{M-1} u_{M-2} \ldots u_2 u_1 u_0, \tag{6.1}
\]

with $\ell = M \delta \ell$. The *unitary transformation at step $k$* is then defined as

\[
u_k \equiv \exp(-\eta_k \delta \ell), \tag{6.2}
\]

where $\eta_k$ is the *generator at step $k$*, which in turn depends on $H_k$, the *Hamiltonian at step $k*". These operators, $H_k$, $\eta_k$ and $u_k$, and the operations on them can be formulated in the tensor network language and truncated at each step $k$ as we show in the following:

---

1 PEPO is the operator representation in the PEPS language.
Figure 6.1: Original Hamiltonian and generator written as MPOs.

Figure 6.2: Approximation of $u_k$.

1. **Initialization:**
   In the initial step, $k = 0$, we write the original Hamiltonian $H_0 ≡ H(\ell = 0)$ as an MPO with a bond dimension $D_{H_0}$. Depending on the choice of the generator, the original generator $\eta_0 ≡ \eta(\ell = 0)$ can be either constructed analytically or obtained numerically from the definition of $\eta$ using $H_0$. We write it as an MPO with bond dimension $D_{\eta_0}$. The MPOs are depicted in Fig. 6.1. In the following we denote approximated operators with a prime.

2. **Main loop:** for $k = 0, 1, ..., M - 1$, iterate the following steps:
   (i) **Approximate $u_k$:** evaluate $u_k$ using a Taylor expansion:
   
   $$u_k = \exp(-\eta_1 k \delta \ell)$$
   $$= 1 - \eta_k \delta \ell + \frac{1}{2} \eta_k^2 \delta \ell^2 - \frac{1}{6} \eta_k^3 \delta \ell^3 + O(\delta \ell^4). \quad (6.3)$$

   Notice that the above equation includes the addition and the multiplication of MPOs. That means the bond dimension of the MPOs will be either added or multiplied. The bond dimension of $u_k$ will then be approximated by $D_{U_k}$. If we stop at a first order Taylor expansion, we have

   $$\exp(-\eta_1 k \delta \ell) = 1 - \eta_k \delta \ell + O(\delta \ell^2) \sim 1 - \eta_k' \delta \ell \sim u_k' \quad (6.4)$$

   as depicted in MPO representation in Fig. 6.2. There are two approximations here, the Taylor expansion and the truncation of the MPO. Later, we will see that higher orders of the Taylor expansion reduce the errors significantly.
(ii) Approximate $H_{k+1}$: transform the Hamiltonian with $u_k'$

$$H_{k+1} = u_k^\dagger H_k u_k \sim u_k'^\dagger H_k' u_k' \sim H_{k+1},$$  \hspace{1cm} (6.5)

as depicted in Fig. 6.3. This means we evolve the Hamiltonian approximately by a step $\delta \ell$. The result of the unitary transformation will be an MPO with a bond dimension which is the product of the bond dimensions of $u_k', H_k'$ and $u_k'$. It is crucial to approximate $H_{k+1}$ with an MPO with bond dimension $D_H$.

(iii) Approximate $\eta_{k+1}$: compute the generator $\eta_{k+1}$ from $H_{k+1}$, e.g. for Wegner’s generator compute:

$$\eta_{k+1} = [(H_{k+1})_d, H_{k+1}] \sim [(H_k')_d, H_k'] \sim \eta_{k+1}'.$$  \hspace{1cm} (6.6)

The resulting generator for the step $k+1$ is approximated by an MPO with bond dimension $D_\eta$. This is shown in Fig. 6.4.

By iterating the main loop, we obtain the operators for each successive step:

$$u_k' \rightarrow H_k' \rightarrow \eta_{k+1}' \rightarrow u_k' \rightarrow H_k' \rightarrow \cdots \rightarrow H_{M-1}'$$  \hspace{1cm} (6.7)
and evolve the Hamiltonian by $\delta \ell$.
For sufficiently large $M$, the Hamiltonian $H'_{M-1}$ should converge to a form defined by the generator, e.g. to a (block) diagonal form in Wegner’s case. The pseudocode is shown in Alg. 1.

**Algorithm 1 eCUT**

initialize MPO for $H_0$ and $\eta_0$
approximate $u_0$
for $k \leftarrow 0, M$ do
  unitary transformation and approximation: $H'_{k+1} = u_k^\dagger H'_k u_k$
  compute and approximate $\eta_k$
  compute and approximate $u_k$
end for

We will use the canonical form of the MPOs to truncate them. That means, whenever we have to approximate an MPO with a lower bond dimension, we first have to bring it in canonical form using successive SVDs. The singular values are then truncated, e.g. by choosing a fixed bond dimension, that is, by including only a fixed amount of singular values and disregarding the rest. This implies an approximation of the MPO.

### 6.2 Implementation for a Small System

As we can see, the algorithm comprises several operations on MPOs which increase the bond dimensions. The truncation scheme only works efficiently if we are able to approximate the resulting MPOs with a lower bond dimension. Therefore, we start by implementing the algorithm for the TFIM for a small system size (up to $N = 8$), where we can omit matrix approximations. This allows us to analyze the singular value spectra during the flow, that is, the operator entanglement.

We modify the algorithm to that effect that we contract the bond indices of the MPO after each operation and use successive SVDs to return to the MPO form. The unitary transformation for example consists of the steps depicted in Fig. 6.5.

Although the matrices are not truncated, the algorithm still includes an approximation in form of the Taylor expansion in Eq. (6.3). The implementation uses up to three orders of the Taylor expansion.

We start with Wegner’s generator $\eta^w$ defined in Eq. (4.12) and proceed with the block-generator $\eta^b$ defined in Eq. (4.37) for $r = 0$ ($\eta^b \equiv \eta^{deo}$) and $r = 1$. 

