



VRIJE  
UNIVERSITEIT  
BRUSSEL



Dissertation for the degree of Bachelor in Physics and Astronomy

# ENTANGLEMENT ENTROPY EVOLUTION IN A QUANTUM ISING SPIN CHAIN WITH LONGITUDINAL AND TRANSVERSAL MAGNETIC FIELD

Floriano Tori

2018-2019

Promotor: Prof. Dr. B. Craps  
Co-promotor: Dr. S. Khetrpal

**Sciences and Bio-Engineering Sciences**

## Acknowledgements

First I would like to thank my promotor Prof. Ben Craps for giving me the opportunity to study this fascinating domain of physics. Importantly I would like to thank my co-promoter Dr. Surbhi Khetrapal, without whom this work would not have been possible, for her help and guidance throughout the year.

Lastly, I would also like to thank my parents and sister for their support throughout this year and for providing me with the necessary amount of coffee needed to persevere.

# Contents

<b>1</b>	<b>Introduction</b>	<b>2</b>
1.1	Density operator and density matrices . . . . .	3
1.1.1	Density operator . . . . .	3
1.1.2	Reduced density matrix . . . . .	5
1.2	Entanglement . . . . .	6
1.2.1	Entangled states . . . . .	6
1.2.2	Entanglement Entropy . . . . .	6
1.3	The Ising model . . . . .	8
1.4	Explicit computation of entanglement entropy for the Ising model . . . . .	9
1.4.1	Diagonalising the Hamiltonian . . . . .	9
1.4.2	Scaling of the entropy for the ground state . . . . .	12
1.5	Quantum mutual information . . . . .	13
1.6	Time evolution . . . . .	13
1.7	Quantum quench . . . . .	14
1.7.1	Example: Particle in a box . . . . .	14
<b>2</b>	<b>Numerical computation of the Entanglement entropy</b>	<b>15</b>
2.1	Entanglement entropy for two sites . . . . .	16
2.1.1	The non-interacting Hamiltonian $H_0$ . . . . .	16
2.1.2	The complete Hamiltonian . . . . .	17
2.1.3	Explicit calculation of $\rho$ and $\rho_{L/2}$ for $L = 2$ . . . . .	18
2.2	Algorithm for the numerical computation . . . . .	19
2.2.1	Generating the matrix representation of the Hamiltonian . . . . .	19
2.2.2	Computing the Entanglement Entropy . . . . .	21
<b>3</b>	<b>Results</b>	<b>22</b>
3.1	Entanglement entropy evolution under $H$ . . . . .	22
3.1.1	Non-integrable case . . . . .	22
3.1.2	Integrable cases . . . . .	23
3.1.3	Evolution of Néel state . . . . .	25
3.1.4	Evolution of Néel state for different values of the coupling constant $g$ . . . . .	25
3.2	Evolution of quantum mutual information after a quench . . . . .	26
3.2.1	Time evolution under $H_2$ . . . . .	27
3.2.2	Time evolution under $H$ . . . . .	27
<b>4</b>	<b>Conclusion</b>	<b>28</b>
	<b>Appendix</b>	<b>29</b>
	<b>References</b>	<b>39</b>

# 1 Introduction

Entanglement is a fundamental property of quantum mechanics which was first received with notable uncertainty [1]. The results of a measurement performed on two particles which are entangled, even if they are spatially separated, show an immediate correlation. In order to quantify entanglement between two systems, the notion of entanglement entropy was introduced. The study of entanglement entropy plays an important role in, for example, domains such as quantum-many body physics or quantum information processing [2]. Entanglement entropy plays for example an important role in the study of quantum phase transitions [3]. Consider the ground state of a Hamiltonian (e.g. a 1-dimensional spin  $\frac{1}{2}$  chain) at absolute zero. The ground state can, due to a change in a physical property of the system like an external magnetic field, transition to a different ground state with different macroscopic properties. Quantum phase transitions differ from classical, thermal transitions since they are not the result of temperature fluctuations but are transitions in the ground state of a quantum many-body system due to quantum fluctuations like a variation in a physical parameter of the system [4]. Near the critical point, where a quantum phase transition takes place, there seems to develop long range correlation which, according to [4] is due to the development of entanglement in the ground state. The study of entanglement entropy in spin systems and its link with quantum phase transition has therefore been an active domain of study [2, 5, 6].

Entanglement in quantum many-body system also plays an important role in domains such as quantum computation and information, that is, the transmission and processing of information using quantum mechanical systems [7]. An example of this would be quantum teleportation where unknown quantum states are teleported over long distances, without the object itself physically travelling [8, 9]. Entanglement entropy can help in investigating and characterizing entanglement in those system which could help gain insights in ways to entangle larger numbers of particles [2]. Finally, the general study of time dependent phenomena like quench dynamics can be of particular interest in other domains, not only in condensed matter physics.

In section 1 of this project an introduction to entanglement entropy, and the necessary theoretical background to define it, namely density matrices, is given. Since entanglement entropy evolution is often studied for integrable models, an example of this, for the Ising model, is also worked out in section 1. The main focus of this work was to study the evolution of the entanglement entropy in a non-integrable system. Starting from a non-entangled product state, one can ask how the entropy of a subsystem grows under unitary time evolution. The system studied was first presented in [10] and a first goal was therefore to corroborate the results obtained in [10]. In order to perform this, since the system was non-integrable, an algorithm was written to compute the evolution of the entropy numerically. The process of writing this algorithm is discussed in section 3. In order to compare the results obtained in the first part with an integrable case, the evolution of entanglement entropy was studied numerically under an integrable Hamiltonian. Finally, the results obtained in [11] where the evolution of quantum mutual information, a quantity dependent on the entanglement entropy, was computed for different Hamiltonians are reproduced making use of the previously written algorithm. Subsequently the evolution of the same quantity in the original system was studied. Section 4 is devoted to discussing and interpreting the results obtained.

## 1.1 Density operator and density matrices

In order to define entanglement entropy, it is necessary to understand density operators, which we will therefore study in this subsection. In the formalism of quantum mechanics we distinguish two different kinds of ensembles which are collections of physical systems, we can make statistical predictions on. These are:

- Mixed state/ensemble: A fraction of the systems in the ensemble are characterized by a certain state ket and other fractions by different kets. The ensemble can therefore not be described by a linear combination of state kets. A concrete example of this is the spin orientation of an unpolarized beam of electrons. Each electron can have a random fixed spin orientation and we can therefore not describe its states as a linear combination of up ( $|S_z, +\rangle = |+\rangle$ ) and down ( $|S_z, -\rangle = |-\rangle$ ) states.
- Pure state/ensemble: Each physical system part of the ensemble is characterized by an identical state ket (e.g. group of atoms all in a spin state parallel with the z-axis).

