Entanglement Entropy in 1D Noninteracting Fermionic Systems

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Eidesstattliche Erklärung

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

Aachen, den 14. September 2012

(Daniel Weigand)
Abstract

This bachelor thesis examines entanglement in various 1-D non-interacting fermionic systems. After a short introduction on entanglement in general, we introduce the Schmidt rank and the entanglement entropy as two examples for entanglement measures in bipartite systems. After that, we discuss entanglement in fermionic systems. This discussion will focus mainly on the consequences of the fermionic statistics if the fermions are not separated by distance or a sufficiently large energy barrier, and adjust the entanglement measures to address those consequences. This will be done by introducing the Slater rank, a generalization of the Schmidt rank, and generalizing the entanglement entropy to second quantization.

In the second part of this thesis, we will derive an algorithm to compute the entanglement entropy for a 1-D fermionic system. This algorithm will be used later on to first retrieve known results, e.g. the logarithmic scaling of the entanglement entropy if the system is at a critical point, and then examine various non-interacting bipartite 1-D fermionic systems, especially the toy model introduced by Kitaev in [1]. Of special interest will be the entanglement of a block of size $L$ with the rest of the system for disturbances in the chemical potential and the superconductivity gap for periodic boundary conditions as well as open boundaries.

We show that the entanglement entropy for one of the phases of the Kitaev wire is very stable. It increases only slightly for varying parameters and shows a very small dependence on disorder, even if the disorder is large.
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1. Introduction

The notion of entanglement is one of the most astonishing features of quantum mechanics. It allows correlations between locally separated locations, reliable even over huge distances. This correlation, titled as “spooky” in the first days of quantum mechanics, even used by its opposers as an argument that the theory of quantum mechanics cannot be complete, is nowadays well-established not only as a curiosity of the theory but as a valuable resource.

The main motivation for this thesis is that it is very difficult to store qubits reliably. One possible solution may be to store that qubit with Majorana particles, as these are relatively robust with respect to disorder.

The plan for this thesis will be the following: In Section 2, we will discuss entanglement in quantum systems in general, entanglement measures (especially the entanglement entropy) and the consequences of fermionic statistics of entanglement if the entangled entities are not separated by a large energy barrier. In Section 3, we will go on to Kitaev’s toy model, which he introduced in [1] as well as a few modifications we will use later on. Section 4 will be dedicated to derive an algorithm to compute the entanglement entropy for a bipartite 1-D system, namely of a block of size $L$ in a system of size $N$. The actual computations will be presented in Section 5.

To make reading easier, some proofs are moved to appendix A and the actual Matlab code used in the computations will be shown and explained in appendix B.
2. Entanglement in Quantum Systems

While its consequences can be quite complex and there are plenty of applications, the concept of entanglement itself is simple. In this chapter, we will define entanglement and examine some of its properties. After introducing entanglement measures for distinguishable entangled entities, we will discuss entanglement for fermions and introduce the entanglement measures of Slater rank and entanglement entropy in second quantization. This chapter is only a short discussion of the topic and it is neither feasible nor intended for it to be complete. For further reading on entanglement, see the lengthy, but highly recommendable review by R., P., M. and K. Horodecki [2].

2.1. Definition of Entanglement

Definition 1. Let \(|\Psi\rangle\) be a state of multiple physical systems and \(|\Phi_i\rangle\) a state in system \(i\). Then, \(|\Psi\rangle\) is called entangled if it cannot be expressed as a product of \(|\Phi_i\rangle\) for any set of \(|\Phi_i\rangle\).

If \(|\Psi\rangle\) is not entangled, it is called separable. If \(|\Psi\rangle\) is a product of \(|\Phi_i\rangle\), \(|\Psi\rangle\) is called a product state. All product states are separable.

For example, one can easily check that the following state \(|\Psi\rangle\) is entangled:

\[
|\Psi\rangle = \frac{|11\rangle + |00\rangle}{\sqrt{2}} \neq (a|1\rangle + b|0\rangle) \otimes (a'|1\rangle + b'|0\rangle) \quad \forall a, b, a', b'
\]

Another Approach

A second, more experimentalist approach to the definition of entanglement is based on the way how entanglement can be obtained. Consider two experimental setups \(A\) and \(B\). As these setups are separate, they may only apply local operations. They may use classical communication to coordinate those operations. Then, entanglement can be defined by these operations [3]:

Definition 2. If a shared state \(\rho\) can be obtained by two parties \(A\) and \(B\) using only local operations and classical communication, \(\rho\) is a separable state.

Note that these two definitions of entanglement are equivalent.

Qubits

As it is a property of the state function, entanglement can in principle occur for every physical entity that can be described by such a quantum mechanical wave function. From
now on, we will refer to these entities as \textit{qubits} in the case of distinguishable entities, and as \textit{fermions} in the case of fermions where the fermionic statistics are relevant.

\textbf{Entanglement and Faster-Than-Light Communication}

One of the great challenges of describing entanglement in the first days was that the effect of a measurement on an entangled state is instantaneous. This seems to imply that an instantaneous transfer of information could be possible by encoding the information in the form of measurements, a clear contradiction to the principle of causality. That dilemma gets solved by the way entanglement changes the state functions after a measurement. The following short discussion is no proof that communication faster than light using entanglement is impossible, but it should make a reasonable case for it.

Suppose there are two sites $A$ and $B$ as well as a shared entangled state with density matrix $\rho = |\Psi\rangle\langle\Psi|$. As shown in section Section 2.2.1, $\rho$ can then be written as

$$\rho = \sum_i \sqrt{\lambda_i \lambda_j} |i_A\rangle\langle j_A| \otimes |i_B\rangle\langle j_B|$$

(2.1.2)

where $\sum_i \lambda_i = 1$, $\lambda_i \geq 0$ and $\lambda_i > 0$ for at least two different $i$. Note that this holds for all bases of $A$ and $B$, so one can assume that $|i_A\rangle$ and $|i_B\rangle$ are eigenstates of $A$ respectively $B$ and that every measurement is taken in the base of these eigenstates.

If a measurement is applied on site $A$, result $i$ occurs with probability $\lambda_i < 1$. As the state function collapses after the measurement, any subsequent measurement will retrieve result $i$ both for site $A$ and site $B$ with probability 1. It is important to note that there is no way to predict the result of the measurement prior to the measurement and no way to retrieve the original state after the measurement is applied.

There are two basic concepts how to encode information, in the frequency of a signal in a common base, or in the alteration of the base at a fixed frequency.

Thus, there is no way to determine if a measurement has been applied to a state without the use of classical communication, it is therefore impossible to encode information in the frequency of measurement.

On the other hand, it is impossible to distinguish nonorthogonal states faithfully. This can also not be done by repeated measurements, as the original state is lost in the process of measurement.

However, it is possible to transmit quantum information respecting the speed of light as a limit using an entangled state. This can be done using the quantum teleportation protocol (see for example [4]). In short, site $A$ applies a series of measurements on an entangled state shared with site $B$ to transmit a second state faithfully. In order to retrieve this second state, site $B$ has to apply a measurement depending on the results of site $A$. These results, however can only be transmitted at the speed of light.

\textbf{2.2. Entanglement Measures}

The need to measure entanglement quantitatively first rose [2] when Bennet et al. described the means to transmit quantum data in [5]. The paper addresses the question what
resources are needed to transmit quantum data faithfully\(1\) over a noisy channel. In short, there are two possible approaches, direct transfer of the qubit over the channel and the use of quantum teleportation. The former would obviously be subject to noise, the latter can be used to transmit a qubit faithfully, but needs a shared, perfectly entangled state to start with.

In previous work \(6\) was shown that entanglement can be concentrated. Thus, \(n\) partially entangled states can be used to create \(m < n\) “more entangled” states, while the distance to the perfectly entangled state can be made arbitrary small for a sufficiently high \(n\). The need for a measure arises when one wants to quantify the number of states needed to get a certain amount of entanglement or to compare two partially entangled states.

Another problem is to detect entanglement between states at all. While our examples are easy to compute, there are a lot of cases where a lot of work is needed to detect entanglement by using its definition directly. Therefore, it is useful to introduce entanglement measures. Such a measure \(E(\rho)\) should fulfill the following properties \(7\):

\begin{enumerate}
\item \(E(\rho) = 0\) if and only if \(\rho\) belongs to a pure state
\item \(\rho \rightarrow E(\rho) \in \mathbb{R}^+_0\)
\item \(E(\rho)\) should be normalized, typical is \(E(\rho) = \log_2(N)\) if \(\rho\) belongs to a maximally entangled state of size \(N\)
\item \(E(\rho)\) should not increase for local operations and classical communication between the two parties
\end{enumerate}

Note that only the first two properties are necessary for an entanglement measure, but the others are very useful.

### 2.2.1. Schmidt Decomposition and Schmidt Rank

The Schmidt rank provides a measure for entanglement of pure states in the case of distinguishable entangled entities. It is derived from the Schmidt decomposition \(4, 8\):

**Theorem 1 (Schmidt decomposition).** Let \(|\Psi\rangle\) be a pure state of a composite system \(AB\). Then, there exists an orthonormal set of states \(|i_A\rangle\) for system \(A\) respectively an orthonormal set of states \(|i_B\rangle\) for system \(B\) such that

\[
|\Psi\rangle = \sum_i \sqrt{\lambda_i} |i_A\rangle |i_B\rangle
\]

(2.2.1)

where \(\lambda_i\) are non-negative real numbers satisfying \(\sum_i \lambda_i = 1\) known as Schmidt coefficients. The number of non-zero Schmidt coefficients is called the Schmidt rank.

\(1\) Faithful means that the influence of noise can be reduced below an arbitrary threshold.

\(2\) We will only discuss entanglement measures for bipartite systems. To examine entanglement in multiparty systems is actually a very hard task that would go beyond this thesis.
The proof can be found in Section A.1 in Appendix A. With Definition 1 follows: $|\Psi\rangle$ is entangled if and only if its Schmidt rank is greater than 1.

2.2.2. Entanglement Entropy

The entanglement entropy is another measure for entanglement. It is computed via the von-Neumann entropy of the reduced density matrix of a subsystem.

**Definition 3.** Let $\rho$ be the density matrix of a composite physical system with subsystems $A$ and $B$. Let $\rho_A$ be the reduced density matrix of system $A$:

$$\rho_A = \text{Tr}_B \rho$$  \hspace{1cm} (2.2.2)

Then, the entanglement entropy is defined by

$$S(\rho_A) = -\text{Tr}(\rho_A \log_2(\rho_A))$$  \hspace{1cm} (2.2.3)

Using the Schmidt decomposition, the entanglement entropy reduces to the Shannon entropy of the Schmidt coefficients:

$$\rho = \sum_{i,j} \sqrt{\lambda_i \lambda_j} |i_A\rangle \langle j_B| \otimes |i_B\rangle \langle j_B|$$

$$\rho_A = \text{Tr}_B \rho = \sum_{i,j} \text{Tr}_B \sqrt{\lambda_i \lambda_j} |i_A\rangle \langle j_B| \otimes |i_B\rangle \langle j_B|$$

$$= \sum_{i,j} \sqrt{\lambda_i \lambda_j} |i_A\rangle \langle j_B| \delta_{ij}$$

$$= \sum_i \lambda_i |i_A\rangle \langle i_A|$$

As the density matrix $\rho_A$ is diagonal, the entanglement entropy reduces to the Shannon entropy of the eigenvalues $\lambda_i$ of the reduced density matrix:

$$S(\rho) = -\sum_j \lambda_j \log_2(\lambda_j)$$  \hspace{1cm} (2.2.4)

Where the entropy for $\lambda_i = 0$ is defined as: $0 \log_2(0) = 0$.

The entanglement entropy has several very useful properties which will proved below.

I. $S(\rho_A) = 0$ if and only if $\rho_A$ is the density matrix of a separable state

II. $S(\rho_A)$ is invariant under base change: $S(\rho) = S(U \rho U^\dagger)$

III. $S(\rho) + S(\rho') = S(\rho \otimes \rho')$ if $\rho$ and $\rho'$ act on disjoint Hilbert spaces

Note that the entanglement entropy of the reduced density matrix $\rho_A$ is the same as the entanglement entropy of $\rho_B$. Nevertheless, we keep the index $A$ to indicate that the entanglement entropy depends on the relative sizes of regions $A$ and $B$. 
Proofs

I. As shown above, the entanglement entropy of a reduced state $\rho_A$ is equivalent to the Shannon entropy of the eigenvalues of the reduced density matrix $\rho_A$. If the reduced density matrix $\rho_A$ is itself the density matrix of a separable state, its only nonzero Schmidt coefficient is $\sqrt{\lambda_1} = 1$. Therefore, the entanglement entropy vanishes as $S(\rho_A) = 1 \log_2(1) = 0$.