6.2 Implementation for a Small System

For Wegner’s generator we choose a stepsize of $\delta \ell = 0.01$ and a first order taylor expansion. This is already enough to show that this generator is not a good choice for our truncation scheme. The eigenbasis of the $\sigma^z$-operator is chosen as the initial basis of the Hamiltonian. We present the results for four and eight sites ($N = 4$ and $N = 8$).

As a measure of convergence, we introduce the residual off-diagonality (ROD)

$$\text{ROD} = \sqrt{\sum_{i \neq j} |h_{ij}|^2},$$

(6.8)

where the sum is over the off-diagonal elements. According to Eq. (4.22), this should be a monotonically decreasing function for Wegner’s generator.

The ROD for different magnetic fields and four sites is depicted in Fig. 6.6. The Hamiltonian converges faster to a diagonal form as the magnetic field increases. This is expected since we initially started in
the eigenbasis of the $\sigma^z$-operator. One specific example is shown in Fig. 6.7. We see that the ROD exhibits a stepwise decrease. The flow first eliminates matrix elements that couple states with large energy difference and proceeds with smaller energy differences [20]. Hence, at different stages of the flow, different subspaces are diagonalized which explains the stepwise decrease of the ROD.

We can further analyze the singular value spectrum of the MPOs for this specific magnetic field. The spectrum in the middle of the chain for the Hamiltonian is shown in Fig. 6.8 and for the generator in Fig. 6.9. Comparing with the ROD in Fig. 6.7, we can make several observations.

The spectrum for the Hamiltonian is very compressed between $\ell \sim 15$ and $\ell \sim 33$. This is the part where the ROD decreases by a large amount. The spectrum for the generator shows a similar behaviour in this sector but the singular values tend to be smaller overall. To account for the big change in the Hamiltonian, that is to decouple the subspaces
in the Hamiltonian, the singular values in the MPOs need to be large. In this sense we can speak of a large entanglement in the MPOs. Increasing the system size confirms these observations (see \(A.1\)). The spectra are very compressed. We do not see that the spectrums decay exponentially fast. A truncation of the singular values does not seem possible without introducing large errors. Furthermore it is not evident how to read off the eigenvalues of the Hamiltonian one is interested in for large systems. Wegner’s generator is not a good choice for our truncation scheme. Mielke’s generator would have the advantage, that it orders the diagonal elements for large \(\ell\). But the spectra for Wegner’s generator suggests that diagonalizing the whole Hamiltonian leads to compressed singular value spectra. A generator that only decouples the ground state or a small subspace might have a spectrum which is not as compressed. We expect it to be easier to find only the ground state energy.

6.2.2 Block Generator \(r = 0\)

We implement the block generator for \(r = 0\) or equivalent to that \(\eta_{\text{deo}}\). This allows us to compute the ground state energy. The step size remains \(\delta \ell = 0.01\). We implement up to three orders of the Taylor expansion. If not specifically mentioned otherwise, the results are presented for the third order. We define the ROD as

\[
\text{ROD} = \sqrt{\sum_{k=1}^{N} |h_{0k}|^2 + |h_{k0}|^2}.
\]

The initial choice of the basis of the Hamiltonian is crucial to the effective convergence of the algorithm. A starting point close to the eigenbasis of the Hamiltonian is expected to lead to a faster convergence. We study two initial bases, the eigenbasis of the \(\sigma^x\)-operator,
Figure 6.10: ROD for the X-basis and $N = 4$. The small window contains a section of the ROD for $h/J = 0.1$ zoomed in.

Figure 6.11: ROD for the X-basis and $N = 4$ in the early phase of the flow.

which we refer to as the $X$-basis, and the eigenbasis of the $\sigma^z$-operator, which we refer to as the $Z$-basis.

The RODs for $N = 4$, the X-basis and different magnetic fields are depicted in Fig. 6.10 and Fig. 6.11. The RODs decrease exponentially fast. Analyzing the early phase of the flow, we see that the RODs for the different strength of the magnetic field decrease at a similar rate in the beginning. This changes during the flow. The RODs for high magnetic fields go to zero faster than for low magnetic fields, e.g. for $h/J = 0.1$, the decrease seems to stop for $\ell > 5$. Zooming in, we notice still a slight decrease. Similar observations are made when increasing the system size to eight sites ($N = 8$). The figures in the appendix (A.2) show the RODs for eight sites and different orders of the Taylor expansion. Fig. 6.12 shows the results for the third order. For $h/J = 0.1$ the flow shows a plateau at $O(10^{-8})$ compared to $O(10^{-4})$ for $N = 4$. The zoomed window shows that the ROD even increases by a small
Figure 6.12: ROD for the X-basis, $N = 8$ and third order Taylor expansion. The small window contains a section of the ROD for $h/J = 0.1$ zoomed in.

amount but this seems to be due to the Taylor approximation as the comparison with Fig. A.3 and Fig. A.4 suggests. The order of the plateau increases as we increase the magnetic field. At $h/J \sim 0.6$ the ROD decreases ocularly again. Further increase of the magnetic field yields a faster drop of the ROD.

These observations can be understood better by looking at the energy gaps that are depicted in Fig. 6.13. The ground state is almost degenerate for low magnetic fields and the algorithm struggles with decoupling the ground state energy, hence we see plateaus. The turning point at $h/J \sim 0.6$ coincides with the point where the degeneracy is lifted ocularly and close to the point where $\Delta E_{02}$ has a minimum. The same is true for the smaller system where the turning point is at $h/J \sim 0.3$. We can say that close to these turning points, the algorithm is not efficient.