The mathematical tool for describing mixed states and allowing to make predictions about the ensemble is the density operator/matrix.

### 1.1.1 Density operator

Suppose we have a system in a certain state characterized by the state ket  $|\psi\rangle$ . We define the density operator  $\hat{\rho}$  as [12]

$$\hat{\rho} \equiv |\psi\rangle \langle\psi|. \quad (1.1)$$

The corresponding matrix can be constructed using a basis  $\{|b_n\rangle\}$

$$\rho_{nm} = \langle b_n | \hat{\rho} | b_m \rangle.$$

The strength of the density operator formalism comes from the fact that it can describe systems which are a mixed ensemble. Consider an ensemble where a fraction of the population  $w_i$  is characterized by the state ket  $|a^{(i)}\rangle$ . In this case we, define the density operator as [12]

$$\hat{\rho} \equiv \sum_i w_i |a^{(i)}\rangle \langle a^{(i)}|. \quad (1.2)$$

Since the coefficients  $w_i$  represent fractions of the total population, they satisfy  $\sum_i w_i = 1$ .

As an example, consider the ensemble of spin  $\frac{1}{2}$  particles where 25% are in the state  $|S_x, +\rangle$  and the other 75% in the state  $|S_z, +\rangle$ . The density operator would, using Eq. (1.2), be written as

$$\hat{\rho} = \frac{1}{4} |S_x, +\rangle \langle S_x, +| + \frac{3}{4} |S_z, +\rangle \langle S_z, +|. \quad (1.3)$$

The state  $|S_x, +\rangle$  can be written [12] as a linear combination of the states  $|S_z, \pm\rangle$  in the following way

$$|S_x, +\rangle = \frac{1}{\sqrt{2}} |S_z, +\rangle + \frac{1}{\sqrt{2}} |S_z, -\rangle. \quad (1.4)$$

The corresponding matrix representation of Eq. (1.3), in the basis  $\{|S_z, +\rangle, |S_z, -\rangle\}$ , is therefore

$$\rho = \begin{pmatrix} \frac{7}{8} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{8} \end{pmatrix}. \quad (1.5)$$

For an observable  $B$  we define the ensemble average [12]

$$[B] = \sum_i w_i \langle \alpha^{(i)} | B | \alpha^{(i)} \rangle, \quad (1.6)$$

where  $|\alpha^{(i)}\rangle$  is the state ket characterizing a fraction of the members of the ensemble with relative population  $w_i$ . Given the matrix representation of an operator  $B$  and the density matrix of the ensemble then the ensemble average  $[B]$  can be computed using [12]

$$[B] = \text{Tr}(\rho B). \quad (1.7)$$

Coming back to the previous example we can compute the ensemble average of the spin along the  $x$ - and  $z$ -axis. Using Eq. (1.7) we obtain

$$[S_x] = \frac{\hbar}{8} \quad \text{and} \quad [S_z] = \frac{3\hbar}{8}. \quad (1.8)$$

We can intuitively make sense of these results. Suppose we chose particles from the ensemble at random and measured their spin component along the  $z$ -axis. What would be the average result of this measurement if repeated multiple times? First we need to consider which particles we would pick at random. From the description of the system above, we know that we have a  $\frac{3}{4}$  chance of picking a particle in a state  $|S_z, +\rangle$  and a  $\frac{1}{4}$  chance of picking a particle in the state  $|S_x, +\rangle$ . The probability of measuring spin up (and obtain  $\frac{\hbar}{2}$ ) if we carry out the measurement on a particle in a state  $|S_z, +\rangle$  is 1. On the other hand, from Eq. (1.4) we know the state  $|S_x, +\rangle$  can be written as a linear combination of states  $|S_z, \pm\rangle$ . The measurement of the spin component along the  $z$ -axis on a particle in the state  $|S_x, +\rangle$  therefore has a  $\frac{1}{2}$  chance of returning  $\frac{\hbar}{2}$  as well as an  $\frac{1}{2}$  chance of returning  $-\frac{\hbar}{2}$ . To obtain the average result we combine those probabilities and their measurements

$$\begin{aligned} S_{z,ave.} &= \frac{3}{4} \left( \frac{\hbar}{2} \right) + \frac{1}{4} \cdot \frac{1}{2} \left( \frac{\hbar}{2} \right) + \frac{1}{4} \cdot \frac{1}{2} \left( \frac{-\hbar}{2} \right) \\ &= \frac{3\hbar}{8}. \end{aligned} \quad (1.9)$$

We obtain exactly the same results as the ensemble average given by Eq. (1.8). It is interesting to see mix of classical probability of picking a certain particle and the quantum mechanical probability of finding a particle in a certain eigenstate of the observable.

**Trace condition [7]** An important property of the density operator of any ensemble is that the trace of it always satisfies the condition

$$\text{Tr}(\hat{\rho}) = 1. \quad (1.10)$$

To see this, suppose we have a density operator

$$\hat{\rho} = \sum_i w_i |a^{(i)}\rangle \langle a^{(i)}|, \quad (1.11)$$

where  $\sum_i w_i = 1$  and let  $\{|b_j\rangle\}$  be an orthonormal basis. The expression for the trace is

$$\begin{aligned} \text{Tr}(\hat{\rho}) &= \sum_j \sum_i w_i \langle b_j | a^{(i)} \rangle \langle a^{(i)} | b_j \rangle \\ &= \sum_i w_i \sum_j \langle b_j | a^{(i)} \rangle \langle b_j | a^{(i)} \rangle^* = \sum_i w_i \sum_j |\langle b_j | a^{(i)} \rangle|^2 \end{aligned} \quad (1.12)$$

$$= \sum_i w_i \langle a^{(i)} | a^{(i)} \rangle. \quad (1.13)$$

The above expression, assuming that the state kets  $|a^{(i)}\rangle$  are all properly normalized, reduces to

$$\text{Tr}(\hat{\rho}) = \sum_i w_i = 1, \quad (1.14)$$

proving that the trace of a density matrix is always equal to 1.

**Pure ensemble** Pure ensembles, as mentioned previously, are ensembles where the system can be described by a state ket  $|\alpha\rangle$ . The density operator is therefore given by Eq. (1.1) and takes the form

$$\hat{\rho} = |\alpha\rangle \langle \alpha|. \quad (1.15)$$

A direct consequence of this is that the density operator in the case of a pure ensemble is idempotent, i.e.  $\hat{\rho}^2 = \hat{\rho}$ , since

$$\begin{aligned} \hat{\rho}^2 &= |\alpha\rangle \langle \alpha| \alpha \rangle \langle \alpha| \\ &= |\alpha\rangle \langle \alpha| = \hat{\rho}, \end{aligned} \quad (1.16)$$

assuming that the state ket  $|\alpha\rangle$  is properly normalized. The operator  $\hat{\rho}$  for a pure ensemble is a projection and has therefore either 0 or 1 as eigenvalues [12]. Since a density operator always satisfies the condition  $\text{Tr}(\rho) = 1$ , it follows that the density matrix of a pure states has only one non-zero eigenvalue and that eigenvalue has the value of 1.