If $\rho$ is the density matrix of an entangled state, there are at least two non-zero Schmidt coefficients $\sqrt{\lambda_i}$ with $\sum_i \lambda_i = 1$ such that $|\Psi\rangle = \sum_i \sqrt{\lambda_i} |i_A\rangle |i_B\rangle$. Then

$$S(\rho) = -\sum_i \lambda_i \log_2(\lambda_i)$$

$$= \sum_i \frac{1}{a_i} \log_2(a_i) > 0$$

where we used $0 < \lambda_i < 1$ and introduced $a_i > 1$ such that $\lambda_i = \frac{1}{a_i}$. □

II. Let $\rho$ be a density matrix, $\tilde{\rho}$ its diagonal form and $U$ the unitary matrix that diagonalizes $\rho$. Then

$$S(\rho) = -\text{Tr}(\rho \log_2(\rho)) = -\text{Tr}(U \tilde{\rho} U^\dagger \log_2(\tilde{\rho}) U^\dagger)$$

$$= -\text{Tr}(U U^\dagger \tilde{\rho} \log_2(\tilde{\rho})) = -\text{Tr}(\tilde{\rho} \log_2(\tilde{\rho}))$$

where we used that matrices in a trace commute. We show that $\log_2(\rho) = U \log_2(\tilde{\rho}) U^\dagger$ in Section A.2 in Appendix A. □

III. Assume $\rho$ and $\rho'$ are two density matrices that act on disjoint Hilbert spaces. Then

$$S(\rho \otimes \rho') = S(U(\rho \otimes \rho') U^\dagger) = S(V \rho V^\dagger \otimes T \rho' T^\dagger) = S(\tilde{\rho} \otimes \tilde{\rho}')$$

where we used in the first step that the entanglement entropy is invariant under base change and in the second step that $\rho$ and $\rho'$ act on disjoint Hilbert spaces. $U$ is defined as

$$U = V \otimes T$$

where $V$ is the unitary matrix that diagonalizes $\rho$ and acts on its Hilbert space, while $T$ is the unitary matrix that diagonalizes $\rho'$ and acts on the Hilbert space of $\rho'$. The eigenvalues of diagonal $\tilde{\rho}$ are $a_j$, the eigenvalues of diagonal $\tilde{\rho}'$ are $b_l$.

$$S(\tilde{\rho} \otimes \tilde{\rho}') = -\sum_{j,l} [a_j \log_2(a_j) + b_l \log_2(b_l)] = -\sum_j a_j \log_2(a_j) - \sum_l b_l \log_2(b_l)$$

$$= S(\rho) + S(\rho')$$

□
2.3. Entanglement in Fermionic Systems

To be able to describe entanglement in a real physical setup, one has to understand the properties of that system and how they affect the state functions. For fermionic systems, there are three important properties affecting the state functions and therefore entanglement:

I. By Pauli’s principle, multiple fermions cannot be in the same state

II. Fermions are indistinguishable

III. Fermionic state functions must be anti-symmetric

To show the consequences on entanglement, we will take a brief look at two examples. For further reading, Eckert et.al. did a decent job at showing those consequences in [8], they consider the spins, too.

Example 1. Let $|\Psi\rangle$ be the state function of a system of two modes filled by a single fermion. We assume there is only one spin direction allowed, e.g. by applying a sufficiently large magnetic field. It follows that

$$|\Psi\rangle = \frac{|1_A\rangle|0_B\rangle - |0_A\rangle|1_B\rangle}{\sqrt{2}}$$

where A and B denote the two modes while 1 labels the filled mode and 0 the empty one (see Figure 2.1). Following Definition 1, it is easy to see that this state is entangled.

What happens if one applies a measurement to one of the two modes? Without loss of generality, assume the measurement is applied to mode A. Then, the state function collapses to one of the two possible outcomes: $|\Psi\rangle = |1_A\rangle|0_B\rangle$ or $|\Psi\rangle = |0_A\rangle|1_B\rangle$. If the measurement of the occupation number of mode A returns 1 (0), then mode B is unoccupied (occupied). Thus, the result is similar to the one of (2.1.1).

\[3\text{Another important property is that the spin-statistics theorem states that fermions have half-integer spin, but that is not of interest for our purposes.}\]
We now modify the previous model by adding a second fermion:

**Example 2.** Let $|\Psi\rangle$ be the state function of a system of two modes, which are filled with two fermions. We assume again that there is only one spin direction allowed. It follows that

$$|\Psi\rangle = \frac{|1_A\rangle|2_B\rangle - |2_A\rangle|1_B\rangle}{\sqrt{2}}$$

Where $A$ and $B$ denote the two modes while 1 and 2 label the two fermions (see Figure 2.2, fermion one is shown as a filled circle, fermion two by the empty circle). Following Definition 2 it is easy to see that this state is entangled, too.

What happens in this case if one applies a measurement on one of the modes?

Again, the state function collapses to one of the two possible outcomes: $|\Psi\rangle = |1_A\rangle|2_B\rangle$ or $|\Psi\rangle = |2_A\rangle|1_B\rangle$.

But as fermions are indistinguishable, the measurement cannot distinguish between label 1 and 2, returning in both cases the same (trivial) result that there is one fermion in each mode: $|\Psi\rangle = |1_A\rangle|1_B\rangle$.

It is important to note that although the state $|\Psi\rangle$ in this example is anti-symmetric and therefore seems to be entangled, there is no measurement that could exploit this entanglement.

In this last computation, we will show that sufficiently localized fermions share no entanglement due to their fermionic properties.

**Example 3.** Let $\Psi(x, x')$ be the state function of two fermions with one fermion in mode $\varphi_A(x)$ at site A and the second in mode $\varphi_B(x')$ at site B, where A and B are separated by a sufficiently large potential $V \gg E$. Let $\Psi(x, x') = \frac{1}{\sqrt{2}}(\varphi_A(x)\varphi_B(x') - \varphi_A(x')\varphi_B(x))$ be their combined state function and let $O$ be a (reasonable) quantum mechanical operator.

---

4 Although fermions are indistinguishable, one has to add a label to be able to write the state function.

5 Reasonable means here that the operator only acts on one of the sites, as they are separated.
acting on $\Psi(x, x')$. Then:

$$ \langle O \rangle = \int \int_{\mathbb{R}^3} \Psi^*(x, x') O \Psi(x, x') \, dx \, dx' $$

$$ = \int \int_{\mathbb{R}^3} \frac{1}{2} [\varphi^*_A(x) \varphi^*_B(x') - \varphi^*_A(x') \varphi^*_B(x)] O [\varphi_A(x) \varphi_B(x') - \varphi_A(x') \varphi_B(x)] \, dx \, dx' $$

$$ = \int \int_{\mathbb{R}^3} \frac{1}{2} \varphi^*_A(x) \varphi^*_B(x') O \varphi_A(x) \varphi_B(x') \, dx \, dx' $$

$$ + \int \int_{\mathbb{R}^3} \frac{1}{2} \varphi^*_A(x') \varphi^*_B(x) O \varphi_A(x') \varphi_B(x) \, dx \, dx' $$

$$ - \int \int_{\mathbb{R}^3} \frac{1}{2} \varphi^*_A(x) \varphi^*_B(x') O \varphi_A(x') \varphi_B(x) \, dx \, dx' $$

$$ - \int \int_{\mathbb{R}^3} \frac{1}{2} \varphi^*_A(x') \varphi^*_B(x) O \varphi_A(x) \varphi_B(x') \, dx \, dx' $$

We required that the operator $O$ does not change the regime of a measurement. As $\varphi_a \approx 0$ in the regime of $B$ and vice versa, $\langle \varphi_A | O | \varphi_B \rangle \approx 0$:

$$ \langle O \rangle \approx \int \int_{\mathbb{R}^3} \frac{1}{2} \varphi^*_A(x) \varphi^*_B(x') O \varphi_A(x) \varphi_B(x') \, dx \, dx' $$

$$ + \int \int_{\mathbb{R}^3} \frac{1}{2} \varphi^*_A(x') \varphi^*_B(x) O \varphi_A(x') \varphi_B(x) \, dx \, dx' $$

$$ = \int \int_{\mathbb{R}^3} \varphi^*_A(x) \varphi^*_B(x') O \varphi_A(x) \varphi_B(x') \, dx \, dx' $$

Note that modes $\varphi_A$ and $\varphi_B$ are no longer necessarily different and that the two fermions do no longer anti-commute but commute. Thus, the fermionic behavior is only important if the fermions are close at some time of the process.

As seen above, the fermionic behavior of particles does not affect a measurement if the fermions are separated. Therefore, we will call a system a fermionic system only if the fermions are close and their fermionic behavior is important for the results.

In Example 1 and Example 2, we showed that there seem to be two kinds of entangled states in such fermionic systems: one of them is useful, as measurable, the other only seems to be entangled, but shows no measurable consequences of this “entanglement”. The definition of entanglement cannot distinguish between those, so one needs to find a new measure to capture useful entanglement only. This is where the entanglement measures come in handy. In the formalism of second quantization, those measures keep their properties towards the “useful” entanglement but absorb the entanglement due to the fermionic behavior of the system.
2.4. Entanglement Measures in Fermionic Systems

2.4.1. Slater Determinants

The first step to distinguish between those kinds of entanglement is to obtain a formalism to simplify the state functions for fermionic systems. The Slater determinant is very useful to describe a fermionic system. It takes account of fermions being indistinguishable and ensures that the resulting state function is antisymmetric. The Slater determinant of \( n \) fermions with state functions \( |\Phi_i\rangle \) is defined by the determinant of the \( n \times n \) square matrix:

\[
\Psi(x_1, \ldots, x_n) = \det \begin{pmatrix}
\Phi_1(x_1) & \Phi_2(x_2) & \ldots & \Phi_n(x_n) \\
\Phi_1(x_1) & \Phi_2(x_2) & \ldots & \Phi_n(x_n) \\
\vdots & \vdots & \ddots & \vdots \\
\Phi_1(x_1) & \Phi_2(x_2) & \ldots & \Phi_n(x_n)
\end{pmatrix}
\] (2.4.1)

In the case of identical (thus indistinguishable) fermions, the Slater determinant can be seen as the generalization of a product state that naturally contains all the states that only seem to be entangled introduced in Section 2.3.

2.4.2. Second Quantization and Majorana Operators

A more elegant approach than the use of Slater determinants is the formalism of second quantization. In this formalism, a fermionic state (rather, a particle in said state) \( |\Psi\rangle \) is created by a set of creation operators \( a_i^\dagger \) that act on the vacuum state \( |0\rangle \). The operator \( a_i^\dagger \) acting on the vacuum state creates a fermion in mode \( i \), the annihilation operator \( a_i \) removes the fermion from mode \( |i\rangle \).

\[
|i\rangle = a_i^\dagger |0\rangle, \quad |0\rangle = a_i |i\rangle
\] (2.4.2)

\[
|\Psi\rangle = \prod_i a_i^\dagger |0\rangle
\] (2.4.3)

The creation and annihilation operators fulfill the following anticommutation relation:

\[
\{a_i, a_j^\dagger\} = \delta_{i,j}
\] (2.4.4)

\[
\{a_i, a_j\} = \{a_i^\dagger, a_j^\dagger\} = 0
\] (2.4.5)

In terms of these operators, it is no more necessary to label the fermions as it is no longer of interest which fermion is in a given mode, but how much fermions are in that mode. Thus, the formalism naturally takes account of fermions being indistinguishable, the anticommutation relations guarantee an antisymmetric state function.

Majorana Operators

For most of the computations later on, it is beneficial to introduce the so-called Majorana operators. They are defined the following way:
Definition 4. Let $a_i^\dagger$ and $a_i$ be fermionic creation and annihilation operators. Then the operators
\begin{align}
c_{2j-1} &= a_j + a_j^\dagger \\
c_{2j} &= i(a_j^\dagger - a_j)
\end{align}
are called Majorana operators. They fulfill the anticommutation relation
\[\{c_i, c_j\} = 2\delta_{i,j}.\]

2.4.3. Slater Rank Criterion

One possible solution to characterize entanglement of indistinguishable particles is the Slater rank criterion. The Slater rank is a generalization of the Schmidt rank, which provides a measure for entanglement. It was introduced in [11] and provides an entanglement measure for two indistinguishable fermions. The following derivation is given by [8]. Note that the entanglement measure introduced here is an entanglement measure for two fermions in a shared n-dimensional single particle space. Therefore, this criterion cannot be used for the means of this thesis, but it gives a good impression of how entanglement measures for fermionic systems can be realized.