Choosing the Z-basis as the initial basis shows a slightly different behaviour. The RODs are depicted in Fig. 6.14 and Fig. 6.15. The RODs decrease much faster compared to the X-basis, also for low magnetic fields. We can see that the algorithm becomes inefficient nearby the turning points. For low magnetic fields the ROD decreases almost as fast as for high magnetic fields. We do not see the plateaus as in the case of the X-basis. This suggests an influence of the direction of the flow, from where the opening gap between the two lowest energies is approached, on the efficiency.

The singular value spectra in the middle of the chain for both basis are shown in the appendix (A.2.1). In contrast to Wegner’s generator the spectra are not as compressed. The magnitude of the singular values ranges from $O(10^2)$ to $O(10^{-16})$ during the flow. During the
Figure 6.13: Gap between the ground state and the first excited state $\Delta E_{02}$ (straight line) and opening gap between the degenerate ground states $\Delta E_{01}$ (dashed line) for $N = 4$ and $N = 8$.

Figure 6.14: ROD for the Z-basis and $N = 4$. 
Figure 6.15: ROD for the Z-basis and $N = 8$.

early phases of the flow, when the ROD drops at a fast rate, the singular values are increasing and decreasing, so that we see a lot of change in the spectrum. This change stops at a certain point depending on the magnetic field and the chosen basis, so that the singular values converge. Qualitatively we can say that, nearby the turning points, the spectra for the Hamiltonian become more dense in the top part. This means the values are higher in magnitude and we would need to keep more singular values to reduce the errors.

The singular values are smaller for low magnetic fields in the X-basis and increase as we increase the magnetic field. For the Z-basis, the singular values decrease as the magnetic field decreases, although not as much as in the case of the X-basis. Especially the singular values for the generator decay exponentially fast when the initial basis is close to the eigenbasis of the Hamiltonian, so that a truncation seems possible without large errors.

The relative deviation of the ground state energy compared to the exact values for several orders of the Taylor expansion is depicted in Fig. 6.16 and Fig. 6.17. Recall that the source of errors is mainly the Taylor expansion and possible numerical errors since no truncation is introduced yet.

We can observe that the deviation depends very much on the order of the Taylor expansion. Higher orders do not have a large effect on the RODs, but reduce the error exponentially. For Taylor orders two and three the deviation peaks around the turning points as expected since the ROD has not vanished for $t = 100$ in this region (see Fig. 6.12). The deviation due to the non-convergence is larger than the Taylor error. In contrast, the deviation for the first order does not show a peak since the error caused by the Taylor expansion is too large.

There is no peak for the Z-basis since the Hamiltonian can be re-
Figure 6.16: Relative deviation of the ground state energy for different orders of the Taylor expansion: X-basis, $N = 8$, $\ell = 100$.

Figure 6.17: Relative deviation of the ground state energy for different orders of the Taylor expansion: Z-basis, $N = 8$, $\ell = 100$. 
garded as converged for all magnetic fields for $\ell = 100$ (see Fig. 6.15). The deviation increases slightly going to the low magnetic field region.

6.2.3 **Block Generator $r = 1$**

We increase the size of the block by setting $r = 1$. This will allow us to compute the two lowest energies. We expect a better convergence for the regime where the ground state is quasi degenerate, since the subspace of the lowest two energies is decoupled from the rest.

Looking at the RODs\(^2\) for the X-basis in Fig. 6.18, this is exactly what we find. We find better convergence for low magnetic fields compared to the results in Fig. 6.12. For high magnetic fields the ROD decreases more slowly. This is the region where the gap between the two lowest energies has already opened up and the energies are far apart. We notice an abrupt drop to zero at $\sim \mathcal{O}(10^{-7})$ which is probably due to numerical instabilities for very small numbers. The RODs show also an increase\(^3\) leading to a peak, which becomes significant as the magnetic field decreases.

The RODs for the Z-basis decreases more slowly as the magnetic field increases. This could be because the gap between $E_1$ and $E_2$ decreases as the magnetic field increases (see Fig. 5.2). The deviations of the obtained energies from the exact values are shown in Fig. 6.20 - Fig. 6.23. We do not see a peak around the turning point for the X-basis since these values also converged. For the X-basis, we observe an increase of the errors when increasing the magnetic field. The opposite is true for the Z-basis. This is likely due

---

\(^2\) The definition of the ROD is adapted to the size of the block.

\(^3\) The ROD only decreases monotonically for large $\ell$. 
Figure 6.19: ROD for the Z-basis and $N = 8$.

Figure 6.20: Relative deviation of the ground state energy for different orders of the Taylor expansion: X-basis, $N = 8$, $\ell = 100$. 
Figure 6.21: Relative deviation of the second lowest energy for different orders of the Taylor expansion: X-basis, $N = 8$, $\ell = 100$.

Figure 6.22: Relative deviation of the ground state energy for different orders of the Taylor expansion: Z-basis, $N = 8$, $\ell = 100$.

Figure 6.23: Relative deviation of the second lowest energy for different orders of the Taylor expansion: Z-basis, $N = 8$, $\ell = 100$. 
to the transformations in the early phase of the flow. Notice that in the early phase the Hamiltonian changes more rapidly and any errors made here have higher weight. The behaviour for the different bases mirrors the different starting points of the flow. This observation is also important regarding any future truncations. It suggests that keeping more singular values in the early stages of the flow will result in smaller errors. On the other hand, reducing the bond dimension in the latter stages of the flow will have less impact on the overall errors. This is also in accordance with the spectra in the appendix (A.2.1), where the singular values decrease for large $\ell$.