### 1.1.2 Reduced density matrix

An important application of density operators is their use in describing subsystems of a composite quantum system, that is a system consisting of two subsystems, through reduced density operators. The reduced density operator of a subsystem  $A$  of a composite system  $AB$  is defined [7] as

$$\hat{\rho}_A \equiv \text{Tr}_B(\hat{\rho}_{AB}). \quad (1.17)$$

Here  $\text{Tr}_B$  is a linear map known as the partial trace. For two vectors  $|a_1\rangle, |a_2\rangle$  in the Hilbert space  $\mathcal{H}_A$  and two vectors  $|b_1\rangle, |b_2\rangle$  in  $\mathcal{H}_B$  the partial trace  $\text{Tr}_B$  is defined [7] as

$$\text{Tr}_B(|a_1\rangle \langle a_2| \otimes |b_1\rangle \langle b_2|) = |a_1\rangle \langle a_2| \text{Tr}(|b_1\rangle \langle b_2|). \quad (1.18)$$

The trace over the outer product  $\text{Tr}(|b_1\rangle \langle b_2|)$  is the inner product  $\langle b_2|b_1\rangle$ . In general let  $O$  be a linear operator defined on a Hilbert space  $\mathcal{H}$ , which in our case would be the density operator, and let  $\mathcal{L}(\mathcal{H})$  denote the space of these operators defined in  $\mathcal{H}$ . If the system studied is a composite system  $AB$ , that is  $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ , then the partial trace taken over subsystem  $B$  is the map [13]

$$\text{Tr}_B : \mathcal{L}(\mathcal{H}) \rightarrow \mathcal{L}(\mathcal{H}_A). \quad (1.19)$$

From [13] we find that obtaining the partial trace of the density matrix, and therefore obtaining the reduced density matrix, using Eq. (1.18) is equivalent to computing the sum

$$\text{Tr}_B(\hat{\rho}) = \sum_{j=1}^{d_B} (\mathbb{1}_A \otimes \langle b_j|) \hat{\rho} (\mathbb{1}_A \otimes |b_j\rangle). \quad (1.20)$$

where  $|b_j\rangle$  is a basis for the subspace  $B$ ,  $\mathbb{1}_A$  the identity operator over subspace  $A$  and  $d_B$  the dimension of the Hilbert space of subsystem  $B$ . The proof of equivalence between Eq. (1.20) and Eq. (1.18) can be found in appendix D.

One can ask oneself why the partial trace is used to describe a part of a larger quantum system. In [7] we can find the following argument. Suppose we want to measure the observable  $M$  on the subsystem  $A$  (for example particle one of the composite system composed of two spin  $\frac{1}{2}$  particles and  $M$  is  $S_z^1$ ). Consider  $M'$  the corresponding observable from the same measurement, measured over the entire system  $AB$ . It can be shown that  $M'$  has to be  $M \otimes \mathbb{1}_B$  and more importantly that the partial trace definition of the reduced density matrix is the unique function such that

$$\text{Tr}(M\hat{\rho}_A) = \text{Tr}(M'\hat{\rho}_{AB}). \quad (1.21)$$

Using Eq. (1.7) we see that the reduced density operator, defined from Eq. (1.17), as a description of a subsystem conserves consistency in measurements.

## 1.2 Entanglement

### 1.2.1 Entangled states

Entanglement is an important property of quantum mechanics that does not arise in classical physics. An entangled state can be defined as a quantum state describing multiple systems that can not be decomposed in a product of states from each individual system. As an example, consider two particles with spin  $\frac{1}{2}$  in a state  $|\Psi\rangle$ . If the state  $|\Psi\rangle$  can be written as a product of two single particle states belonging to the individuals particle Hilbert spaces then the state  $|\Psi\rangle$  is not entangled. An example of this, in a system of two spin  $\frac{1}{2}$  particles would be:

$$|\Psi\rangle = |+\rangle_1 \otimes |+\rangle_2 \equiv |+\rangle_1 |+\rangle_2. \quad (1.22)$$

The state

$$|\Psi\rangle = \frac{1}{\sqrt{2}} (|+\rangle_1 |-\rangle_2 - |-\rangle_1 |+\rangle_2), \quad (1.23)$$

by contrast, can not be written as a product of two single particles states and is therefore an example of an entangled state. To quantify this entanglement we now introduce the concept of entanglement entropy.

### 1.2.2 Entanglement Entropy

To illustrate the concept of entanglement entropy we will use the example of two spin  $\frac{1}{2}$  mentioned above. The density operator of the state given by Eq. (1.23) is calculated using Eq. (1.1). Using  $\{|\pm\rangle_1 |\pm\rangle_2\}$  as an orthogonal basis of the Hilbert space  $\mathcal{H}$  to construct the matrix representation for the density operator we obtain

$$\rho(= [\hat{\rho}]) = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

We can now compute the reduced density matrix of subsystem  $A$ , for example particle 1, by tracing out the second particle in the expression for the density operator defined by Eq. (1.23),

$$\rho_1 = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (1.24)$$



The entanglement entropy of a subsystem  $A$  is defined with the ‘Von-Neumann’ definition of entropy and can be computed as follows:

$$S_{EE}(A) \equiv -\text{Tr}(\rho_A \log_2(\rho_A)). \quad (1.25)$$

If we consider the operator  $\rho_A$  in the basis in which it is diagonal then we can rewrite Eq. (1.25) as

$$S_A = S_{EE}(A) = -\sum_i^N \lambda_i \log_2 \lambda_i, \quad (1.26)$$

where  $\lambda_i$  are the eigenvalues of the operator  $\rho_A$ . Applying this to the previous example we obtain that

$$\begin{aligned} S_1 &= -\left(\frac{1}{2}\right) \log_2 \left(\frac{1}{2}\right) - \left(\frac{1}{2}\right) \log_2 \left(\frac{1}{2}\right) \\ &= 1. \end{aligned}$$

This result indeed confirms that particle one is entangled with particle two in the state given by Eq. (1.23). Repeating the calculations for the state given by Eq. (1.22) results in  $S_A = 0$ , which is consistent with the fact that the given state was not an entangled state. In general we have the following property for the entanglement entropy.