Theorem 2 (Slater Decomposition). Let $|\Psi\rangle = \sum_{i,j=1}^n w_{ij} f_i^\dagger f_j^\dagger |0\rangle$ be a state vector of two identical fermions sharing a single n-dimensional particle space, let $f_i^\dagger$ be their fermionic creation operators. Then, there exists a unitary transformation $U$ such that
\begin{equation}
\tilde{w} = U w U^T = \text{diag}[Z_1, \ldots, Z_r, Z_0], \quad Z_i = \begin{bmatrix} 0 & z_i \\ -z_i & 0 \end{bmatrix}
\end{equation}
where $z_i > 0 \ \forall \ i \in 1, \ldots, r$ and $Z_0$ is an $(n - 2r) \times (n - 2r)$ null matrix. The number $r$ of non-vanishing block-matrices $Z_i$ is called Slater rank.

Proof. Let $|\Psi\rangle$ be a state vector of two identical fermions sharing a single n-dimensional particle space, let $f_i^\dagger$ be their fermionic creation operators. Then, $|\Psi\rangle$ can be written as:
\begin{equation}
|\Psi\rangle = \sum_{i,j=1}^n w_{ij} f_i^\dagger f_j^\dagger |0\rangle
\end{equation}

As the particles are fermions, $\{f_i^\dagger, f_j^\dagger\} = 0$ and $f_i^\dagger f_i^\dagger |0\rangle = 0$. Therefore, $w$ is skew-symmetric. As shown in [11], there exists a unitary transformation $U$ such that:
\begin{equation}
\tilde{w} = U' w U'^T = \text{diag}[Z_1, \ldots, Z_r, Z_0], \quad Z_i = \begin{bmatrix} 0 & z_i \\ -z_i & 0 \end{bmatrix}
\end{equation}
Use $|\Psi\rangle = f^\dagger T w f^\dagger$, where $f^\dagger T = (f_1^\dagger, \ldots, f_n^\dagger)$, and define $U = U'^\dagger$
\begin{equation}
|\Psi\rangle = f^\dagger T w f^\dagger |0\rangle = f^\dagger T U \tilde{w} U^T f^\dagger |0\rangle = e f^\dagger U \tilde{w} c^\dagger |0\rangle
\end{equation}
where we define $c_i^\dagger \equiv U T f_i^\dagger$. Then:

$$|\Psi\rangle = \sum_{k=1}^{n} z_k \left( c_{2k-1}^\dagger c_{2k}^\dagger - c_{2k}^\dagger c_{2k-1}^\dagger \right) |0\rangle$$

Therefore, every block-matrix $Z_i$ corresponds to an elementary Slater determinant. Then, the number $r$ is the minimum number of elementary Slater determinants to express $|\Psi\rangle$ in any base and therefore a direct analogue to the Schmidt number.

### 2.4.4. Entanglement Entropy

In second quantization, the definition of entanglement entropy and its properties remain the same as in Section 2.2.2. Thus, the entanglement entropy of a bipartite state $\rho$ is still the von-Neumann entropy of the reduced density matrix $\rho_A$. However, a state created by fermionic creation operators takes fully account for the fermionic behavior of the fermion. Thus, the eigenstates of the reduced density matrix in second quantization can be distinguished and the entanglement entropy is indeed only greater than zero if the consequences of the entanglement are measurable.
3. Model

Our model is a chain of fermions with \( N \) fermionic sites as introduced by Kitaev in [1]. We assume that there is only one spin direction present, so every site is either empty or occupied with a single fermion. Thus, the Hamiltonian is determined by the chemical potential \( \mu \), the hopping amplitude \( w \) and the superconductivity gap \( \Delta = |\Delta|e^{i\varphi} \). It is sufficient for our purposes to examine the case \( \varphi = 0 \), so we will assume \( \Delta \in \mathbb{R} \) from now on:

\[
H = \sum_j -w \left( a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j \right) - \mu \left( a_j^\dagger a_j - \frac{1}{2} \right) + \Delta a_j a_{j+1} + \Delta a_{j+1}^\dagger a_j^\dagger \quad (3.0.1)
\]

One of our main interests is the question of how the system behaves if there is a disorder in the system. Such a disorder may be applied by replacing \( \mu \) respectively \( \Delta \) with the new site-dependent parameters \( \mu' \) and \( \Delta' \):

\[
\mu' = \mu + \eta u_j \quad (3.0.2) \\
\Delta' = \Delta + \gamma u_j \quad (3.0.3)
\]

where \( \mu \) and \( \Delta \) are constant, \( \eta \) respectively \( \gamma \) are the amplitude of the disorder and \( u_j \) is a uniform random variable: \( u_j = \text{uniform}[\frac{-1}{2}, \frac{1}{2}] \). The result is obtained by taking the average of many such simulations.

3.1. Hopping Hamiltonian

One of the models we will examine closer is the hopping Hamiltonian. It is a very simple Hamiltonian that describes e.g. noninteracting electrons on a 1-dimensional lattice

\[
H = \sum_{j=1}^{N} \left[ -w \left( a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j \right) - \mu \left( a_j^\dagger a_j - \frac{1}{2} \right) \right] \quad (3.1.1)
\]

where \( a_{N+1} = a_1 \). This is the model we will refer to as the **hopping Hamiltonian**.
### 3.1.1. Analytical Discussion

Introducing the operators $b_k = \frac{1}{\sqrt{N}} \sum_j a_j e^{-\frac{2\pi i kj}{N}}$ with $-\frac{N}{2} \leq k \leq \frac{N}{2}$, the hopping Hamiltonian gets diagonal:

$$H = \sum_{k,k'} -w b_k^\dagger b_{k'} \sum_j e^{-\frac{2\pi i j}{N} (k-k')} \left( e^{\frac{2\pi i k'}{N}} + e^{-\frac{2\pi i k'}{N}} \right) - \mu \left( b_k^\dagger b_k - \frac{1}{2} \right)$$

$$= \sum_k \left[ -\mu - 2w \cos \left( \frac{2\pi k}{N} \right) \right] b_k^\dagger b_k + \frac{\mu}{2} \quad (3.1.2)$$

The ground state is defined as the state with the lowest energy. Therefore, the states are filled beginning with the state of lowest energy with a fermion, then filling the next higher energy state with a fermion and so on until all fermions are in a state. The energy $E_k$ of each mode is determined by (3.1.2).

As shown in [10], the correlation matrix $A_{L} = \langle a_m^\dagger a_n \rangle$ with $m, n \leq L$ has the same eigenvalues as the reduced density matrix of the ground state, while it is easy to compute. The correlation matrix $\langle b_k^\dagger b_{k'} \rangle$ can be obtained directly from the ground state\footnote{note that this matrix is diagonal and not block-diagonal, as $b$ are not Majorana but fermionic operators.}:

$$\langle b_k^\dagger b_{k'} \rangle = \begin{cases} \delta_{k,k'} & \text{if } E_k < 0, \text{thus } |k| \leq k_c \\ 0 & \text{if } E_k > 0 \end{cases} \quad (3.1.4)$$

where we defined the Fermi vector $k_c$ such that $E(\pm k_c) = 0$. In order to determine the entanglement entropy, one has to get the correlation matrix $\langle a_m^\dagger a_n \rangle$. That can be done by going back in the Fourier transform:

$$\langle a_m^\dagger a_n \rangle = \sum_{k,k'} \frac{1}{N} e^{-\frac{2\pi i (km-k'n)}{N}} \langle b_k^\dagger b_{k'} \rangle = \sum_{k,k'} \frac{1}{N} e^{-\frac{2\pi i (km-k'n)}{N}} \langle b_k^\dagger b_{k'} \rangle$$

$$= \sum_{|k|<k_c} \frac{1}{N} e^{-\frac{2\pi i k(m-n)}{N}} = \sum_{k=0}^{k_c} \frac{1}{N} \left( e^{-\frac{2\pi i k(m-n)}{N}} + e^{\frac{2\pi i k(m-n)}{N}} \right)$$

$$= \frac{2}{N} \sum_{k=0}^{k_c} \cos \left( \frac{2\pi k}{N} (m-n) \right) \quad (3.1.5)$$

As shown in [10], this sum can be computed as an integral in the limit of large $N$:

$$A_{mn} = \langle a_m^\dagger a_n \rangle = \frac{1}{\pi} \sin(k_c(m-n)) \quad (3.1.6)$$
3.2. Kitaev Wire

The second important variation will be called Kitaev wire, as it is the toy model he discusses in [1]. The Hamiltonian will be expressed in terms of Majorana operators introduced in Section 2.4.2:

\[ H = \frac{i}{2} \sum_j -\mu c_{2j-1}c_{2j} + (w + \Delta) c_{2j}c_{2j+1} + (-w + \Delta) c_{2j-1}c_{2j+2} \quad (3.2.1) \]

3.2.1. Spectrum

In a first step, we analyze the spectrum of (3.0.1), assuming periodic boundary conditions. Introducing again operators

\[ b_k = \frac{1}{\sqrt{N}} \sum_j a_j e^{-2\pi ikj} \]

with \(-N/2 \leq k \leq N/2\), the Hamiltonian becomes:

\[ H = \sum_k \left[ -\mu + 2w \cos \left( \frac{2\pi k}{N} \right) \right] b_k^\dagger b_k + \frac{\Delta}{2} + \sum_{k,k',j} \Delta \left( e^{-2\pi ij(k+k')/N} b_k b_{k'} + e^{2\pi ij(k+k')/N} b_k^\dagger b_{k'}^\dagger \right) \]

Define \( \epsilon_k \equiv \mu + 2w \cos \left( \frac{2\pi k}{N} \right) \) and use \( \sum_{r=-N}^N r(x) = \sum_{r>0} f(x) + f(-x) \):

\[ H = \sum_k \epsilon_k b_k^\dagger b_k + \sum_{k,k'} \Delta \left( e^{-2\pi ik'/N} b_{k-k'} b_{k'} + e^{2\pi ik} b_{-k-k'} b_{k-k'}^\dagger \right) + \frac{\mu}{2} \]

Use \( \sum_{x=-N}^N f(x) = \sum_{x>0} f(x) + f(-x) \):

\[ H = \sum_{k>0} \left[ -\epsilon_k b_k^\dagger b_k - \epsilon_{-k} b_{-k}^\dagger b_{-k} + \Delta e^{2\pi ik} \left( b_k b_{-k} + b_k^\dagger b_{-k}^\dagger \right) \right] + \frac{\mu}{2} \]

use \( b_k, b_{-k} = b_k^\dagger, b_{-k}^\dagger = 0 \):

\[ H = \sum_{k>0} \left[ -\epsilon_k b_k^\dagger b_k + \epsilon_{-k} b_{-k}^\dagger b_{-k} + \Delta \left( e^{2\pi ik/N} - e^{2\pi i(-k)/N} \right) \left( -b_k b_{-k} + b_k^\dagger b_{-k}^\dagger \right) \right] + \frac{\mu}{2} \]

\[ + \sum_{k>0} \epsilon_{-k} \]
Define \( c \equiv \frac{\mu}{2} - \sum_{k>0} \epsilon_{-k} \) and \( \xi_k \equiv 2i\Delta \sin \left( \frac{2\pi k}{N} \right) \):

\[
H = \sum_{k>0} \left[ -\epsilon_k b_k^\dagger b_k - \epsilon_{-k} b_{-k}^\dagger b_{-k} + \xi_k \left( b_{-k} b_k + b_k^\dagger b_{-k}^\dagger \right) \right] + c \quad (3.2.2)
\]

This can be written as:

\[
H = \sum_k \left( b_k^\dagger \frac{\xi_k}{\epsilon_k - \epsilon_{-k}} b_k \right) + c \quad (3.2.3)
\]

As the constant \( c \) can be neglected, the spectrum is determined by the eigenvalues of matrix \( h \)

\[
0 = (-\epsilon_k - E(k)) (\epsilon_k - E(k)) + \xi_k^2
\]

\[
E(k) = \pm \sqrt{\left( \mu + 2w \cos \left( \frac{2\pi k}{N} \right) \right)^2 + \left( 2\Delta \sin \left( \frac{2\pi k}{N} \right) \right)^2}, \quad -\pi \leq \frac{2\pi k}{N} \leq \pi \quad (3.2.4)
\]

where we used that \( \epsilon_{-k} = \epsilon_k \). This spectrum is the same as derived by Kitaev [1].

### 3.2.2. Area Law and Critical Behavior

A system is called critical if its energy gap converges to zero for large system sizes: \( \Delta E \to 0 \) for \( N \to \infty \) [18]. The energy gap \( \Delta E = E_0 - E_1 \) of a system is the difference between the energy of the ground state \( E_0 \) and the first excited state \( E_1 \). If we examine the spectrum of our Hamiltonian, we find that the system is critical for \( |\mu| = |2w| \) and for \( \Delta = 0, |\mu| < |2w| \).