Summary of Results

Our results show that diagonalizing the whole Hamiltonian using Wegner’s Generator does not seem feasible with our truncation scheme, due to the large operator entanglement during the flow. The singular value spectra for the block generator suggest a smaller operator entanglement of the Hamiltonian and show exponential decaying singular values for the generator, hence we will proceed with this generator for further analysis. The errors of the obtained energies decrease exponentially when increasing the order of the Taylor expansion. The efficiency of the method and the errors depend on the initial basis of the Hamiltonian. The X-basis is preferable for low magnetic fields, while the Z-basis is preferable for large magnetic fields.

6.3 IMPLEMENTATION FOR THE GENERIC CASE

In this chapter we implement the full algorithm described in Sec. 6.1 for arbitrary sites, that is, we use our truncation scheme to approximate MPOs. Before we present the results for $N = 8$ and $N = 20$, we will look into some details of the implementation.

6.3.1 Details of the Implementation

A main concern of computational physics is the speed of the used algorithms. It becomes obvious that the bottleneck of eCUT is the SVD. When applying an MPO to an MPO, like in the unitary transformation (see Fig. 6.3), the bond dimensions are multiplied leading to large matrices. We can demonstrate this by looking at the example in Fig. 6.24. After the multiplication of two MPOs the task will be to perform an SVD on matrices like in Fig. 6.24. We labeled the physical dimension as $p$, the bond dimension of the MPOs as $D_H$ and $D_U$.

After applying an MPO to another and subsequently reshaping the resulting tensors, we obtain matrices of the dimension

$$(D_U \cdot D_H \cdot p^2 \times D_U \cdot D_H \cdot p^2).$$
6.3 Implementation for the Generic Case

For simplicity we assume $D := D_U = D_H$, thus the matrices will be of dimension $(D^2 \cdot p^2 \times D^2 \cdot p^2)$. The full SVD of a $(m \times n)$ matrix has a computational complexity of $O(mn^2)$. The computational complexity in our case would be of order $O(p^6D^6)$. In comparison, the updating procedure of an MPS in the TEBD algorithm has a complexity of order $O(p^3D^3)$ [15]. That means the bond dimension is a huge limiting factor, even more so than in TEBD, but on the other hand, it also sets the accuracy of our truncation.

To overcome this we use a randomized singular value decomposition (rSVD) which is described in Ref. [37] and implemented for MATLAB in Ref. [38]. The rSVD allows an approximate calculation of the desired amount of singular values. An analysis of the speedup and accuracy in the case of TEBD can be found in Ref. [1]. For eCUT we also find a significant speedup. For a comparison of the accuracy with the full SVD we show an example for a calculation with the variational generator and a fixed bond dimension of $D = 15$ for all MPOs. The deviation of the results for the ground state energy from both SVD variants is shown in Fig. 6.25. The deviation from the exact values for both variants is depicted in Fig. 6.26 and Fig. 6.27 respectively.

Comparing the three plots we can see that the deviation of the results of rSVD from the results of SVD are generally an order of magnitude smaller than the overall error of the algorithm. One exception is the point at $h/J = 1.15$ for the third order. But this large deviation seems to be a numerical error as Fig. 6.26 suggests. The overall accuracy is sufficient to demonstrate that our algorithm works, hence we will use rSVD for our simulations. But the rSVD has to be considered as another source of error when interpreting the results.
Figure 6.25: The relative deviation of the ground state energy computed with the rSVD compared to the results with the full SVD for: X-basis, N = 8, D = 15 and several orders of the Taylor expansion.

Figure 6.26: The relative deviation of the ground state energy computed with the full SVD compared to the exact results for: X-basis, N = 8, D = 15.

Figure 6.27: The relative deviation of the ground state energy computed with the rSVD compared to the exact results for: X-basis, N = 8, D = 15.
6.3 Implementation for the Generic Case

Figure 6.28: Ground state energy for the X-basis, Z-basis and exact results for: N=8, D = 10, Taylor order = 3.

6.3.2 Results for the Block Generator

Block Generator N=8 r=0

We calculate the ground state energy using the block generator for r = 0. The simulations are run till ℓ = 20 with δℓ = 0.01 for up to the third order in the Taylor expansion. We use the same fixed bond dimensions D for all operators, that is D := D_H = D_U = D_η. Note that the spectra in appendix A.2.1 suggest that this might not be necessary, e.g. D_U and D_η could be chosen smaller than D_H which would also reduce the computational cost. We leave this analyses for future work.

The ground state energy for the two initial bases is depicted in Fig. 6.28. When comparing with the exact results, we can immediately see that the energies for the Z-basis are very inaccurate towards low magnetic fields. We will analyze the accuracy further by plotting the relative deviations. The results are shown for the X-basis (Fig. 6.29 and Fig. 6.30) and Z-basis (Fig. 6.37 and Fig. 6.38). From the previous results we know that the errors of the ground state energy in the first order Taylor expansion are very large. To study the influence of the truncation, we consider the results for the third order and start with the X-basis (see Fig. 6.30).

The errors for different bond dimensions are of the same order for low magnetic fields. For h/J < 0.2 the largest bond dimension produces the lowest errors. This behaviour changes as the magnetic field increases. As the magnetic field rises the deviation increases by a large amount. Comparing with Fig. 6.12, we know that this is mainly due to the fact that the ROD shows plateaus around h/J ~ 0.6. So the deviation is rather a matter of non-convergence than truncation.

In the strong field region, the deviation for the different bond dimensions spreads over several orders of magnitude. In addition to the
Figure 6.29: Relative deviation of the ground state energy for several bond dimensions for: $N = 8$, X-basis, Taylor order = 1.

Figure 6.30: Relative deviation of the ground state energy for several bond dimensions for: $N = 8$, X-basis, Taylor order = 3.
non-convergence of the simulation for $\ell = 20$, the truncation plays also a role. In Fig. 6.31 - Fig. 6.36 the singular value spectra for the Hamiltonian and the generator for several values of the magnetic field are plotted.