**Property 1:** *The entanglement entropy is non-negative. And  $S_{EE}(\rho_\psi) = 0$  if  $\rho_\psi$  describes a pure state [7].*

Proving this can be done using the fact, showed in section 1.1.2, that the eigenvalues of the density matrix of a pure state are either 0 or 1. The entanglement entropy for a pure state, using Eq. (1.26), is, assuming the density matrix is a  $N \times N$  matrix and therefore has  $N$  eigenvalues,

$$S_{EE} = 1 \log_2 1 + \sum_{i=1}^{N-1} 0 \log_2 0 = 0. \quad (1.27)$$

The positivity of the entanglement entropy follows from the fact that the eigenvalues of a density matrix are real numbers between 0 and 1 [12]. Their logarithm will therefore be smaller or equal to 0 which, using Eq. (1.26), implies that  $S_{EE}$  is greater than zero.

Using this property we can show that the entanglement entropy is indeed well defined. Consider for example the subsystems of a composite system  $AB$  which is described by a product state  $|\psi\rangle = |a\rangle \otimes |b\rangle$  where  $|a\rangle$  and  $|b\rangle$  are the state kets of the subsystems  $A$  and  $B$ . Since both subsystems are described by a state ket they are a pure state, and the entanglement entropy computed with their density matrix is subsequently, using property 1, zero. This result is exactly what we would expect since the total system is described by a product state which by definition means that the subsystems are not entangled.

**Property 2:** *Given a composite system  $AB$  in a pure state, the entanglement entropy of the subsystem  $A$  is equal to that of subsystem  $B$  [10]. Or, in other words:*

$$S_A = S_B. \quad (1.28)$$

In order to prove this property, it is necessary to use the Schmidt Decomposition theorem:

*Let  $|\psi\rangle$  be a pure state in the Hilbert space  $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ . Then there exist an orthonormal basis  $\{|i_A\rangle\}$  in  $\mathcal{H}_A$  and an orthonormal basis  $\{|i_B\rangle\}$  in  $\mathcal{H}_B$  such that*

$$|\psi\rangle = \sum_i^n \lambda_i |i_A\rangle |i_B\rangle, \quad (1.29)$$

where  $\lambda_i \in \mathbb{R}_0$  satisfying  $\sum_i^n \lambda_i^2 = 1$  and  $n \leq \min \{\dim(\mathcal{H}_A), \dim(\mathcal{H}_B)\}$ . A proof of this theorem can be found in Appendix E.

Going back to property 2, we can directly see why Eq. (1.28) holds. If the system AB is in a pure state  $|\psi\rangle$  then the density matrix  $\hat{\rho}_{AB}$  of AB is given by  $\hat{\rho}_{AB} = |\psi\rangle\langle\psi|$ . Using the decomposition theorem we can rewrite this as

$$\hat{\rho}_{AB} = \sum_i^n \lambda_i^2 |i_A\rangle |i_B\rangle \langle i_A| \langle i_B|. \quad (1.30)$$

The reduced density matrices of the subsystem are therefore given by

$$\hat{\rho}_A = \sum_i^n \lambda_i^2 |i_A\rangle \langle i_A| \quad \text{and} \quad \hat{\rho}_B = \sum_i^n \lambda_i^2 |i_B\rangle \langle i_B|. \quad (1.31)$$

Both reduced density matrices will have the same non-zero eigenvalues and will therefore result in the same entanglement entropy.

### 1.3 The Ising model

The Ising Hamiltonian is given by [3]

$$H_{Is.} = -J \sum_i \sigma_i^z \sigma_{i+1}^z + Jg \sum_i \sigma_i^x, \quad (1.32)$$

where the first sums considers the spin-spin interaction between pairs of nearest neighbours. The Pauli spin matrices appearing in Eq. (1.34) are defined as follows:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The constant  $J$  and  $g$  in the definition are both positive and  $g$  is called a coupling constant. To study the Ising model analytically it is often found to be convenient to rotate the axis by  $90^\circ$  around the  $y$ -axis so that

$$\sigma^z \rightarrow \sigma^x \quad \text{and} \quad \sigma^x \rightarrow -\sigma^z, \quad (1.33)$$

which does not influence the results obtained [3]. We then obtain

$$H_{Is.} = -J \sum_i \sigma_i^x \sigma_{i+1}^x - Jg \sum_i \sigma_i^z, \quad (1.34)$$

as expression for the Hamiltonian. The Ising model is a special case of the more general XY model [2]

$$H_{XY} = -Jg \sum_i \left( \frac{1+\gamma}{2} \sigma_i^x \sigma_{i+1}^x + \frac{1-\gamma}{2} \sigma_i^y \sigma_{i+1}^y \right) - Jg \sum_i \sigma_i^z, \quad (1.35)$$

where the factor  $\gamma$  determines the degree of anisotropy in spin-spin interaction along the XY plane. We can see that by setting  $\gamma = 1$ , Eq. (1.35) becomes the Ising Hamiltonian.

The Ising Hamiltonian is interesting to study for different reasons. First, like will be shown in §1.4, analytical results for its entanglement entropy are obtainable, and offer therefore the possibility to compute the entropy numerically for high values of the chain length. Secondly, according to S. Sachdev [3], the Ising model also displays a quantum phase transition for a certain critical value of  $g = g_c$ . The quantum Ising model is also an important model since it can be studied experimentally in  $\text{CONb}_2\text{O}_6$  crystals [14], for example, where the Ising spin resides on the  $\text{C}^{++}$  ion.

## 1.4 Explicit computation of entanglement entropy for the Ising model

An analytical solution for the entanglement entropy is not always available. For example, the system described by the Hamiltonian given by Eq. (2.1) is not integrable for a range of parameters. On the other hand, for some models, in particular the XY (and XXZ model), expressions for the entanglement entropy of a block of  $L$  spins are known and can be found for example in [2, 15, 16]. In this work we present the method for evaluating entanglement entropy for the Ising Hamiltonian, though the procedure can be used for the more general XY model.

### 1.4.1 Diagonalising the Hamiltonian

The derivation for the analytical solution to the Ising model presented here is based on [2] where the more general XY model was analysed and the derivation in [3]. Consider the Ising Hamiltonian from Eq. (1.34) but rewrite the parameters as [15]

$$H_{\text{Ising}} = -\frac{1}{2} \sum_{l=0}^{N-1} \sigma_l^x \sigma_{l+1}^x - \frac{1}{2} \lambda \sum_{l=0}^{N-1} \sigma_l^z, \quad (1.36)$$

where  $N$  is the number of spins and  $\lambda$  is the transverse magnetic field. First we will define new operators using the spin matrices with what is called the Jordan-Wigner transformation. The end of the chain for the Ising Hamiltonian can be treated with periodic boundary conditions (i.e.  $\sigma_N^x = \sigma_1^x$ ) but where the correction term arising from this boundary condition is neglected for large number of spins (often referred to as the ‘c-cyclic’ problem [17, 18]).