The one-dimensional fermion chain is a well-studied model and it is known that the entanglement will obey the area law for non-critical systems. The area law states that the entanglement of a region \( A \) with its surroundings \( B \) scales with the surface of \( A \), i.e. in 1-d systems, the entanglement entropy is constant.

However, if a system is at a critical point, it shows a logarithmic scaling of the entanglement entropy \( S(L) \approx \log(L) \). Wolf has shown that this logarithmic scaling holds not only for 1-dimensional systems, but for all dimensions [12].

Thus, we expect a logarithmic scaling of the entanglement entropy along the critical lines and a fast saturation for all other values of \( \mu \) and \( \Delta \).

### 3.2.3. Phases

In his paper, Kitaev introduces two phases of pairing of the Majorana operators. The boundaries of these phases are the same as the critical lines identified in the spectrum:

The first phase can be seen e.g. in the trivial case, \( w = \Delta = 0 \):

\[
H = \frac{i}{2} \sum_j -\mu c_{2j-1} c_{2j} = \sum_l -\mu a_l^\dagger a_l \quad (3.2.5)
\]
Abbildung 3.1.: Pairing of operators in the two phases of the Kitaev wire. On the left side is the phase $|\mu| > |2w|$, on the right side the phase $|\mu| < |2w|, \Delta \neq 0$. The zero energy mode corresponds to the two unpaired operators $c_1$ and $c_L$. The figure is originally used by Kitaev in [1].

The Majorana operators of each site are bound together, there is no interaction between different sites at all. As shown above, the Hamiltonian becomes diagonal by simply going back to the original fermionic operators. Thus, the ground state is either completely filled or empty, depending on the sign of $\mu$.

The second phase of pairing appears e.g. for $\Delta = w > 0, \mu = 0$. The Hamiltonian becomes:

$$H = \frac{i}{2} \sum_j 2wc_{2j}c_{2j+1} \quad (3.2.6)$$

Now, the Majorana operators of different sites are bound together. By introducing new fermionic operators $\tilde{a}_l = \frac{1}{2}(c_{2l} + ic_{2l+1})$ and $\tilde{a}^\dagger_l = \frac{1}{2}(c_{2l} - ic_{2l+1})$ the Hamiltonian becomes diagonal [1]:

$$H = \sum_{l=1}^{L-1} 2w\tilde{a}^\dagger_l \tilde{a}_l - \frac{1}{2} \quad (3.2.7)$$

Note that operators $\tilde{a}^\dagger_L$ and $\tilde{a}_L$ do not appear in this Hamiltonian, leaving an additional mode $L$ with zero energy. Therefore, the ground state is degenerate.

In terms of Majorana operators, the operator $\tilde{a}^\dagger_L$ becomes $\frac{1}{2}(c_{2L} - ic_1)$. The pairing of operators in these phases can be seen in Figure 3.1.

In his paper, Kitaev examines arbitrary values for $\mu$, $w$ and $\Delta$ [1]. He shows that the first phase appears when $|\mu| > |2w|$ while the second phase appears when $|\mu| < |2w|, \Delta \neq 0$. The line $|\mu| < |2w|, \Delta = 0$ is the simple hopping Hamiltonian in a normal metal phase we examined above.
4. Deriving an Algorithm

Now that we have set the foundations, we will develop an algorithm to get the entanglement entropy. In Section 4.1 we will take a look at the necessary steps, while Section 4.2 explains the implementation in detail. A shortened, commented version of the Matlab code will be presented in Appendix B.

4.1. Main Algorithm

To get the entanglement entropy for given Hamiltonian $H$, system size $N$ and block size $L$, one must follow these steps:

I. Any quadratic Hamiltonian can be written as $H = \frac{i}{2} c^T A c$, where $c^T = (c_1, c_2, ..., c_{2N})$ and $c_i$ are Majorana operators. Construct the skew-symmetric matrix $A$ that determines eq. (3.2.1).

II. Any real skew-symmetric real matrix $A$ can be block-diagonalized with an orthonormal matrix $R$: $A = R S R^T$, where $S$ is block-diagonal (see Section ?? in Appendix A). In terms of $S$, the Hamiltonian becomes

$$H = \frac{i}{2} c^T A c = \frac{i}{2} c^T R S R^T c = \frac{i}{2} b^T S b \quad (4.1.1)$$

where $c$ and $b$ relate via $c = R b$.

III. The next step is to determine the ground state $\rho$. This can be done using the block diagonal form of the Hamiltonian: Every block of the matrix $S$ corresponds to an eigenvalue of the Hamiltonian, while the corresponding operator $b^\dagger$ to that mode is the creation operator of the corresponding eigenfunction. As the ground state is defined as the state with the lowest energy, every eigenmode of $H$ with negative energy will be occupied, those with positive energy will be empty.

IV. Construct the block-diagonal correlation matrix $M_R$ in the rotated basis of $b$. The correlation matrix $M$ of two operators $c_i, c_j$ acting on the system defined by density matrix $\rho$ is defined by $M_{ij} = i \text{Tr}(c_i c_j \rho)$.

V. The eigenvalues of the reduced density matrix $\rho_A$ relate to the eigenvalues of the submatrix $M_A$ of $M$ in the basis of $c$ via $11.2.3$. Therefore, the next step is to rotate $M_R$ back to the basis of $c$ to get the correlation matrix $M$.

\[ ^1 \text{Although the eigenfunction itself is not of interest here} \]
VI. As the relation between the eigenvalues of the reduced density matrix and the ones of the $2L \times 2L$ submatrix $M_A$ of $M$ is known, the next step is to take that submatrix.

VII. Since the entanglement entropy is invariant under base change and reduces to the Shannon entropy for diagonal $\rho$, it is necessary to block-diagonalize $M_A$. The entanglement entropy can then simply be computed from the Shannon entropy of the eigenvalues of the $2 \times 2$-blocks within $M_A$ using the known relation between eigenvalue $\mu_i$ of block $M_A$ and eigenvalue $p_i$ of the reduced density matrix $\rho_A$

$$p_i = \frac{|\mu_i| + 1}{2}$$

$$S_L = \sum_{i=1}^{L} -p_i \log_2 p_i - (1 - p_i) \log_2 (1 - p_i)$$

where $\pm \mu_i$ are the (purely imaginary) eigenvalues of the i-th block in $M_A$.

4.2. Details

4.2.1. Step I.: Form of a Quadratic Hamiltonian

An arbitrary quadratic Hamiltonian is of the form:

$$H = \sum_{i,j} \left( \begin{array}{c} a_i \\ a_j^\dagger \end{array} \right) \left( \begin{array}{cc} h_{ii} & h_{ij} \\ h_{ji} & -h_{jj} \end{array} \right) \left( \begin{array}{c} a_i^\dagger \\ a_j \end{array} \right) + k$$

(4.2.1)

Using the Majorana operators $c_{2i}$ and $c_{2i-1}$, the Hamiltonian becomes:

$$H = \sum_{i,j} \frac{1}{4} \left( \begin{array}{c} c_{2i-1} - i c_{2i} \\ c_{2i-1} + i c_{2i} \end{array} \right) \left( \begin{array}{cc} h_{ii} & h_{ij} \\ h_{ji} & -h_{jj} \end{array} \right) \left( \begin{array}{c} c_{2i-1} + i c_{2i} \\ c_{2i-1} - i c_{2i} \end{array} \right) + k$$

Execute the matrix multiplication and we are done.

4.2.2. Step II.: Block-Diagonalizing a Skew-Symmetric Matrix

It is difficult to block-diagonalize a skew-symmetric matrix utilizing Matlab directly, as the transformation matrix $R$ obtained in this procedure is not necessarily unitary let alone orthonormal. This leads to numerical issues while computing the inverse of $R$. A useful workaround is the use of the Schur decomposition.

**Theorem 3** (Real Schur Decomposition). Let $A$ be a normal square matrix of order $n$. Then, there exists an orthogonal matrix $R$ such that

$$S = R^T A R = \begin{pmatrix} S_{11} & S_{12} & \cdots & S_{1m} \\ 0 & S_{22} & \cdots & S_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & S_{mm} \end{pmatrix}$$

(4.2.2)
where the matrices $S_{ii}$ on the diagonal are either of order 1 or of order 2.

The proof can be found in [9, p. 246] and in Section A.3 in Appendix A.

There are numerical algorithms (e.g. the QR-algorithm) that determine the Schur decomposition of a matrix as a sequence of orthogonal matrices $Q$:

$$S = Q_1^T Q_2^T \cdots Q_k^T A Q_k \cdots Q_1$$

where $S$ is approximately of the form of (4.2.2) and $Q_i$ is orthogonal for all $i$. Note that the product of orthogonal matrices is orthogonal, so we can write:

$$S = R^T A R, \quad R \equiv \prod_i Q_i \quad (4.2.3)$$

This guarantees a real transformation matrix $R$ and gives the Schur decomposition $S$ of the initial matrix $A$. In the case of a normal matrix $A$, the matrix $S$ is already a block diagonal matrix $S$ with $2 \times 2$ blocks of the form of (2.4.8) and unpaired zeros on the diagonal (see Section A.4 in Appendix A), e.g.:

$$
\begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & \lambda & 0 \\
0 & -\lambda & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}
$$

To avoid computational issues, one must re-arrange the unpaired zeros so they become paired. In our case, this is always possible because the matrix $S$ is $2N \times 2N$, thus always leaving an even number of unpaired zeros.

4.2.3. Step IV.: Constructing the Correlation Matrix

The matrix $M$ is defined by its elements the following way:

$$M_{ij} = \frac{1}{2} \text{Tr}([c_i, c_j] \rho) \quad (4.2.4)$$

It completely determines the density matrix $\rho$ of a state. Furthermore, the eigenvalues $\mu_i$ of a submatrix $M_A$ relate to the eigenvalues $p_i$ of a reduced density matrix $\rho_A$ via:

$$p_i = \frac{|\mu_i| + 1}{2} \quad (4.2.5)$$

Now we come to construct the correlation matrix. It is possible to obtain the entry $M_{2i-1, 2i}$ of the correlation matrix from the expectation value of the occupation number of fermionic mode $i$ and vice versa:

$$
\langle n_i \rangle = \langle a_i^\dagger a_i \rangle = \text{Tr} \left( a_i^\dagger a_i \rho \right) = \text{Tr} \left( i c_{2i-1} c_{2i} + I \frac{1}{2} \rho \right) = \frac{1}{2} (1 + i \text{Tr} (c_{2i-1} c_{2i} \rho))
$$

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With \( (4.2.4) \), we obtain:

\[
\langle n_i \rangle = \frac{1 + M_{2i-1,2i}}{2} \tag{4.2.6}
\]

In the ground state, every mode with negative energy is filled, while every mode with a positive energy is empty. If a mode is occupied, then \( \langle n_i \rangle = 1 \), thus \( M_{2i-1,2i} = 1 \). If a mode is empty, \( M_{2i-1,2i} = -1 \). The element \( M_{2i,2i-1} = -M_{2i-1,2i} \) can be obtained using that \( M \) is skew-symmetric. As the Hamiltonian in the basis of \( b_k \) is block-diagonal, there is no coupling between operators of different \( k \) at all. Thus, all other coefficients of the correlation matrix are zero.