The blue straight lines show the singular values without truncation and the dashed orange lines show the singular values for $D = 20$, that is, the largest 20 singular values. Comparing the spectra of the Hamiltonian, we find that for $h/J = 0.1$ a bond dimension of $D = 20$ covers singular values of $O(10^{-7})$ resulting in small errors. For $h/J = 0.8$ the order is $O(10^{-3})$ and for $h/J = 1.4$ it is $O(10^{-1})$. This shows that the further the initial basis is from the final one, the larger the bond dimension has to be to reduce the errors.

Turning to the spectra for the generator, we can see that, without truncation, the singular values decay exponentially fast when the magnetic field is low. However, the truncated spectra deviate from the
Figure 6.33: Singular values for the Hamiltonian in the middle of the chain for: $N = 8$, X-basis, Taylor order = 3, $h/J = 0.8$.

Figure 6.34: Singular values for the generator in the middle of the chain for: $N = 8$, X-basis, Taylor order = 3, $h/J = 0.8$.

Figure 6.35: Singular values for the Hamiltonian in the middle of the chain for: $N = 8$, X-basis, Taylor order = 3, $h/J = 1.4$. 
Figure 6.36: Singular values for the generator in the middle of the chain for: N = 8, X-basis, Taylor order = 3, h/J = 1.4.

Figure 6.37: Relative Deviation of the ground state energy for several bond dimensions for: N = 8, Z-basis, Taylor order = 1

full spectra, which becomes very apparent for e.g. h/J = 1.4, where the singular values of the truncated spectrum increase instead of decreasing. This seems to be a significant source of error. One needs to study the behaviour for larger bond dimensions, but given the computational complexity of the algorithm this becomes impracticable within the scope of this thesis.

Our observations strongly suggest that eCUT is only efficiently applicable when choosing an initial basis close to the basis for ℓ → ∞.

For an analysis of the influence of the truncation for the Z-basis we regard the results for the third order Taylor expansion plotted in Fig. 6.38. Considering the behaviour of the ROD in Fig. 6.15, we see that for ℓ = 20 the RODs are of O(10^{-8}) or smaller and thus the results can be considered as converged. We see that the errors of the ground state energy increase when decreasing the magnetic field. Comparing
with the results for the X-basis, we would expect that the largest bond dimension gives the smallest errors for the Z-basis in the strong field regime. This is not the case here since the magnetic field is not sufficiently large. Looking at the singular value spectrum for e.g. $h/J = 1.5$ in Fig. 6.39, we see that for $D = 20$ the singular values drop only to $O(10^{-3})$. A much larger bond dimension is needed to significantly reduce the errors. For $h/J \to \infty$ we expect a similar behaviour in the strong field regime like in the low field regime for the X-basis. To study this, rewriting the Hamiltonian with a parametrization of the Ising coupling like

$$ H = - \sin(\alpha) \sum_{j=1}^{N} \sigma_j^z - \cos(\alpha) \sum_{j=1}^{N-1} \sigma_j^x \sigma_{j+1}^x, $$

(6.10)
would be useful. For $\alpha = 0$ we have the limit with a vanishing magnetic field and for $\alpha = \pi/2$ we have the limit with a vanishing coupling.

**Block Generator N=8 r=1**

We set $r = 1$ to compute the two lowest energies $E_0$ and $E_1$. We run the simulations for $\ell = 30$ since the RODs should be sufficiently small (see Fig. 6.18 and Fig. 6.19).

Examples of the obtained energies are depicted in Fig. 6.40 and Fig. 6.41.

We see that the results for the Z-basis become inaccurate towards low magnetic fields. The same is expected for the X-basis for large magnetic fields. Fig. 6.42 shows the relative errors of the ground state energy for the X-basis in third order Taylor expansion. Comparing this with the results for $r = 0$ (see Fig. 6.30), we see an overall increase...
of the error. Additionally the results for different bond dimensions are scattered over several orders of magnitude even for low magnetic fields, where the X-basis should deliver good results. These observations can be explained by looking at the comparison of the singular value spectra in Fig. 6.43. We can see that the singular values for $r = 1$ are several orders of magnitude larger during the flow than the singular values for $r = 0$. We can conclude that a larger bond dimension is needed when increasing $r$. Otherwise the truncation will lead to larger errors.

Fig. 6.44 shows the errors for the second lowest energy. Qualitatively the errors show the same trend as for the ground state energy with regard to the strength of the magnetic field.

Fig. 6.45 shows a comparison between the errors of the ground state energy for both block sizes and the second lowest energy. The interesting part is the section up to $h/J \sim 0.6$. The ground state energy for
6.3 IMPLEMENTATION FOR THE GENERIC CASE

Figure 6.44: Relative deviation of the second lowest energy $E_1$ for several bond dimensions for: $N = 8$, X-basis, Taylor order = 3.

Figure 6.45: Relative deviation of the energies obtained for $r = 0$ and $r = 1$: $N = 8$, X-basis, Taylor order = 3, $D = 20$. 
Figure 6.46: Relative deviation of the ground state energy $E_0$ for several bond dimensions for: $N = 8$, Z-basis, Taylor order = 3.

Figure 6.47: Relative deviation of the second lowest energy $E_1$ for several bond dimensions for: $N = 8$, Z-basis, Taylor order = 3.

$r = 0$ shows the smallest errors. For $r = 1$ the error of the second lowest energy is smaller than the error for the ground state energy. Fig. 6.46 and Fig. 6.47 show the results for the Z-basis in third order. The observations we made for the X-basis can be transferred to the Z-basis, taking the asymmetry of the bases regarding the chosen magnetic fields into account.