**Jordan-Wigner transformation** The Jordan-Wigner transformation maps the system of interacting spin  $\frac{1}{2}$  into a system of interacting fermions [15]. Using the Pauli matrices, we define the following operator

$$a_l = \left( \prod_{m=0}^{l-1} \sigma_m^z \right) \frac{\sigma_l^x - i\sigma_l^y}{2}. \quad (1.37)$$

To ensure that these new operators  $a_l$  (and  $a_l^\dagger$ ) are indeed fermionic it is necessary to check that they fulfil the canonical commutation relations (CCR), i.e.

$$\{a_j, a_k^\dagger\} = \delta_{kj} \mathbb{1} \quad \{a_j, a_k\} = 0. \quad (1.38)$$

Writing the operators out explicitly in the case of  $n$  interacting spin:

$$\begin{aligned} a_l &= \sigma_0^z \otimes \dots \otimes \sigma_{l-1}^z \otimes \sigma_l^- \otimes \mathbb{1}_{l+1} \otimes \dots \otimes \mathbb{1}_n \\ a_l^\dagger &= \sigma_0^z \otimes \dots \otimes \sigma_{l-1}^z \otimes \sigma_l^+ \otimes \mathbb{1}_{l+1} \otimes \dots \otimes \mathbb{1}_n, \end{aligned}$$

where we used that  $\sigma_l^\pm = (\sigma_l^x \pm i\sigma_l^y)/2$  and  $(\sigma_i^z)^\dagger = (\sigma_i^z)$ . Writing out the definition of the anticommutator we obtain

$$\begin{aligned} \{a_k, a_l^\dagger\} &= a_k a_l^\dagger + a_l^\dagger a_k \\ &= (\sigma_0^z \otimes \dots \otimes \sigma_{k-1}^z \otimes \sigma_k^- \otimes \mathbb{1}_{k+1} \otimes \dots \otimes \mathbb{1}_n) (\sigma_0^z \otimes \dots \otimes \sigma_{l-1}^z \otimes \sigma_l^+ \otimes \mathbb{1}_{l+1} \otimes \dots \otimes \mathbb{1}_n) \\ &\quad + (\sigma_0^z \otimes \dots \otimes \sigma_{l-1}^z \otimes \sigma_l^+ \otimes \mathbb{1}_{l+1} \otimes \dots \otimes \mathbb{1}_n) (\sigma_0^z \otimes \dots \otimes \sigma_{k-1}^z \otimes \sigma_k^- \otimes \mathbb{1}_{k+1} \otimes \dots \otimes \mathbb{1}_n). \end{aligned} \quad (1.39)$$

Using from [20] the fact that  $(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$  and supposing that  $k > l$  we can rewrite the previous expression as

$$\begin{aligned}
&= (\mathbb{1} \otimes \dots \otimes \mathbb{1}_{l-1} \otimes \sigma_l^z \sigma_l^+ \otimes \sigma_{l+1}^z \otimes \dots \otimes \sigma_{k-1}^z \otimes \sigma_k^- \otimes \mathbb{1}_{k+1} \otimes \dots \otimes \mathbb{1}_n) \\
&+ (\mathbb{1} \otimes \dots \otimes \mathbb{1}_{l-1} \otimes \sigma_l^+ \sigma_l^z \otimes \sigma_{l+1}^z \otimes \dots \otimes \sigma_{k-1}^z \otimes \sigma_k^- \otimes \mathbb{1}_{k+1} \otimes \dots \otimes \mathbb{1}_n) \\
&= (\mathbb{1} \otimes \dots \otimes \mathbb{1}_{l-1} \otimes (\sigma_l^z \sigma_l^+ + \sigma_l^+ \sigma_l^z) \otimes \sigma_{l+1}^z \otimes \dots \otimes \sigma_{k-1}^z \otimes \sigma_k^- \otimes \mathbb{1}_{k+1} \otimes \dots \otimes \mathbb{1}_n) \quad (1.40)
\end{aligned}$$

since  $\sigma_m^z \sigma_m^z = \mathbb{1}$ . Calculating the product  $(\sigma_l^z \sigma_l^+ + \sigma_l^+ \sigma_l^z)$  explicitly results in

$$\begin{aligned}
\sigma_l^z \sigma_l^+ + \sigma_l^+ \sigma_l^z &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\
&= 0. \quad (1.41)
\end{aligned}$$

Eq. (1.40) is therefore equal to 0. Repeating the calculations for  $k = l$  shows that

$$\begin{aligned}
\{a_l, a_l^\dagger\} &= a_l a_l^\dagger + a_l^\dagger a_l \\
&= (\mathbb{1} \otimes \dots \otimes \mathbb{1}_{l-1} \otimes (\sigma_l^- \sigma_l^+ + \sigma_l^+ \sigma_l^-) \otimes \mathbb{1}_{l+1} \otimes \dots \otimes \mathbb{1}_n) \quad (1.42)
\end{aligned}$$

The product  $(\sigma_l^- \sigma_l^+ + \sigma_l^+ \sigma_l^-)$  is equal to  $\mathbb{1}_l$ . The case where the index of  $a^\dagger$  is smaller than  $a$  can be verified by taking the conjugate transpose of Eq. (1.40) and checking that the product  $(\sigma_k^- \sigma_k^z + \sigma_k^z \sigma_k^-) = 0$ . The previous results taken together confirm that the operator  $a_l$  satisfies one of the CCR. The second CCR, namely

$$\{a_k, a_l\} = a_k a_l + a_l a_k = 0 \quad (1.43)$$

can be checked in an analogous way. Assuming that  $k > l$  we can write that

$$\begin{aligned}
\{a_l, a_k\} &= (\mathbb{1} \otimes \dots \otimes \mathbb{1}_{l-1} \otimes \sigma_l^z \sigma_l^- \otimes \sigma_{l+1}^z \otimes \dots \otimes \sigma_{k-1}^z \otimes \sigma_k^- \otimes \mathbb{1}_{k+1} \otimes \dots \otimes \mathbb{1}_n) \\
&+ (\mathbb{1} \otimes \dots \otimes \mathbb{1}_{l-1} \otimes \sigma_l^- \sigma_l^z \otimes \sigma_{l+1}^z \otimes \dots \otimes \sigma_{k-1}^z \otimes \sigma_k^- \otimes \mathbb{1}_{k+1} \otimes \dots \otimes \mathbb{1}_n) \\
&= (\mathbb{1} \otimes \dots \otimes \mathbb{1}_{l-1} \otimes (\sigma_l^z \sigma_l^- + \sigma_l^- \sigma_l^z) \otimes \sigma_{l+1}^z \otimes \dots \otimes \sigma_{k-1}^z \otimes \sigma_k^- \otimes \mathbb{1}_{k+1} \otimes \dots \otimes \mathbb{1}_n). \quad (1.44)
\end{aligned}$$