If the energy of the mode is zero, the ground state is degenerate. This degeneracy has to be broken so one is actually able to compute the entanglement entropy, this can be done by either filling in a fermion or leaving it out. Thus, to get the correlation matrix \( M_R \) in the ground state from the block-diagonal Hamiltonian, one takes the block-diagonal matrix \( S \) and replaces its values the following way:

- if \( \lambda_k = S_{2k-1,2k} > 0 \): \( S_{2k-1,2k} \to -1, S_{2k,2k-1} \to 1 \)
- if \( \lambda_k < 0 \): \( S_{2k-1,2k} \to 1, S_{2k,2k-1} \to -1 \)
- if \( \lambda_k = 0 \) it does not matter:
  \( S_{2k-1,2k} \to -1, S_{2k,2k-1} \to 1 \) OR \( S_{2k-1,2k} \to 1, S_{2k,2k-1} \to -1 \)

4.2.4. Step V.: Rotating the Correlation Matrix

The correlation matrix is defined by:

\[
M_{ij} = i \text{Tr} \left( c_i c_j \rho \right) = i \text{Tr} \left( c_i c_j e^{-\beta c^T A c} \right) = i \text{Tr} \left( c_i c_j e^{-\beta b^T S b} \right)
\]

Use \( c = R b \) and \( \text{Tr}(\alpha A + \beta B) = \alpha \text{Tr}(A) + \beta \text{Tr}(B) \):

\[
M_{ij} = i \text{Tr} \left( \sum_{k,l} R_{ik} b_k R_{jl} b_l e^{-\beta b^T S b} \right) = \sum_{k,l} R_{ik} R_{jl} i \text{Tr} \left( b_k b_l e^{-\beta b^T S b} \right)_{M_R,kl}
\]

Thus, \( M = RM_R R^T \) and \( M = -M^T \)

4.2.5. Step VII.: Computing the Entropy from the Correlation Matrix

While the algorithm for the entropy is based on block-diagonalizing \( M_A \), one can get the eigenvalues of the blocks more directly from \( M_A \)

\[
\mu_i = \text{Im}(\lambda_{2i-1}) \tag{4.2.7}
\]

where \( i = 1 \ldots L \) and \( \lambda_k \) is the \( k \)-th eigenvalue of \( M_A \). One selects only every second eigenvalue because they come in pairs (two for each block), the imaginary part is taken because the eigenvalues of \( M_A \) are purely imaginary, while those of a block are real.
4.2.6. Checking Results

As Matlab uses numerical approaches, it is necessary to check the results. On the other hand, the computation time should not be significantly increased by these checks. Here are a few useful properties to implement such checks:

- The eigenvalues of the Hamiltonian have to come in pairs. Check if $\epsilon_{2k} + \epsilon_{2k-1} = 0$
- The rotation matrix $R$ has to be orthonormal. Check if $RR^T = I$
- Matrices $S$ and $M$ should be skew-symmetric. Check if $S + S^T = 0$ and $M + M^T = 0$
- The eigenvalues of Matrix $M_A$ have to come in pairs, too
5. Simulations

In this chapter, we will discuss the actual numerical results. In the first section, we will introduce the entanglement length and the maximum entanglement entropy, these are used in the following sections to describe the behavior of the entanglement entropy. In the second section, we will retrieve known results to check if the algorithm works as intended. In the last section, we will do further simulations on the Kitaev wire to examine it in detail.

In order to deal with the number of plots, we will write a Hamiltonian of the form of (3.0.1) respectively (3.2.1) above each group of plots. The values in this Hamiltonian are the actual values used in the simulation. If appropriate\footnote{1}{1\footnote{Meaning if the number of data points is not too large.}}, the data points in a plot are marked by a small cross.

If not mentioned otherwise, the default for the hopping Hamiltonian is $w = 1$, $\mu = \Delta = 0$, the default for the Kitaev wire is $w = \Delta = 1$, $\mu = 0$.

5.1. Scaling of the Entanglement Entropy

It is a difficult task to compare the scaling of the entanglement entropy for different parameters or a disorder directly. This is simply due to the number of plots that would be involved and the lack of an objective value to compare. We note that the entanglement entropy in our model always scales monotonous with the system size $L$. Furthermore, we note that the scaling is in all encountered plots logarithmic until $L$ gets close to some critical length where the entanglement entropy becomes constant.

To be able to describe this scaling, a new parameter will be introduced, the entanglement length. It describes how far two particles can be apart to share entanglement. If this length is smaller than the size of the block, the particles are completely localized in one of the subsystems and therefore do not change the entanglement (see Section 2.3). As such, the entanglement length would be ideally the subsystem size $L$ at which the entanglement entropy no longer increases.

The second parameter we introduce is the maximum entanglement entropy. This is the value the entanglement entropy converges to when the block size exceeds the entanglement length.

The behavior of the entanglement entropy for a given system is (at least in the context of our model) completely determined by the maximum entanglement entropy along with the entanglement length and the knowledge of the logarithmic scaling for small blocks: A system with an entanglement length close to zero has a constant entanglement entropy throughout the whole system, the maximum entanglement entropy is the constant value.
Abbildung 5.1.: An example for the use of entanglement length and maximum entanglement entropy. On the left side, there are markers for the values of entanglement length and maximum entanglement entropy on the line $\eta = 1$, on the right side for the line $\eta = 0$. The plot itself is only an example, it will be discussed later.

A critical system with logarithmic scaling has an entanglement length very close to $N^2$, where $N$ is the total system size. The maximum entanglement entropy is the value of the entanglement entropy at its turning point at $N^2$.

Dealing with Computational Errors

As some measurements require the use of random variables, the entanglement entropy shows a small variance for these measurements. There is no longer a (reliable) maximum of the entropy and the entropy is no longer monotonous.

In order to deal with these issues, we define the entanglement length as the subsystem size where the difference between the entanglement entropy and the maximum entanglement entropy gets smaller than some small threshold. The maximum entanglement entropy will be defined as the mean value of all subsystems larger than the entanglement length.

To obtain precise results, this computation will be repeated several times for each plot, using old the results as input.

Note that due to this definition, the obtained values for both the entanglement length and the maximum entanglement entropy are always smaller than the correct one would be. Therefore, the entanglement length is always smaller than half the system, even for a pure logarithmic scaling of the entanglement entropy.

5.2. Retrieving Known Results

5.2.1. Pure Hopping Hamiltonian

The first step to check the algorithm is the search for known results. In order to do that, we take a look at a pure hopping Hamiltonian with some hopping amplitude $w$.
and chemical potential $\mu$:

$$H = \sum_j -w \left( a_{j+1}^\dagger a_j + a_j^\dagger a_{j+1} \right) - \mu \left( a_j^\dagger a_j - \frac{1}{2} \right)$$  \hspace{1cm} (5.2.1)

In this section, we will briefly analyze the spectrum of its ground state and an alternate approach on its entanglement entropy discussed in detail by Latorre and Riera in [10]. Afterwards we will compare the results of our algorithm to those of these alternate approaches.

**Entanglement Entropy of a Block**

Following the steps in Section 3.1.1, Latorre and Riera compute a logarithmic scaling of the entropy of the form

$$S(L) = \frac{1}{3} \log(L) + a$$  \hspace{1cm} (5.2.2)

where $a$ is a constant depending on the applied chemical potential $\mu$. If $|\mu| > |2w|$, the entanglement entropy saturates to 0, as the ground state is a product state where all modes are filled ($\mu > 0$) respectively empty ($\mu < 0$).

Applying our algorithm, we get the same logarithmic scaling for $S$ in dependence of $L$ for sufficient small $L$ (see Figure 5.2). The pure logarithmic scaling only applies for the limit $N \to \infty$, therefore the fit is only accurate for $L \ll N$. As expected, the constant $a$ is exactly symmetric with respect to $\mu$.

**Occupation Number**

An additional check is the occupation number of the Hamiltonian in dependence of $\mu$. One expects to find a filled Fermi-sea, thus one fermion per site with $E_k < 0$. As shown in Section 4.2.3, the expectation value of the occupation number $n_i$ of mode $i$ is given by

$$\langle n_i \rangle = 1 + \frac{M_{2i-1,2i}}{2}$$  \hspace{1cm} (5.2.3)

where $M$ is the correlation matrix from section Section 4.1. We get for the occupation number of the system

$$\langle N \rangle = \langle \sum_i n_i \rangle = \text{Tr}(\sum_i n_i \rho) = \sum_i \text{Tr}(n_i \rho) = \sum_i \langle n_i \rangle$$  \hspace{1cm} (5.2.4)

and therefore

$$\langle N \rangle = \sum_i 1 + \frac{M_{2i-1,2i}}{2}$$  \hspace{1cm} (5.2.5)

As seen in Figure 5.3, the numerical result is perfectly consistent with the analytical approach.

---

2 This has been proven analytically in [16]. They also determine the constant $a$ analytically.

3 Since the occupation number of the Hamiltonian is symmetric with respect to $\mu$.
\[ H = \sum_{j} - \left( a_{j}^\dagger a_{j+1} + a_{j+1}^\dagger a_{j} \right) - \mu \left( a_{j}^\dagger a_{j} - \frac{1}{2} \right) \]

Abbildung 5.2.: Entanglement Entropy for the hopping Hamiltonian dependent on block size computed using our algorithm (left) and computed by Latorre and Riera in [10] (right).

Abbildung 5.3.: Analytical and numerical result for the number of fermions in the system. Note that the number of fermions must be a natural number or zero, so the correct analytical result is actually not continuous in \( \langle N \rangle \), too. However, the continuous function is plotted for the sake of legibility.
5.2.2. Hopping Hamiltonian with Disorder

The next phenomenon we recover will be the Anderson localization. It is an effect of disorder affecting wave functions on lattices, named after P. Anderson. Originally describing waves of electrons in a metal to describe vanishing conductivity in presence of a sufficient large disorder, the effect was shown to appear in all sorts of waves on a lattice. In our case, the fermions become localized on the chain until some of them no longer participate to the entanglement as they are completely localized in one of the blocks. Thus, one expects the entanglement entropy to increase logarithmic with block size as before (yet the overall entanglement should be smaller) and saturate to a constant value as the block size exceeds the localization length.

In order to show the effect of Anderson localization in our model, we will add a small uniform random disorder with amplitude $\eta$ to our chemical potential and taking the average of many simulations. The Hamiltonian becomes

$$H = \sum_j \left[ -w \left( a_j a_{j+1} + a_{j+1}^\dagger a_j \right) - (\mu + \eta u_j) \left( a_j^\dagger a_j - \frac{1}{2} \right) \right]$$

(5.2.6)

where $u_j$ is a uniform random variable $u_j = \text{uniform}\left[ -\frac{1}{2}, \frac{1}{2} \right]$. As shown in Figure 5.4, the entanglement entropy shows the same qualitative behavior as expected: The entanglement length decreases for increasing disturbance (see Figure 5.2.2), and as less fermions are entangled, the maximum entropy decreases over all as well (see Figure 5.2.2).

5.2.3. Kitaev Wire

In the Kitaev wire, it is convenient to write the Hamiltonian in terms of Majorana operators. As shown in Section 3, the Hamiltonian becomes:

$$H = \frac{i}{2} \sum_j \left[ -\mu c_{2j-1} c_{2j} + (w + \Delta) c_{2j} c_{2j+1} + (-w + \Delta) c_{2j-1} c_{2j+2} \right]$$

(5.2.7)

In this model, it is of interest to examine both periodic and open boundary conditions.

Trivial Case

In the case Kitaev calls the trivial case, $\Delta = w = 0$. Then:

$$H = \frac{i}{2} \sum_j -\mu c_{2j-1} c_{2j} \quad \left( = \sum_l -\mu a_l^\dagger a_l \right)$$

(5.2.8)

The Majorana operators of each site are bound together, there is no interaction between different sites at all. As shown above, the Hamiltonian becomes diagonal by simply going back to the original fermionic operators. Thus, the ground state is either completely filled or empty, depending on the sign of $\mu$. The entanglement entropy is expected to be zero for all block sizes as this ground state is a product state. The simulation retrieves this behaviour for both open and periodic boundary conditions.
\[ H = \sum_j -\left( a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j \right) - (0 + \eta u_j) \left( a_j^\dagger a_j - \frac{1}{2} \right) \]

Abbildung 5.4.: Entanglement Entropy with Anderson localization. Note that the small variance for enabled disturbance is a numerical issue, it decreases for increased computation time.

Abbildung 5.5.: Entanglement length (left) and maximum entanglement entropy (right) for the hopping Hamiltonian with Anderson localization.
\[ H = \frac{i}{2} \sum_j -0c_{2j-1}c_{2j} + 2c_{2j}c_{2j+1} + 0c_{2j-1}c_{2j+2} \]

Abbildung 5.6.: Entanglement Entropy for the pure case in the Kitaev wire

“Pure” Case

In the case we will call the “pure” case, \( \Delta = w > 0, \mu = 0 \). The Hamiltonian becomes:

\[ H = \frac{i}{2} \sum_j 2wc_{2j}c_{2j+1} \quad (5.2.9) \]

Now, the Majorana operators of different sites are bound together. By introducing new fermionic operators \( \tilde{a}_l = \frac{1}{2} (c_{2l} + ic_{2l+1}) \) and \( \tilde{a}^\dagger_l = \frac{1}{2} (c_{2l} - ic_{2l+1}) \) the Hamiltonian becomes diagonal \[1\]:

\[ H = \sum_{l=1}^{L-1} \left[ 2w\tilde{a}_l^\dagger \tilde{a}_l - \frac{1}{2} \right] \quad (5.2.10) \]

Note that operators \( \tilde{a}_L^\dagger \) and \( \tilde{a}_L \) do not appear in this Hamiltonian, leaving an additional mode \( L \) with zero energy. Therefore, the ground state is degenerate. As seen in Figure 5.6, the entanglement entropy is constant one, independent of block size \( L \).