Block Generator $N=20$, $r=0$

We proceed by increasing the system size to 20 sites. Note that for a spin-1/2 system, the Hamiltonian is a matrix of size $m \times m = 2^{20} \times 2^{20}$. If we want to store this matrix on a computer using double precision, we would need about 8.8 Terabyte of memory. The computational complexity is of $O(m^3)$. So for $N \sim 20$ the limit of what is possible on a computer is reached. This is why we would like our
method to be able to handle matrices beyond that limit. We run the computations with the same parameters as in Sec. 6.3.2. In order to reduce the runtime, we choose again a fixed amount of steps, that is, we run the algorithm till $\ell = 18$. Considering the RODs for $N = 8$, that means that it is not guaranteed that the RODs have vanished. This non-convergence has to be taken into account. An example for the ground state energy is depicted in Fig. 6.48. We can see a large deviation for the Z-basis for low magnetic fields. A further analysis will show unstable results for both bases. The relative errors for the X-basis are depicted in Fig. 6.49 (first order) and Fig. 6.50 (third order). In addition to observations made for $N = 8$, we see a lot of data points missing when increasing the bond dimension. This is because these values diverged. For $D = 15$ and $D = 20$ the truncation leads to instabilities and thus to larger er-
errors or diverging values. For $D = 10$ the algorithm seems to be more stable and exhibits smaller errors, which seems surprising. To find a systematic behaviour it is necessary to run computations with a wide range of bond dimensions. Our results so far suggest that the range of bond dimensions we studied is lower than the necessary dimension to properly approximate the operators, so that the algorithm is very sensitive to the bond dimension at which we truncate. We think that, in simulations with much larger bond dimensions, the errors should decrease as the bond dimension increases, as one would expect.

For completeness we show the results for the Z-basis in Fig. 6.51 (first order) and Fig. 6.52 (third order). We can make analogous observations as for the X-basis. Increasing the magnetic field should further decrease the errors but the most significant problem stays the insufficient bond dimension. These results should be regarded as a first
proof of concept. A more thorough benchmark with larger bond dimensions and longer runtime is definitely necessary. We conclude with showing again a main result in Fig. 6.53. The simulation was run until \( \ell = 10 \) instead of \( \ell = 18 \), so that the results are not converged yet, but also did not diverge. We clearly see that the initial choice of the basis effects the efficiency of the algorithm.

6.4 Summary of results

We briefly summarize and discuss our results, mention what we missed and what improvements we suggest for further analysis of the method. We have implemented a test code for small system sizes without approximations of operators during the flow, that is, without any truncation of the singular values. This allowed us to study the effect of
the order of the Taylor expansion in Eq. (6.3), as well as the singular value spectra during the flow. The analysis was done for four and eight sites ($N = 4$ and $N = 8$).

The results for Wegner’s generator show that diagonalizing the whole Hamiltonian with our method seems impractical for two reasons. One reason is the long runtime which is necessary to sufficiently decrease the ROD. But more importantly, the singular value spectra are too compressed, that is, they do not show an exponential decay. A proper truncation seems impossible. A more thorough analysis using a modified Hamiltonian like in Eq. (6.10) would be useful to study the behaviour for different initial bases (X-basis and Z-basis).

Mielke’s generator was not implemented since it is yet unclear how to construct this generator as an MPO. We expect it to behave similarly to Wegner’s generator, regarding runtime and singular value spectra. Nevertheless, it would be interesting to study this generator since, in contrast to Wegner’s generator, the diagonal elements of the Hamiltonian are ordered for large $\ell$.

We have implemented the block generator defined in Eq. (4.37) for $r = 0$ and $r = 1$. This allowed us to calculate the two lowest energies. The results demonstrate that increasing the order of the Taylor expansion reduces the errors exponentially. Most importantly, the singular value spectra are not as compressed as in the case of Wegner’s generator and show an exponential decay especially for the generator. This motivated us to use the block generator in the fully implemented eCUT algorithm described in Sec. 6.1.

Finally we have implemented eCUT using the block generator for $r = 0$ and $r = 1$. We have identified the bottleneck of the algorithm and sketched it in Fig. 6.24. The computational cost of the depicted step goes with at worst $D^6$, where $D$ is the bond dimension of the involved operators. This motivated us to use a $rSVD$ for speedup which must also be considered as a source of error. To eliminate this source, it is advisable to use a stable SVD algorithm in future works, which comes at the cost of a longer runtime.

Truncations were done for fixed bond dimensions: $D = 10$, $D = 15$ and $D = 20$. The same bond dimension was chosen for the Hamiltonian, the generator and the unitaries. There are several points that influence the operator entanglement during the flow and hence the quality of the approximation of the operators.

- The choice of the initial basis is very important. If it is close to the final basis ($\ell \rightarrow \infty$) the bond dimension can be kept low. If the initial basis is far from the final basis the flow requires a larger bond dimension. This is evident from the plots for the relative error for the X-basis and Z-basis.

- The operator entanglement is large nearby the points we referred to as the turning points. For $N \rightarrow \infty$ these points would be critical points, hence cannot be represented with a finite bond
dimension in the MPS formalism. Our findings are in accordance with that.

- The transition from $r = 0$ to $r = 1$ shows that in the latter case a larger bond dimension is required.

- When comparing the results for $N = 8$ and $N = 20$ it becomes apparent that a larger bond dimension is needed, the larger the system size is.

The last two points are related to the number of off-diagonal elements that have to be eliminated. If this number increases the bond dimension should increase as well.

An extended analysis is necessary in this area. This can be done by studying a wide range of fixed bond dimensions. Additionally the bond dimensions for the three operators should be chosen separately. For $\ell \to \infty$ the unitary operators should become the unity operator with bond dimension one. In this respect an adapted bond dimension that adapts to the requirements of the flow would be beneficial. The truncation is then performed based on a threshold for the singular values. A positive effect of this procedure is that it speeds up the flow for large $\ell$. An implementation was done but did not produce stable results for the chosen thresholds and thus was disregarded. Nevertheless we think this way of truncation is preferable to the fixed bond dimension method.