Since  $(\sigma_k^- \sigma_k^z + \sigma_k^z \sigma_k^-) = 0$  then Eq. (1.44) is also equal to 0. The case where  $k = l$  can be checked by noting that

$$(\sigma_l^-)^2 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = 0. \quad (1.45)$$

We can therefore conclude that the operator  $a_l$  satisfies both CCR and is therefore a fermionic operator. Transforming the Hamiltonian given by Eq. (1.36) requires the inverse relation, namely the Pauli matrices expressed in function of the operator  $a_l$ . It can be shown (Appendix A.1) that the following holds:

$$\sigma_l^z = 2a_l^\dagger a_l - 1 \quad \text{and} \quad \sigma_l^x \sigma_{l+1}^x = -(a_l^\dagger - a_l)(a_{l+1}^\dagger + a_{l+1}). \quad (1.46)$$

With the relations above we can rewrite the Hamiltonian given by Eq. (1.36)

$$\begin{aligned}
H_I &= -\frac{1}{2} \sum_{l=0}^{N-1} \left( -(a_l^\dagger - a_l)(a_{l+1}^\dagger + a_{l+1}) \right) - \frac{\lambda}{2} \sum_{l=0}^{N-1} (2a_l^\dagger a_l - 1) \\
&= -\frac{1}{2} \sum_{l=0}^{N-1} (-a_l^\dagger a_{l+1}^\dagger - a_l^\dagger a_{l+1} + a_l a_{l+1}^\dagger + a_l a_{l+1}) + \sum_{l=0}^{N-1} \lambda (a_l a_l^\dagger - \frac{1}{2}), \quad (1.47)
\end{aligned}$$

where in the second equality the relation  $\{a_l, a_l^\dagger\} = 1$  was used. Using the other CCR Eq. (1.47) can be rewritten as

$$H_I = -\frac{1}{2} \sum_{l=-(N-1)/2}^{(N-1)/2} \left[ (a_l a_{l+1}^\dagger + a_{l+1} a_l^\dagger + a_l a_{l+1} + a_{l+1}^\dagger a_l^\dagger) - 2\lambda(a_l a_l^\dagger - \frac{1}{2}) \right], \quad (1.48)$$

where the summation convention from [2] was used. Since  $l$  only serves as a indexing of the site it doesn't influence the Hamiltonian but makes the following Fourier transformation easier.

**CCR and unitary transformation** In [21] we find the following reasoning to conclude that unitary transformations do not change the commutation relations. Suppose  $V$  is a finite dimensional vector space and  $a_1, \dots, a_n$  are operators satisfying the fermionic canonical commutation relation. We now define new operators  $b_i$  as follows

$$b_i = \sum_{k=1}^n \beta_{ik} a_k. \quad (1.49)$$

To find a condition for the transformation  $\beta$  such that the new operators satisfy the CCR we compute

$$\{b_j, b_k^\dagger\} = \left\{ \sum_l^n \beta_{jl} a_l, \sum_p^n \beta_{kp}^* a_p^\dagger \right\} \quad (1.50)$$

$$= \sum_{l,p}^n \beta_{jl} \beta_{kp}^* \{a_l, a_p^\dagger\}. \quad (1.51)$$

Using Eq. (1.38) we can rewrite this as

$$\begin{aligned} \{b_j, b_k^\dagger\} &= \sum_p^n \beta_{jp} \beta_{kp}^* \mathbb{1} \\ &= \sum_p^n \beta_{jp} \beta_{pk}^\dagger \mathbb{1} \\ &= (\beta \beta^\dagger)_{jk} \mathbb{1}. \end{aligned} \quad (1.52)$$

Using the linearity of the anticommutator again we can derive that

$$\begin{aligned} \{b_j, b_k\} &= \sum_{l,p}^n \beta_{jl} \beta_{kp}^* \{a_l, a_p\} \\ &= 0, \end{aligned} \quad (1.53)$$

where Eq. (1.38) was used. It therefore follows, from Eq. (1.52) that the transformation  $\beta$  must satisfy  $(\beta \beta^\dagger) = \mathbb{1}$  or thus that  $\beta$  must be an unitary transformation for the new operators to satisfy the CCR.

**Fourier transform** Exploiting the translational symmetry of the system, we can introduce a new set of operators, namely the Fourier transform of the operators  $a_l$ . Explicitly we define

$$d_k = \frac{1}{\sqrt{N}} \sum_{j=-(N-1)/2}^{(N-1)/2} a_j e^{-i \frac{2\pi}{N} k j}, \quad (1.54)$$

or writing the inversion relation

$$a_j = \frac{1}{\sqrt{N}} \sum_{k=-(N-1)/2}^{(N-1)/2} d_k e^{i \frac{2\pi}{N} k j}. \quad (1.55)$$

Since the Fourier transform is a unitary transformation it follows immediately that these new operators follow the commutation relations. Replacing  $a_l$  in equation Eq. (1.48) results in the Hamiltonian taking the form

$$H_I = \sum_{k=-(N-1)/2}^{(N-1)/2} \left[ \left( \lambda - \cos \left( \frac{2\pi k}{N} \right) \right) d_k d_k^\dagger + \frac{i \sin \left( \frac{2\pi k}{N} \right)}{2} \left( d_k d_{-k} + d_k^\dagger d_{-k}^\dagger \right) - \frac{\lambda}{2} \right]. \quad (1.56)$$

The exact computations to derive Eq. (1.56) can be found in the appendix A.2.

**Bogoliubov transformation** Finally, a last transformation of operators, called a Bogoliubov transformation, is needed to obtain the Hamiltonian in a diagonal form. We define

$$\gamma_k = u_k d_k - i v_k d_{-k}^\dagger, \quad (1.57)$$

where  $u_k, v_k$  are real numbers satisfying  $u_k^2 + v_k^2 = 1$ ,  $u_{-k} = u_k$  and  $v_{-k} = -v_k$ . The fact that these new operators satisfy the commutation relations follows from the relations for the operators  $d_k$ . The exact computation can be found in the Appendix A.3. We define the constants as  $u_k = \cos(\theta_k/2)$ ,  $v_k = \sin(\theta_k/2)$  and chose  $\theta_k$  such that the new Hamiltonian does not contain terms like  $\gamma_k \gamma_k$  or  $\gamma_k^\dagger \gamma_k^\dagger$ . The inverse relation of Eq. (1.57) are

$$d_k = u_k \gamma_k + i v_k \gamma_{-k}^\dagger \quad (1.58)$$

$$d_k^\dagger = u_k \gamma_k^\dagger - i v_k \gamma_k, \quad (1.59)$$

which results (see Appendix A.4) in the Hamiltonian taking the diagonal form

$$H_I = \sum_{k=\frac{-(N-1)}{2}}^{\frac{N-1}{2}} \Lambda_k \left( \gamma_k^\dagger \gamma_k - 1/2 \right). \quad (1.60)$$

This coincides with the results from [2] and [3].