5.3. Further Simulations on the Kitaev Wire

The main interest of this thesis is the supposed robustness of the two phases of entanglement in Kitaev’s toy model with respect to disorder. In this section, we will examine this system further. On the one hand, we vary \( \mu \) or \( \Delta \) in the case without disturbance, on the other hand we examine the behavior for a small disturbance in \( \mu \) or \( \Delta \) for a fixed mean value. Since the general behavior of the system only depends on the relations of \( \mu, \Delta \) and \( w \), we will keep \( w \) fixed.
5.3.1. Phase Transitions

To examine the behavior of the entanglement entropy at the phase transition, we will compute the entanglement length as well as the entanglement entropy. As seen in Figure 5.7, the behavior of open and periodic boundary conditions in terms of entanglement length is very similar. The maximum entanglement entropies resemble each other as well, but the maximum entropy falls much more quickly after the phase transition for open boundary conditions (see Figure 5.8). It is notable furthermore that both the entanglement length and especially the entanglement entropy remain very stable inside the phase with zero-energy modes, $|2w| > |\mu|, \Delta \neq 0$.

5.3.2. Disorder in $\mu$

In this section we will examine the behavior of the entanglement entropy for disturbance in $\mu$. For both periodic and open boundary conditions the entanglement entropy increases slightly with the disturbance in $\mu$. It is notable that the behavior for a disturbance with amplitude $\eta$ in $\mu$ is very similar to the behavior for a constant value of $\mu = \frac{\eta}{2}$, for both open and periodic boundary conditions (See Figure 5.12 and Figure 5.11). We can conclude from this minor difference that the influence of a rising expectation value of $|\mu|$ is much greater than the influence of any random disturbance. It is very likely that the increase of the entanglement entropy for disorder in $\mu$ is actually not an effect of disorder, but an effect of a rising mean absolute value of $\mu$. As seen in Figure 5.10, the Majorana fermions remain very localized and the entanglement length increases only slightly even for relatively big disturbances.

5.3.3. Disturbance in $\Delta$

The next parameter we vary will be to add a small disturbance in the superconductivity Gap $\Delta$. As seen in Figure 5.13, the entanglement length remains small, so the entropy still saturates after a block length of a few fermions. The maximum entanglement entropy on the other hand increases up to 10%. While this effect is very small compared to the maximum entanglement entropy at a phase transition, it greatly exceeds the effects of a variation of $\mu$ or a disturbance in $\mu$.

Nevertheless, this effect is still much smaller than the increase if $\Delta$ is shifted by a constant (see Figure 5.9). While a direct comparison is not possible, as the maximum entanglement entropy as a function of $\Delta$ is not symmetric at $|\Delta| = 1$, the values for a disorder are of the same order as the values for a constant shift.
\[ H = \frac{i}{2} \sum_{j} \left( -\mu c_{2j-1}c_{2j} + 2c_{2j}c_{2j+1} + 0c_{2j-1}c_{2j+2} \right) \]

Abbildung 5.7.: Entanglement Length in the Kitaev wire for \( \mu \), periodic (left) and open boundaries (right)

Abbildung 5.8.: Maximum entanglement entropy in the Kitaev wire for \( \mu \), periodic (left) and open boundaries (right)

\[ H = \frac{i}{2} \sum_{j} \left( -0c_{2j-1}c_{2j} + \left( 1 + \Delta \right) c_{2j}c_{2j+1} + \left( -1 + \Delta \right) c_{2j-1}c_{2j+2} \right) \]

Abbildung 5.9.: Entanglement length (left) and maximum entanglement entropy (right) in the Kitaev wire for \( \Delta \) and periodic boundary conditions. There is no difference to open boundaries.
\[ H = \frac{i}{2} \sum_{j} - (0 + \eta u_j) c_{2j-1}c_{2j} + 2c_{2j}c_{2j+1} + 0c_{2j-1}c_{2j+2} \]

Abbildung 5.10.: Entanglement length in the Kitaev wire for disorder in \( \mu \), periodic (left) and open (right) boundaries

Abbildung 5.11.: Maximum entanglement entropy in the Kitaev wire for disorder in \( \mu \), periodic (left) and open (right) boundaries

\[ H = \frac{i}{2} \sum_{j} - \mu c_{2j-1}c_{2j} + 2c_{2j}c_{2j+1} + 0c_{2j-1}c_{2j+2} \]

Abbildung 5.12.: A zoom at the maximum entanglement entropy for varying \( \mu \) without disorder with periodic (left) and open (right) boundaries. Note the similarities between these plots and the plots for a disorder in \( \mu \)
Abbildung 5.13.: Entanglement length (left) and maximum entanglement entropy (right) in the Kitaev wire for various disturbances in $\Delta$. 
6. Conclusions and Future Research

In this thesis, we derived an algorithm to compute the entanglement entropy in various 1d non-interacting fermionic systems. We showed that the algorithm works as intended by retrieving known results, for example the Anderson localization in the hopping Hamiltonian with disorder.

We then examined the entanglement entropy in the Kitaev wire in detail by varying the system parameters or applying a disorder. It was shown that the entanglement entropy in the Kitaev wire for varying chemical potential $\mu$ remains mostly constant\(^1\) inside the different phases and increases to a logarithmic scaling close to the phase transition at $\mu = 2$ (see Figure 5.8). Furthermore, it was shown that the entanglement entropy increases indeed for a small disorder in $\Delta$ of $\mu$ (see Figure 5.11 and Figure 5.13), but the effect is very small, even for large disorders. On the other hand, the entanglement entropy for the hopping Hamiltonian decreases by around 30 % for a similar disorder. However, it was suggested that these effects of disorder are not actually effects of disorder, like the Anderson localization, but effects of a shifting mean absolute value of the parameters.

**Future Research**

A rather surprising result is that the entanglement entropy in the Kitaev wire is not continuous for small $\mu$ (see Figure 5.12). It is yet to be seen if this is an effect of the system size, or if this effect increases for large systems.

The Algorithm used in this thesis may be used to address such questions about the effect of system size in principle, but the current version simply takes a lot of time for a large system. While it was not necessary for the means of this thesis, it would be possible to optimize computation time.

A promising approach is to lower the precision of the entanglement entropy for big subsystems by simply skipping some subsystem-sizes. For each block size $L$, a matrix of size $2L$ is diagonalized. On the other hand, the matrix of the total system only has to be diagonalized a single time. Thus, there are two possible solutions:

Examine only small\(^2\) block sizes $L$.

If the block size gets large, one could skip some block sizes. The entanglement entropy would be less precise in $L$, but the computation time would decrease linear to the proportion of sites skipped.

This is mainly a task of finding the right balance between computation time and precision.

---

\(^1\)although with increasing localization length

\(^2\)Note that small means here absolute size. The algorithm can deal with blocks of up to 200 sites in about an hour on a desktop computer.
A. Proofs

A.1. Schmidt decomposition

Theorem (Schmidt decomposition). Let $|\Psi\rangle$ be a pure state of a composite system $AB$. Then, there exists an orthonormal set of states $|i_A\rangle$ for system $A$ respectively an orthonormal set of states $|i_B\rangle$ for system $B$ such that

$$
|\Psi\rangle = \sum_i \sqrt{\lambda_i} |i_A\rangle |i_B\rangle
$$

(A.1.1)

where $\lambda_i$ are non-negative real numbers satisfying $\sum_i \lambda_i = 1$ known as Schmidt coefficients. The number of non-zero Schmidt coefficients is called the Schmidt rank.

Proof. Let $|\Psi\rangle$ be a pure state of a composite physical system of subsystems $A$ with dimension $m$ and $B$ with dimension $n$. Let $|\Phi_j\rangle$ and $|\Phi'_k\rangle$ be an arbitrary fixed orthonormal base for $A$ respectively $B$. Then:

$$
|\Psi\rangle = \sum_{j=0}^{m-1} \sum_{k=0}^{n-1} c_{j,k} |\Phi_j\rangle |\Phi'_k\rangle,
$$

(A.1.2)

By singular value decomposition, $C = UDV$, where $C$ is a $m \times n$ complex matrix, $U$ is $m \times m$ unitary and $V$ is $n \times n$ unitary and $D$ is $m \times n$ matrix e.g. of the form:

$$
\begin{pmatrix}
    d_0 & 0 & 0 & \ldots & 0 \\
    \vdots & \ddots & \ddots & \vdots & \ddots \\
    0 & \cdots & \cdots & \cdots & \cdots \\
    0 & \cdots & \cdots & \cdots & \cdots \\
\end{pmatrix}
$$

Where $\lambda_i$ are non-negative and $r = \min(m, n)$. In these terms, $|\Psi\rangle$ becomes:

$$
|\Psi\rangle = \sum_{j=0}^{m-1} \sum_{k=0}^{r-1} u_{j,i} d_{i,i} v_{i,k} |\Phi_j\rangle |\Phi'_k\rangle,
$$

(A.1.3)

Define $|\varphi^A_i\rangle \equiv \sum_j u_{j,i} |\Phi_j\rangle, |\varphi^B_i\rangle \equiv \sum_k v_{i,k} |\Phi'_k\rangle$ and $\lambda_i \equiv d_{i,i}$. Then:

$$
|\Psi\rangle = \sum_{i=0}^{r-1} \lambda_i |\varphi^A_i\rangle |\varphi^B_i\rangle
$$

(A.1.4)

\[\square\]

1 This is a generalization of the proof by [4] p. 109 where the case dim(A)=dim(B) is shown.
2 In this example is $n > m$
A.2. Properties of Entanglement Entropy

Logarithm of a density matrix

\[ \rho = U \tilde{\rho} U^\dagger = \sum_n U \frac{\ln(\tilde{\rho})^n}{n!} U^\dagger \]

\[ = \sum_n \frac{(U \ln(\tilde{\rho}) U^\dagger)^n}{n!} = \exp(U \ln(\tilde{\rho}) U^\dagger) \]

Therefore, \( \ln(\rho) = U \ln(\tilde{\rho}) U^\dagger \), where \( \tilde{\rho} = U \rho U^\dagger \) is diagonal.

A.3. Real Schur Decomposition

**Theorem.** Let \( A \) be a square matrix of order \( n \). Then, there exists an orthogonal matrix \( R \) such that

\[ S \equiv R^T A R = \begin{pmatrix} S_{11} & S_{12} & \cdots & S_{1m} \\ 0 & S_{22} & \cdots & S_{2m} \\ \vdots & \ddots & \ddots \\ 0 & 0 & \cdots & S_{mm} \end{pmatrix} \]  

(A.3.1)

where the matrices \( S_{ii} \) on the diagonal are either of order 1 or of order 2.

**Proof.** Let \( \lambda \) be a real eigenvalue of \( A \) with normalized eigenvector \( x \). Then, there exists an orthonormal base \( r_i \) of \( \mathbb{R}^{n-1} \) that is orthogonal to \( x \). Define \( R_1 \equiv (x, \tilde{R}_1) \) with \( \tilde{R}_1 = (r_i), \tilde{R}_1 \in \mathbb{R}^{n \times n-1} \). Then

\[ R_1^T A R_1 = \begin{pmatrix} x^T \\ \tilde{R}_1^T \end{pmatrix} A \begin{pmatrix} x \\ \tilde{R}_1 \end{pmatrix} \]

(A.3.2)

\[ = \begin{pmatrix} \lambda & x^T \tilde{A} R_1 \\ 0 & \tilde{R}_1^T A R_1 \end{pmatrix} \equiv A_1 \]

(A.3.3)

where we used that \( x^2 = 1, \ x \perp r_i \ \forall \ i \).

Let \( \mu = \alpha + i \beta \) be a complex eigenvalue of \( A \) and \( x = u + i v \) be its normalized eigenvector. It is easy to see \( \mu^* \) is an eigenvalue with eigenvector \( x^* \). Then:

\[ A(u \pm iv) = (\alpha \pm i\beta)(u \pm iv) \]

(A.3.4)

For real and imaginary part

\[ Au = \alpha u - \beta v, \ Av = \beta u + \alpha v \]

(A.3.5)
As \( \mathbf{x} \) and \( \mathbf{x}^* \) are linear independent vectors, \( \mathbf{u} \) and \( \mathbf{v} \) must be linear independent vectors, too. Define \( Y \equiv (\mathbf{u}, \mathbf{v}) \), \( Y \in \mathbb{R}^{n \times 2} \). With (A.3.5) follows:

\[
AY = Y \begin{pmatrix} \alpha & \beta \\ -\beta & \alpha \end{pmatrix} \equiv YT \tag{A.3.6}
\]

In the space with base \( \mathbf{u} \) and \( \mathbf{v} \), there are two orthonormal vectors \( \mathbf{x}_1 \) and \( \mathbf{x}_2 \) that form a matrix \( X \) such that:

\[
Y = XC \tag{A.3.7}
\]

In these terms, (A.3.6) can be written as:

\[
AX = XCTC^T \equiv XS_1 \tag{A.3.8}
\]

As \( C \) is an orthonormal matrix, \( S_1 \) has the same eigenvalues as \( Y \). There exists an orthonormal base \( r_i \) of \( \mathbb{R}^{n-2} \) that is orthogonal to \( \mathbf{x}_1 \) and \( \mathbf{x}_2 \). Define \( R_2 \equiv (\mathbf{x}_1, \mathbf{x}_2, \mathbf{R}_1) \) with \( \mathbf{R}_1 = (r_i) \). Define \( \mathbf{R}_1 \in \mathbb{R}^{n \times n-2} \). Then:

\[
R_2^T AR_2 = \begin{pmatrix} X^T \\ \mathbf{R}_2^T \end{pmatrix} A \begin{pmatrix} X \\ \mathbf{R}_2 \end{pmatrix}
\]

\[
= \begin{pmatrix} S_1 & X^T \mathbf{R}_2 \\ 0 & \mathbf{R}_2^T \mathbf{R}_2 \end{pmatrix} \equiv A_2 \tag{A.3.9}
\]

Where we used that \( x_{1,2}^2 = 1 \), \( x_{1,2} \perp r_i \) \( \forall i \).