In addition to an adaptive bond dimension we can use an adaptive stepsize $\delta \ell$. We have chosen a fixed value, $\delta \ell = 0.01$, throughout the flow. The ROD decreases exponentially. At the beginning of the flow the ROD is reduced by a large amount and the algorithm is more sensitive to errors than in later stages of the flow. Taking this into account we can choose a smaller stepsize at the start and increase $\delta \ell$ at later stages. This can further reduce errors.

For $N = 20$ we could not produce satisfactory results due to limited time and resources. We suggest further computations with larger bond dimensions and longer runtime.

A way of stabilizing the method would be to normalize the tensors in the MPOs. This is a standard procedure when dealing with MPS and easily realized due to the nature of states but is more complicated when dealing with operators. One needs to keep track of the normalization constants during the flow.
7 CONCLUSIONS AND FURTHER WORK

7.1 COMPARISON WITH OTHER METHODS

We discussed several advantages and disadvantages of eCUT and want to give a brief comparison of the algorithm with other tensor network algorithms and other truncation schemes for CUT.

Two prominent and well studied tensor network methods are DMRG and TEBD. We have already discussed some properties of TEBD. The computational complexity of TEBD is smaller than the computational complexity of eCUT, but it allows only the computation of the ground state and energy, whereas with eCUT we can in theory obtain an effective Hamiltonian that allows the computation of excitations as well. With DMRG, the computation of excitations is also possible. A significant difference to eCUT is that DMRG is a variational method. The flow equation method itself is not variational.

In comparison with self-similar CUT, where the truncation has to be adapted to the problem on a case-by-case basis, eCUT is a more general tool. In contrast to perturbative approaches it does not require a small expansion parameter. We saw that its limitations are the entanglement properties of the Hamiltonian.

7.2 CONCLUSIONS

In this thesis a new algorithm for quantum many-body physics was introduced. We formulated the CUT method in TN language and utilized tensor network approximations of operators as a truncation scheme for CUT. This truncation scheme stands out from existing schemes for CUT since it is based on the entanglement content of operators. Thus, it is subject to very different limitations than the existing ones.

In the first part, we introduced the basic concepts of entanglement and the TN formalism. Our focus was on the framework for 1d systems, that is, we focused on MPS and MPO. We gave an overview over the CUT approach and several generators for unitary transformations in the context of CUT were discussed. A new generator called block generator that can target the low energy spectrum, hence especially suitable for tensor network algorithms, was described.

In the second part of the thesis, the 1d TFIM model was reviewed. A solution of the model was given using known results and a benchmark using the well-known TN algorithm TEBD was performed.

In the third part the new algorithm eCUT was described and the imple-
mentation for a finite 1d system was explained. First benchmarking results using TFIM, a spin-1/2 system with N sites, were presented. The benchmark was divided into two parts. In the first part a variation of the algorithm for small system sizes, that is, for up to eight sites, was implemented. This allowed the study of the operator entanglement without truncation and the influence of a Taylor expansion that is necessary for the algorithm. The analysis was done for Wegner’s generator and the block generator for block sizes one and two. The former allowed a diagonalization of the whole Hamiltonian and the latter the computation of the two lowest energy eigenvalues. Our findings suggested that the operator-entanglement in the case of Wegner’s generator is too large and a truncation is not feasible. The results for the block generator showed low and exponentially decaying singular values depending on the initial basis of the Hamiltonian. Additionally we saw an exponential decrease of the errors of the obtained energies when increasing the order of the Taylor expansion from one to two and three.

In the second part of the benchmark the full eCUT algorithm with truncations was analyzed for eight and 20 sites. The block generator was used which allowed the computation of the ground state energy and the second lowest energy. Only the ground state energy was computed for the simulation of TFIM with 20 sites. The truncation was done for fixed bond dimensions. This was sufficient to demonstrate the feasibility of the truncations scheme provided the initial basis of the Hamiltonian is close to the basis of the desired effective Hamiltonian.

We conclude by stating that the results of this thesis should be regarded as a proof of concept. To demonstrate the viability of eCUT further analysis is necessary, especially for larger system sizes.

7.3 Outlook

In Sec. 6.4 we suggested some improvements regarding the analysis in this thesis. Once the algorithm is well understood, future works could include several proposals. The system size could be increased. Certainly we are interested in studying larger system sizes. Going beyond the limit of exact diagonalization would be definitely beneficial. The computational complexity is a limiting factor here. Infinite systems could be studied using a translational invariant unit cell analogous to iTEBD. This would also get rid of the computational overhead for finite systems since the SVD has to be applied only on the unit cells instead of the whole chain.

In case of the block generator we could increase the size of the block we want to decouple, that is, increase the parameter r. This would allow us to compute more eigenvalues of the Hamiltonian.
Our results suggest that eCUT is not very efficient if the initial basis of the Hamiltonian is far apart from the final basis\(^1\), so that a notion of the problem at hand and its properties is necessary. One could think about rough approximation or other transformations to block-diagonalize the Hamiltonian beforehand which should increase the efficiency of eCUT. In this respect, one could also think about implementing symmetries.

As discussed in the introduction to CUT, observables other than the energy can also be computed in similar fashion. Additionally one can think about computing states by passing from the Heisenberg picture to the Schrödinger picture\(^2\) as done in Sec. 4.3.5. If the transformation of the Hamiltonian is known, then it is sufficient to apply this transformation backwards to the states.