#### 1.4.2 Scaling of the entropy for the ground state

Through the use of Majorana operators, correlation functions and Toeplitz matrices it is possible using the diagonal form Eq. (1.60) to derive an analytical expression for the entanglement entropy of a block of length  $\ell$  when the spin chain is in its ground state. The exact derivation and results can be found in for example [2, 15]. The behaviour obtained for the Ising model given by Eq. (1.36) for the critical value of  $\lambda = 1$  is

$$S_\ell^{Is.} = \frac{1}{6} \log_2(\ell) + a. \quad (1.61)$$

The scaling law is not a unique property of the Ising model. For the same value of the magnetic field it is also found in the more general XY-model

$$S_\ell^{XY} = \frac{1}{6} \log_2(\ell) + a(\gamma), \quad (1.62)$$

where the parameter  $a$  now depends on the degree of anisotropy present in spin-spin interaction in the XY-plane.

The time-evolution of the entanglement entropy of a pure state  $|\psi_0\rangle$  evolved by a Hamiltonian  $H$  of which  $|\psi_0\rangle$  is not an eigenstate was studied by Calabrese and Cardy in [16] for the Ising model. In their analyses, numerical and analytical, the entanglement entropy of a block of length  $\ell$  increases linearly until a time  $t^* \approx \ell/2$  and subsequently saturates to a value dependent on the length of the block and the quench.

## 1.5 Quantum mutual information

Another quantity that can be defined with the entanglement entropy of a system is the mutual information. Suppose we have a system with  $A$  and  $B$  as subsystems, then the quantum mutual information is defined [7] as

$$I_{A:B} \equiv S_A + S_B - S_{A \cup B}, \quad (1.63)$$

where  $S$  is the von Neumann entropy of the subsystem.  $S_{A \cup B}$  is the entanglement entropy of the composite system  $AB$ . The mutual information gives a measure for the amount of information subsystem  $A$  and  $B$  have in common [7].

## 1.6 Time evolution

Suppose we have a state ket  $|\alpha\rangle$  at a certain time  $t_0$ , and under the influence of a Hamiltonian  $H$  we wish to know what the states evolves to after a certain time  $t$ . Writing this concisely we want to describe the process

$$|\alpha, t_0; t_0\rangle \longrightarrow |\alpha, t_0; t\rangle. \quad (1.64)$$

We introduce the time evolution operator  $\mathcal{U}(t, t_0)$  as

$$|\alpha, t_0; t\rangle = \mathcal{U}(t, t_0) |\alpha, t_0; t_0\rangle. \quad (1.65)$$

An important property the time evolution operator has to possess, is unitary. This guarantees that if the state ket at time  $t_0$  is normalized it will stay normalized under time evolution, and will therefore conserve probability. Furthermore, we require the time evolution operator to posses the decomposition property, namely

$$\mathcal{U}(t_2, t_0) = \mathcal{U}(t_2, t_1) \mathcal{U}(t_1, t_0) \quad (t_2 > t_1 > t_0). \quad (1.66)$$

Defining the infinitesimal time evolution operator, the Schrödinger equation for the time-evolution operator can be derived [12]

$$i\hbar \frac{\partial}{\partial t} \mathcal{U}(t, t_0) = \hat{H} \mathcal{U}(t, t_0). \quad (1.67)$$

Eq. (1.67) can be used to find explicit expressions for the time-evolution operator. In the simplest case, where the Hamiltonian does not depend on time,  $\mathcal{U}(t, t_0)$  can be expressed as

$$\mathcal{U}(t, t_0) = e^{\frac{-iH(t-t_0)}{\hbar}}. \quad (1.68)$$

We can see that this expression for the time evolution operator satisfies Eq. (1.67).

## 1.7 Quantum quench

The dynamics and evolution of parameters of a many-body quantum system following a sudden change in the Hamiltonian is a topic often studied, see for example [11, 22, 23]. Such a change is referred to as a quench in the Hamiltonian. If a system with Hamiltonian  $\hat{H}$  is in the eigenstate  $|\psi\rangle$  of  $\hat{H}$  before the quench then  $|\psi\rangle$  will not be an eigenstate of the quenched Hamiltonian  $\hat{H}'$ . The system will, on the other hand, be a linear combination

$$|\Psi(t)\rangle = \sum_{n'} a_{n'} e^{-iE_{n'}t} |n'\rangle \quad (1.69)$$

of the eigenstates  $|n'\rangle$  of the new Hamiltonian. Suppose the quench happened at a time  $t = 0$ . Then the coefficients  $a_{n'}$  can be determined by noting that at the time  $t = 0$  the state  $|\Psi(0)\rangle$  should be equal to  $|\psi(0)\rangle$ . This equality implies that the coefficients are given by

$$a_{n'} = \langle n' | \psi(0) \rangle. \quad (1.70)$$

As an example we will now examine the system of a particle in a box where the length  $L$  of the box is suddenly changed to a length  $L'$  as an example of a quantum quench.

### 1.7.1 Example: Particle in a box

Suppose we have a particle with mass  $M$  in a box of length  $L$ . The potential of this situation is

$$V(x) = \begin{cases} 0 & 0 \leq x \leq L \\ \infty & \text{otherwise} \end{cases}. \quad (1.71)$$

Finding the stationary states of this system therefore reduces to finding the eigenstate of the Hamiltonian with  $V = 0$ , imposing the boundary condition that  $\psi(x) = 0$  for  $x = 0$  and  $x = L$  and subsequently adding the exponential factor for time evolution. Completing these calculations results in [19]

$$\psi(x, t)_n^b = \begin{cases} \sqrt{\frac{2}{L}} \sin(k_n x) e^{-i\frac{\hbar k_n^2 t}{2M}} & 0 \leq x \leq L \\ 0 & \text{otherwise} \end{cases}, \quad (1.72)$$

where  $k_n = \frac{n\pi}{L}$  ( $n \in \mathbb{N}_0$ ). If the length of the box is suddenly changed to  $L'$  then the new stationary of this system will be given by

$$\psi(x, t)_{n'}^a = \begin{cases} \sqrt{\frac{2}{L'}} \sin(k_{n'} x) e^{-i\frac{\hbar k_{n'}^2 t}{2M}} & 0 \leq x \leq L' \\ 0 & \text{otherwise,} \end{cases} \quad (1.73)$$

where  $k_{n'} = \frac{n'\pi}{L'}$  ( $n' \in \mathbb{N}_0$ ). We now suppose the system was in the ground state  $\psi_1^b(x, t)$  before the system was quenched at a time  $t = 0$ . The general state of the system after the quench will therefore be