The eigenvalues of matrix \( A \) are completely determined by \( \lambda \) respectively the eigenvalues of \( S_1 \) and the eigenvalues of the submatrix \( \mathbf{R}_1^T A \mathbf{R}_1 \) respectively \( \mathbf{R}_2^T \mathbf{R}_2 \). The procedure can be repeated by applying a new orthogonal matrix \( V \) that transforms these submatrices to the form of \( A_1 \) respectively \( A_2 \):

\[
V \equiv \begin{pmatrix} I & 0 \\ 0 & \mathbf{V}_i \end{pmatrix} \tag{A.3.11}
\]

The matrix \( A \) can be transformed to the form of \( \lambda, \) the orthogonal transformation matrix \( R \) is the product of the transformation matrices obtained in the process. \( \square \)

**A.4. Schur Decomposition of a Real Normal Matrix**

A real normal matrix is a matrix that commutes with its transposed matrix. In particular, skew-symmetric matrices are normal.

**Lemma 1.** Let \( A \) be a normal square matrix of order \( n \). Then, the Schur decomposition of \( A \) is of the form

\[
S \equiv R^T AR = \begin{pmatrix} S_{11} & 0 & \ldots & 0 \\ 0 & S_{22} & 0 & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \ldots & S_{mm} \end{pmatrix} \tag{A.4.1}
\]
where the matrices $S_{ii}$ on the diagonal are either single unpaired zeros or square matrices of order 2.

Proof. The eigenvectors of a normal matrix of dimension $n$ form an orthogonal base of $\mathbb{R}^n$. Therefore, the matrix $S_1$ in the proof of the Schur decomposition is equivalent to the matrix $\Gamma$. As the columns of matrices $\tilde{R}_i$ are the eigenvectors of $A$, $\mathbf{x}^T A \tilde{R}_1 = X^T A \tilde{R}_2 = 0$.

Note that the eigenvalues of a skew-symmetric matrix are purely imaginary, the block matrices $S_{ii}$ are therefore of the form:

$$S_{ii} = \begin{pmatrix} 0 & \lambda_i \\ -\lambda_i & 0 \end{pmatrix} \quad (A.4.2)$$
B. Matlab code

In this section, the Matlab code will be shown. At first, we take a look at the main script, afterwards follow the subroutines in order of appearance.

B.1. Main Script (Rahmen.m)

The first section defines the variables $a, b, c$ which are defined by (3.2.1):

$$H = \frac{i}{2} \sum_j -ac_{2j-1}c_{2j} + bc_{2j}c_{2j+1} + cc_{2j-1}c_{2j+2} \quad (B.1.1)$$

where $a = \mu, b = w + \Delta$ and $c = -w + \Delta$. The parameter $d$ is the amplitude of a small random disturbance on $a$ for each site:

$$a_i = a + \frac{d}{N} (2 \times \text{rand} - 1) \quad (B.1.2)$$

where ‘rand’ is a uniform random scalar $\in [0...1]$.

```matlab
1 %Main script
2 clear all; %Reset all variables
3 hold all; %start timer
4 tic;
5 scrsz = get(0, ’ScreenSize’);
6 set(0,’DefaultAxesColorOrder’, [0 0 0], ’DefaultAxesLineStyleOrder’, ’-|’’-|’’-|’’, ’DefaultLineWidth’, 2, ’DefaultFigurePosition’, [scrsz(3)/2 100 scrsz(3)/2 scrsz(4)/2])
7 %fixed parameters
8 a=0; %mu
9 w=1; %w+delta
10 delta=0; %w+delta
11 d=0; %lifts degeneracy
12 e=0; %Amplitude of disturbance in \mu
13 f=0; %Amplitude of disturbance in \Delta
14 b=w+delta;
```
18 c=delta−w;
19
20 % sets minimum, maximum and step−size for N
21 Nmax=100;
22 Nmin=100;
23 Nstep=1;
24
25 % sets minimum, maximum and step−size for one of the other variables
26 Varmax=2;
27 Varmin=−2;
28 Varstep=0.01;
29
30 % sets minimum, maximum and step−size for one of the other variables
31 Var2max=1;
32 Var2min=1;
33 Var2step=1;
34
35 % switches
36 switch_pb=1; % periodic boundaries 1=on.
37 switch_Var_N=1; % N/Var−Plot 0=N, 1=Var.
38 switch_Var=1; % a=1, w=2, delta=3, d=4, e=5, f =6, 0=off,
39 switch_Var2=0;
40 switch_NN=2; % 0=off, 1=put out N, 2=hopping
41
42 switch_fit=0;
43 switch_loclength = 0;
44 Nrepeat=1; % Number of repetitions
45 bLmax=0.45;
46 aLmax=0.5;
47 lstep=0;
48 Lmax=round(Nmax*aLmax); % sets the maximum Value for L
49 Loctemp=bLmax;
50 Fitmax=round(Nmax*0.1);
51
52 %---------------------------------------------------------------------
53 fig1=1;
54 fig2=2;
55 fig3=3;
for Var2=Var2min : Var2step : Var2max
% switch which is the Variable to go through
switch switch_Var2
  case 1
    a=Var2;
  case 2
    w=Var2;
    b=w+delta;
    c=delta−w;
  case 3
    delta=Var2;
    b=w+delta;
    c=delta−w;
  case 4
    d=Var2;
  case 5
    e=Var2;
  case 6
    f=Var2;
end

%initialize counting variables
indVar=0;
indN=0;
ind1=0;
ind2=0;
indLoc=0;
bug=0;
bugcount=0;
bugloopVar=1;
bugloopN=1;
cont=1;
contb=1;

[switch_Var , switch_average , Nmin , Nmax , Nstep , NN , Varmin , Varmax , Varstep , VarN , X , H] = Init (switch_Var , switch_Var_N , Nrepeat , Nmin , Nmax , Nstep , Varmin , Varmax , Varstep);
HR=zeros(Nmax, Nrepeat);
eN=zeros(3, VarN);
for Var=Varmin : Varstep : Varmax
indVar=indVar+1;

% switch which is the Variable to go through
switch switch_Var
  case 1
    a=Var;
  case 2
    w=Var;
    b=w+delta;
    c=delta−w;
  case 3
    delta=Var;
    b=w+delta;
    c=delta−w;
  case 4
    d=Var;
  case 5
    e=Var;
  case 6
    f=Var;
end

indN=0;

for N=Nmin:Nstep:Nmax
  for indR=1:Nrepeat
    indN=indN+1;
    A=Matrix_fuellen(a,b,c,N,d,e,f,switch_pb); % subroutine , Get Matrix A
    [R,RI,S]=Matrix_block(A,N); % subroutine , block−diagonalize A
    [M,MR,bug]=Corr_Matrix(R,RI,S,N,bug); % subroutine , gets rotated correlation−matrix
    HR(:,indR)=Entropy(M,Lmax,Nmax);
  end
  time=toc;
  switch switch_Var_N
    case 0
      H(:,indN)=mean(HR,2);
      eta=time(NN*Nrepeat/((indN−1)*Nrepeat+indR−1));
    case 1
      H(:,indVar)=mean(HR,2);
      eta=time*(VarN*Nrepeat/((indVar−1)*Nrepeat+indR−1));
  end
end

end
printf( 'eta%d seconds', eta); 
switch switch_NN 
  case 1 
    eN=Erw_N(N,M); 
    printf( 'eN(N=%d) = %d', N, eN); 
  case 2 
    eN(1,indVar)=Erw_N(N,M); 
    eN(2,indVar)=Erw_N hop(a,N); 
    eN(3,indVar)=a; 
    K=N*acos(-a/2)/(pi); 
    eN(4,indVar)=1+N-K; 
    if K==0 
      eN(4,indVar)=N; 
    end 
  end 
end 
if switch_loclength 
  indLoc=indLoc+1; 
  switch switch_Var_N 
  case 0 
    Loc(indLoc)=loc_length(N,aLmax,bLmax, 
                      lstep,Lmax,H(:,indN),Loctemp)/N; 
  case 1 
    Loc(indLoc)=loc_length(N,aLmax,bLmax, 
                      lstep,Lmax,H(:,indVar),Loctemp)/N; 
  end 
end 
Loctemp=Loc(indLoc); 
end 
figure(fig1); 
hold all; 
switch switch_loclength 
  case 0 
    if switch_Var2==0 
      hold all; 
      plot_HmaxVar(H,aLmax,bLmax,Nmax,Varmin, 
                  Varmax,Varstep,Var2min,Var2max,Var2step, 
                  switch_Var2,switch_Var_N,a,b,c,e); 
    end 
    hold all; 
    if switch_Var2==0 
      if switch_fit
logfit = fittype('g+h*log2(x)');
fitobject = fit(X(1:Fitmax,1),H(1:Fitmax,1),
    logfit,'StartPoint',[0, 1]);
options.Method='NonlinearLeastSquares';
coeffnames(fitobject);
coeffvalues(fitobject)

hold all;
graph=plot(fitobject);
set(graph,'LineSmoothing','on');

plot_HL(X,H,aLmax,Nmin,Nmax,Nstep,Varmin,Varmax,
    Varstep,switch_Var_N,switch_Var,a,b,c,e,f);
interpreter', 'latex', 'FontSize', 18);
    case 5
    xlabel('\eta', 'FontSize', 28);
    title('[\$H = \sum_j - (', num2str(w), ') \left( a^\dagger_j a_{j+1} + a^\dagger_{j+1} a_j \right) - (', num2str(a), '+ \eta u_{j+1}) \left( a^\dagger_j a_j - \frac{1}{2} \right) + (', num2str(delta), ' + \gamma u_j) \left( a_j a_{j+1} + a^\dagger_{j+1} a^\dagger_j \right) $]', 'interpreter', 'latex', 'FontSize', 18);
end
    case 6
    xlabel('\gamma', 'FontSize', 14);
    title('[\$H = \sum_j - (', num2str(w), ') \left( a^\dagger_j a_{j+1} + a^\dagger_{j+1} a_j \right) - (', num2str(a), ') \left( a^\dagger_j a_j - \frac{1}{2} \right) + (', num2str(delta), ') + \gamma u_j) \left( a_j a_{j+1} + a^\dagger_{j+1} a^\dagger_j \right) $]', 'interpreter', 'latex', 'FontSize', 18);
end
    set(gca, 'FontSize', 24);
    figure(fig2);
    hold all;
    plot_Hmax(Loc, H, Varmin, Varstep, Varmax, VarN, aLmax, N, a, w, delta, e, f, switch_Var)
end
    if switch_NN == 2
    figure(fig3);
    hold all;
    plot(eN(3,:), eN(1,:));
    plot(eN(3,:), eN(4,:));
    ylabel('[\$\langle N \rangle_{\text{range}} \rangle $', 'FontSize', 24, 'interpreter', 'latex');
    xlabel('\mu', 'FontSize', 28);
    legend('[\$\langle N \rangle_{\text{range}} \rangle ', 'Analytical result '); set(legend, 'FontSize', 28, 'Location', 'NorthEast');
end
end