Other 1d models, where the Hamiltonian can be efficiently expressed as an MPO, can be studied. Since the scheme is independent of the type of interactions (short range, long range, . . .) in the Hamiltonian, one could also study e.g. next-to-nearest neighbours etc. The generalization to the PEPS framework should be straightforward which would allow the study of models with a higher spatial dimension using PEPOs. For 2d this would be interesting, since there are not too many options to compute excitations.

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\(^1\) This is a general problem of CUT and not specifically related to eCUT.

\(^2\) In the literature Heisenberg picture and Schrödinger picture are defined in the case where time is the continuous parameter. In our case the continuous parameter is \(\ell\) but everything is analogous.
Part IV

APPENDIX
A.1 Wegner’s Generator

Figure A.1: Singular Values of the MPO for the Hamiltonian in the middle of the chain during the flow for $h/J = 0.2$ and $N = 8$.

Figure A.2: Singular Values of the MPO for the generator in the middle of the chain during the flow for $h/J = 0.2$ and $N = 8$.  

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A.2 Block Generator

Figure A.3: ROD for the X-basis, \( N = 8 \) and first order Taylor expansion.

Figure A.4: ROD for the X-basis, \( N = 8 \) and second order Taylor expansion.

Figure A.5: ROD for the X-basis, \( N = 8 \) and third order Taylor expansion in the early phase of the flow.
A.2.1 Singular Value Spectra Block Generator $r = 0$

Figure A.6: $H$ (left) and $\eta^{\text{deo}}$ (right), $N = 8$, X-basis, $h/J = 0.1$.

Figure A.7: $H$ (left) and $\eta^{\text{deo}}$ (right), $N = 8$, X-basis, $h/J = 0.3$.

Figure A.8: $H$ (left) and $\eta^{\text{deo}}$ (right), $N = 8$, X-basis, $h/J = 0.5$.

Figure A.9: $H$ (left) and $\eta^{\text{deo}}$ (right), $N = 8$, X-basis, $h/J = 0.6$. 
Figure A.10: H (left) and $\eta^{\text{deo}}$ (right), $N = 8$, X-basis, $h/J = 0.7$.

Figure A.11: H (left) and $\eta^{\text{deo}}$ (right), $N = 8$, X-basis, $h/J = 0.9$.

Figure A.12: H (left) and $\eta^{\text{deo}}$ (right), $N = 8$, X-basis, $h/J = 1.3$.

Figure A.13: H (left) and $\eta^{\text{deo}}$ (right), $N = 8$, X-basis, $h/J = 1.5$. 
Figure A.14: $H$ (left) and $\eta^{deo}$ (right), $N = 8$, Z-basis, $h/J = 0.1$.

Figure A.15: $H$ (left) and $\eta^{deo}$ (right), $N = 8$, Z-basis, $h/J = 0.3$.

Figure A.16: $H$ (left) and $\eta^{deo}$ (right), $N = 8$, Z-basis, $h/J = 0.5$.

Figure A.17: $H$ (left) and $\eta^{deo}$ (right), $N = 8$, Z-basis, $h/J = 0.6$. 
Figure A.18: H (left) and $\eta^{\text{deo}}$ (right), $N = 8$, Z-basis, $h/J = 0.7$.

Figure A.19: H (left) and $\eta^{\text{deo}}$ (right), $N = 8$, Z-basis, $h/J = 0.9$.

Figure A.20: H (left) and $\eta^{\text{deo}}$ (right), $N = 8$, Z-basis, $h/J = 1.1$.

Figure A.21: H (left) and $\eta^{\text{deo}}$ (right), $N = 8$, Z-basis, $h/J = 1.3$. 

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**Implementation for Small Systems**
A.2 block generator

Figure A.22: H (left) and $\eta_{deo}$ (right), $N = 8$, Z-basis, $h/J = 1.5$.

A.2.2 Singular Value Spectra Block Generator $r = 1$

Figure A.23: H (left) and $\eta_{deo}$ (right), $N = 8$, X-basis, $h/J = 0.1$.

Figure A.24: H (left) and $\eta_{deo}$ (right), $N = 8$, X-basis, $h/J = 0.3$.

Figure A.25: H (left) and $\eta_{deo}$ (right), $N = 8$, X-basis, $h/J = 0.5$. 
Figure A.26: H (left) and $\eta^{deo}$ (right), $N = 8$, X-basis, $h/J = 0.6$.

Figure A.27: H (left) and $\eta^{deo}$ (right), $N = 8$, X-basis, $h/J = 0.7$.

Figure A.28: H (left) and $\eta^{deo}$ (right), $N = 8$, X-basis, $h/J = 0.9$.

Figure A.29: H (left) and $\eta^{deo}$ (right), $N = 8$, X-basis, $h/J = 1.3$. 
Figure A.30: $H$ (left) and $\eta^{\text{deo}}$ (right), $N = 8$, X-basis, $h/J = 1.5$.

Figure A.31: $H$ (left) and $\eta^{\text{deo}}$ (right), $N = 8$, Z-basis, $h/J = 0.1$.

Figure A.32: $H$ (left) and $\eta^{\text{deo}}$ (right), $N = 8$, Z-basis, $h/J = 0.3$.

Figure A.33: $H$ (left) and $\eta^{\text{deo}}$ (right), $N = 8$, Z-basis, $h/J = 0.5$. 
Figure A.34: H (left) and $\eta^{\text{deo}}$ (right), $N = 8$, Z-basis, $h/J = 0.6$.

Figure A.35: H (left) and $\eta^{\text{deo}}$ (right), $N = 8$, Z-basis, $h/J = 0.7$.

Figure A.36: H (left) and $\eta^{\text{deo}}$ (right), $N = 8$, Z-basis, $h/J = 0.9$.

Figure A.37: H (left) and $\eta^{\text{deo}}$ (right), $N = 8$, Z-basis, $h/J = 1.5$. 
BIBLIOGRAPHY