B.2. Subroutines

B.2.1. Create Matrices, Fill Default Values

This subroutine simply saves space in the main script. There are no computations in here.
function [switch_Var, switch_average, Nmin, Nmax, Nstep, NN, Varmin, Varmax, Varstep, VarN, X, H] = Init(switch_Var, switch_Var_N, Nrepeat, Nmin, Nmax, Nstep, Varmin, Varmax, Varstep)

switch_average = 0;
if Nrepeat ~ = 1
    switch_average = 1; % takes average. 1=on.
end

if Nmax == Nmin
    NN = 1;
else
    NN = (Nmax - Nmin) / Nstep + 1; % gets the number of values for N
end

if Varmax == Varmin
    VarN = 1;
else
    VarN = round((Varmax - Varmin) / Varstep + 1); % gets the number of values for Var
end

switch switch_Var_N
    case 0 % switch is on "N"
        Varmin = Varmax;
        Varstep = 1;
        VarN = 1;
        switch_Var = 0;
        X = ones(Nmax, NN);
        for N = Nmin:Nstep:Nmax
            ind1 = ind1 + 1;
            for ind2 = 1:N
                X(ind2, ind1) = ind2 / N;
                % X(ind2, ind1) = ind2;
            end
        end
    case 1 % switch is on "Var"
        Nmin = Nmax; % assures there is a fixed N
        Nstep = 1;
        NN = 1;
        X = ones(Nmax, VarN);
        for Var = Varmin:Varstep:Varmax
            for ind1 = 1:Nmax
                X(ind1, 1:VarN) = ind1 / Nmax;
            end
        end
end

end

46
% X(ind1,1:VarN)=ind1;
end
end
end
% creates the Matrix H to store the entropy.
% Each column is a separate line in the plot.
switch switch
  case 0 % switch is on "N"
    H=zeros(Nmax,NN);  % plot N
  case 1 % switch is on "Var"
    H=zeros(Nmax,VarN);  % plot Var
end
HR=zeros(Nmax,Nrepeat);

B.2.2. Determine Hamiltonian (Matrix_fuellen.m)

function A = Matrix_fuellen(a,b,c,N,d,e,f,switch_pb)
  A=zeros(2*N,2*N);
  for ind=1:N-1
    r=rand;
    A(2*ind-1,2*ind)=a+d/N*(2*rand-1)+e*(2*r-1);
    a=\mu
    A(2*ind,2*ind+1)=b+f*(2*r-1);
    b=\omega+\delta
    A(2*ind-1,2*ind+2)=c-f*(2*r-1);
    c=\delta-\omega
  end
  A(2*N-1,2*N)=a+d/N*(2*rand-1)+e*(2*rand-1);
  if switch_pb % fill in the periodic boundary condition
    r=rand;
    A(2*N,1)=b+f*(2*r-1);
    A(2*N-1,2)=c-f*(2*r-1);
  end
  A=A-A';  % make A skew-symmetric

B.2.3. Block-Diagonalize a Matrix (Matrix_block.m)

function [R,RI,S] = Matrix_block(A,N)
% block-diagonalizes a Matrix A
[U,D]=schur(A);  % get eigenvalues of A
E=ordeig(D);

42   X(ind1,1:VarN)=ind1;
43     end
44     end
45
46 % creates the Matrix H to store the entropy.
47 % Each column is a separate line in the plot.
48 switch switch
49     case 0 % switch is on "N"
50       H=zeros(Nmax,NN);  % plot N
51     case 1 % switch is on "Var"
52       H=zeros(Nmax,VarN);  % plot Var
53     end
54
55 B.2.2. Determine Hamiltonian (Matrix_fuellen.m)

1 % Gets the matrix A which determines the hamiltonian
2 function A = Matrix_fuellen(a,b,c,N,d,e,f,switch_pb)
3     A=zeros(2*N,2*N);
4     for ind=1:N-1
5        r=rand;
6        A(2*ind-1,2*ind)=a+d/N*(2*rand-1)+e*(2*r-1);
7            a=\mu
8        A(2*ind,2*ind+1)=b+f*(2*r-1);
9            b=\omega+\delta
10       A(2*ind-1,2*ind+2)=c-f*(2*r-1);
11           c=\delta-\omega
12     end
13     A(2*N-1,2*N)=a+d/N*(2*rand-1)+e*(2*rand-1);
14
15     if switch_pb % fill in the periodic boundary condition
16        r=rand;
17        A(2*N,1)=b+f*(2*r-1);
18        A(2*N-1,2)=c-f*(2*r-1);
19     end
20
21     if switch_pb % make A skew-symmetric
22         A=A-A';
23
B.2.3. Block-Diagonalize a Matrix (Matrix_block.m)

1 function [R,RI,S] = Matrix_block(A,N)
2 % block-diagonalizes a Matrix A
3     [U,D]=schur(A);  % get eigenvalues of A
4     E=ordeig(D);
[R, S] = ordschur(U, D, abs(E) < 1000*eps);
RI = R';
m = max(max(R*RI - eye(2*N)));
if m > 100*eps
    fprintf('R not unitary, N: %d, Maximum: %d\n', N, m)
end

C = R*S*RI - A;
m = max(max(abs(C)));
if m > 10^eps;
    fprintf('R Transformiert S nicht korrekt, N: %d, Maximum: %d\n', N, m)
end

B.2.4. Determine the Correlation Matrix (Corr_matrix.m)

    %gets the correlation−matrix MR and rotates it

    MR = zeros(2*N, 2*N);  % block−diagonal matrix
    M = zeros(2*N, 2*N);   % skew−symmetric matrix

    for ind = 1:N;
        if S(2*ind - 1, 2*ind) > 0  % \mu_{i} > 0
            MR(2*ind - 1, 2*ind) = 1;
            MR(2*ind, 2*ind - 1) = -1;
        elseif S(2*ind - 1, 2*ind) < 0  % \mu_{i} < 0
            MR(2*ind - 1, 2*ind) = -1;
            MR(2*ind, 2*ind - 1) = 1;
        elseif S(2*ind - 1, 2*ind) == 0  % \mu_{i} = 0
            MR(2*ind - 1, 2*ind) = -1;
            MR(2*ind, 2*ind - 1) = 1;
        end
    end

    M = R*MR*RI;  % rotate MR
    bug = Check_Skewsym(M, 'M', N, bug);  % subroutine, check M

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B.2.5. Compute the Shannon-Entropy (Entropy.m)

```matlab
function HV = Entropy(M, Lmax, Nmax)
% gets the entropy
HV=zeros(Nmax, 1);
for L=1:Lmax
    h=0;
    MA=M(1:2*L, 1:2*L);
    E=imag(eig(MA));
    for j=1:L
        p=(E(2*j-1)+1)/2;
        if abs(p-1)<10^(-10);
            continue;
        end
        if abs(p)<10^(-10);
            continue;
        end
        h=h-p*log2(p)-(1-p)*log2(1-p);
    end
    HV(L)=h;
end
```

B.2.6. Get the Expectation Value of the Number of Fermions

Numerical Variant

```matlab
function eN = Erw_N(N,M)
% gets
eN=N/2;
for ind =1:N
    eN=eN-M(2*ind-1, 2*ind )/2;
end
```

Variant for the Hopping Hamiltonian Based on the Energy

```matlab
function eN_hop = Erw_N_hop(a, N)
% gets N for a hopping Hamiltonian
eN_hop=0;
for k=1:N
    E=a-2*cos(2*pi*k/N);
    if E<0
        eN_hop=eN_hop+1;
    end
end
```
B.2.7. Determine Entanglement Length (loc_length.m)

```matlab
function l = loc_length(N, aLmax, bLmax, lstep, Lmax, H, Loctemp)

aLmax = round(aLmax * N);
blmax = round(bLmax * N);
Loctemp = round(Loctemp * N);
lstep = round(lstep * N);
Hmax = mean(H(Loctemp: aLmax));

if lstep == 0
    for l = 1:Lmax
        if abs(Hmax - H(l)) < 2*10^-3
            return;
        end
    end
    return;
end
lstep = round(lstep * N);

for l = 1:Lmax
    maxl = l + lstep;
    if maxl < Lmax
        lmean = mean(H(1:maxl));
    else
        lmean = mean(H(1:Lmax));
    end
    if abs(Hmax - lmean) < 10^-2
        return;
    end
end
```

B.2.8. Plots

Variant for Maximum Entanglement Entropy and Two Variables (plot_HmaxVar.m)

```matlab
function plot_HmaxVar(H, aLmax, bLmax, Nmax, Varmin, Varmax, Varstep, Var2min, Var2max, Var2step, switch_Var2, switch_Var_N, a, b, c, e)

Lmax = round(aLmax * Nmax);
Lmin = round(bLmax * Nmax);
lm = H(Lmin:Lmax,:);
HM = mean(lm);
```
function plot_Hmax(Loc,H,Varmin,Varstep,Varmax,VarN,aLmax,N,a,w,delta,e,f,switch_Var)
Loc=round(Loc*N);
Lmax=round(aLmax*N);

Variant for Maximum Entanglement Entropy and One Variable (plot_Hmax.m)
```matlab
for ind = 1:VarN
    Hmax(ind) = mean(H(Loc(ind):Lmax, ind));
end

vec = Varmin: Varstep: Varmax;
graph = plot(vec, abs(Hmax));
set(graph, 'LineSmoothing', 'on');
ylabel('Maximum Entanglement Entropy', 'FontSize', 24);
switch switch_Var
    case 1
        xlabel('\mu', 'FontSize', 28);
        title(['$\displaystyle H=\sum_{j}\left(\Delta_{j} + a_{j+1}\overset{\dagger}{a}_{j}\right) - \left(\Delta_{j} + a_{j+1}\overset{\dagger}{a}_{j}\right) + a_{j+1}\overset{\dagger}{a}_{j}\right)$', 'Interpreter', 'latex', 'FontSize', 18);
    case 2
        xlabel('\Omega', 'FontSize', 28);
        title(['$\displaystyle H=\sum_{j}\left(\Delta_{j} + a_{j+1}\overset{\dagger}{a}_{j}\right) - \left(\Delta_{j} + a_{j+1}\overset{\dagger}{a}_{j}\right) + a_{j+1}\overset{\dagger}{a}_{j}\right)$', 'Interpreter', 'latex', 'FontSize', 18);
    case 3
        xlabel('\Delta', 'FontSize', 28);
        title(['$\displaystyle H=\sum_{j}\left(\Delta_{j} + a_{j+1}\overset{\dagger}{a}_{j}\right) - \left(\Delta_{j} + a_{j+1}\overset{\dagger}{a}_{j}\right) + a_{j+1}\overset{\dagger}{a}_{j}\right)$', 'Interpreter', 'latex', 'FontSize', 18);
    case 5
        xlabel('\eta', 'FontSize', 28);
        title(['$\displaystyle H=\sum_{j}\left(\Delta_{j} + a_{j+1}\overset{\dagger}{a}_{j}\right) - \left(\Delta_{j} + a_{j+1}\overset{\dagger}{a}_{j}\right) + a_{j+1}\overset{\dagger}{a}_{j}\right)$', 'Interpreter', 'latex', 'FontSize', 18);
    case 6
        xlabel('\gamma', 'FontSize', 14);
        title(['$\displaystyle H=\sum_{j}\left(\Delta_{j} + a_{j+1}\overset{\dagger}{a}_{j}\right) - \left(\Delta_{j} + a_{j+1}\overset{\dagger}{a}_{j}\right) + a_{j+1}\overset{\dagger}{a}_{j}\right)$', 'Interpreter', 'latex', 'FontSize', 18);
end
```
Variant for Entanglement Entropy vs. Block Size (plot_HL.m)

```matlab
function plot_HL(X,H,aLmax,Nmin,Nmax,Nstep,Varmin,Varmax,
                Varstep,switch_Var_N,switch_Var,a,b,c,e,f)

plot(X,real(H),'LineSmoothing','on') % plot L vs entanglement-entropy
xlim([0 aLmax])
title(['\omega=','num2str((b-c)*0.5) ', '\Delta=','num2str((b+c) *0.5) ','Disturbance in \mu =','num2str(e) ','Disturbance in \Delta is ','num2str(f) ','Disturbance in \mu is ','num2str(e) '], 'FontSize',24);
ylabel('entanglement entropy', 'FontSize', 28);
xlabel('block size/system size', 'FontSize', 28);
set(gca,'FontSize',24);

switch switch_Var_N
    case 0
        vec=(Nmin:Nstep:Nmax) ';
        legend([repmat('N=','length(vec),1) num2str(vec)]);
    case 1
        vec=(Varmin:Varstep:Varmax) ';
        switch switch_Var
            case 0
                legend('off');
                return;
            case 1
                legend([repmat('\mu=','length(vec),1) num2str(vec)]);
            case 2
                legend([repmat('\{\mu+\Delta\}+\mu=','length(vec),1) num2str(vec)]);
            case 3
                legend([repmat('-\{\mu+\Delta\}+\mu=','length(vec),1) num2str(vec)]);
            case 4
                legend([repmat('d=','length(vec),1) num2str(vec)]);
            case 5
                legend([repmat('\eta=','length(vec),1) num2str(vec)]);
end
```

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title(['\omega=',num2str((b-c)*0.5),',\Delta=',num2str((b+c)*0.5),'.\eta:\text{Disturbance in }\mu\text{ is }\zeta.\Delta:\text{Disturbance in }\Delta\text{ is }f.','FontSize',24)];

legend([repmat('zeta=',length(vec),1)
num2str(vec)]);

end

set(legend,'FontSize',28,'Location','NorthWest');
Literaturverzeichnis