$$\Psi(x, t)^a = \sum_{n'} \langle n' | \psi_1^b(x, 0) \rangle e^{-i\frac{\hbar k_{n'}^2 t}{2M}} |n'\rangle, \quad (1.74)$$

where we used Eq. (1.70) to write the coefficients explicitly. This coefficient can be written out as

$$\begin{aligned} a_{n'} &= \langle n' | \psi_1^b(x, 0) \rangle = \int_{-\infty}^{\infty} \psi_{n'}^a(x, 0)^* \psi_1^b(x, 0) dx \\ &= \int_0^L \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}\right) \sqrt{\frac{2}{L'}} \sin\left(\frac{n'\pi}{L'}\right) dx, \end{aligned} \quad (1.75)$$



where we assumed  $L < L'$  and used the fact that  $\psi_{n'}^a(x, 0)$  is equal to zero for  $x < 0$  or  $x > L$ . This integral can be solved (Appendix B) and one obtains the expression

$$a_{n'} = \frac{\sqrt{LL'}}{\pi} \frac{L'}{(L'^2 - n'^2 L^2)} \sin\left(\frac{n' \pi L}{L'}\right) \quad (1.76)$$

for the coefficients. The expectation value of the energy for this state can now be determined using the expression

$$E = \sum_{n'} |a_{n'}|^2 E_{n'}. \quad (1.77)$$

We can rewrite this expression using the fact that the energy  $E_{n'}$  is given by  $\hbar^2 k_{n'}^2 / 2M$  and that the coefficients are given by Eq. (1.76). The expected value for the energy after the quench is therefore

$$\begin{aligned} E &= \sum_{n'} 4 \frac{LL'}{\pi^2} \frac{L'^2}{(L'^2 - n'^2 L^2)} \sin^2\left(\frac{n' \pi L}{L'}\right) \frac{\hbar^2 \pi^2 n'^2}{2ML^2} \\ &= \sum_{n'} \frac{2\hbar^2}{M} \frac{LL'n'^2}{(L'^2 - n'^2 L^2)} \sin^2\left(\frac{n' \pi L}{L'}\right). \end{aligned} \quad (1.78)$$

We can therefore see how a quench in the Hamiltonian can result in a change in an observable, such as for example the energy. Using the theory examined in this first section we can now compute the time evolution of the entanglement entropy in a specific system.

## 2 Numerical computation of the Entanglement entropy

A first goal of this project is to study the unitary time evolution of the entanglement entropy in a spin chain where the states are evolved by a Hamiltonian

$$H = \sum_{i=1}^L g \sigma_i^x + \sum_{i=2}^{L-1} h \sigma_i^z + (h - J)(\sigma_1^z + \sigma_L^z) + \sum_{i=1}^{L-1} J \sigma_i^z \sigma_{i+1}^z. \quad (2.1)$$

The parameters  $g, h$  and  $J$  were chosen so that the system would remain non-integrable. From [10] we attributed the values  $J = 1$ ,  $h = 0.8090$  and  $g = 0.9045$  to the parameters. To compute the evolution of the entropy we let the system evolve from initial states, which are a product of random spin states

$$|s_i\rangle = \cos\left(\frac{\theta_i}{2}\right) |+\rangle_i + e^{i\phi_i} \sin\left(\frac{\theta_i}{2}\right) |-\rangle_i, \quad (2.2)$$

where  $\theta_i \in [0, \pi)$  and  $\phi_i \in [0, 2\pi)$ . Since these starting states are product states they are by definition not entangled and the subsystem, namely the left half of the chain, has zero entanglement entropy. Computing the entropy at different times therefore amounts to studying its growth with time in a non-integrable system. This is then also an example of quenched evolution, since the starting states given by Eq. (2.2) are not eigenstates of the Hamiltonian given by Eq. (2.1).

Because the system described by the Hamiltonian given in Eq. (2.1) is non-integrable it is only possible to study the evolution numerically. We follow the same procedure as in [10] and for each time  $t$  we generate 200 random starting states, let them evolve with the time evolution operator given by Eq. (1.68) and subsequently compute the entanglement entropy of the left

half of the spin chain. The side of the chain we chose to compute the entanglement entropy from would not change the obtained result. This is a consequence of property 2 in §1.2 since the starting state of the spin chain is chosen to be a product state (and the system is therefore in a pure state) and because unitary time transformation will maintain the system in a pure state [24]. Finally, we average the entropies over the 200 random starting states for each different time.

The program was written in the Python programming language. Since the computational time needed grows rapidly for increasing lengths of the spin chain the VUB cluster ‘Hydra’ [25] was used to run the programs.

## 2.1 Entanglement entropy for two sites

First we derive an explicit expression for the reduced density matrix of a single spin in the case where the chain consists of two sites. This way the output of the algorithm can be checked in the  $L = 2$  case and a confirmation of its accuracy can be obtained.

### 2.1.1 The non-interacting Hamiltonian $H_0$

Setting  $J = 0$  and regrouping the terms in Eq. (2.1) per site results in

$$H_0 = (g\sigma_1^x + h\sigma_1^z) + (g\sigma_2^x + h\sigma_2^z), \quad (2.3)$$

as Hamiltonian. As a basis for a general spin state we represent the spin-up ( $|+\rangle$ ) and spin-down ( $|-\rangle$ ) along the z-axis as

$$|+\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (2.4)$$

and subsequently use the following as a basis for a chain with two sites.

$$\begin{aligned} |+\rangle \otimes |+\rangle &= |++\rangle & , & |+\rangle \otimes |-\rangle = |+-\rangle \\ |-\rangle \otimes |+\rangle &= |-+\rangle & , & |-\rangle \otimes |-\rangle = |--\rangle. \end{aligned}$$

Using the matrix representation we note the effect of the Pauli matrices on the spin states:

$$\sigma^z |+\rangle = |+\rangle, \quad \sigma^x |+\rangle = |-\rangle \quad \text{and} \quad \sigma^z |-\rangle = -|-\rangle, \quad \sigma^x |-\rangle = |+\rangle.$$

**Matrix representation of  $H_0$**  The goal now is to construct the matrix representation of the Hamiltonian  $H_0$ . This will be done by calculating the following terms:

$$\begin{array}{cccc} \langle ++ | H_0 | ++ \rangle & \langle +- | H_0 | ++ \rangle & \langle -+ | H_0 | ++ \rangle & \langle -- | H_0 | ++ \rangle \\ \langle ++ | H_0 | +- \rangle & \langle +- | H_0 | +- \rangle & \langle -+ | H_0 | +- \rangle & \langle -- | H_0 | +- \rangle \\ \langle ++ | H_0 | -+ \rangle & \langle +- | H_0 | -+ \rangle & \langle -+ | H_0 | -+ \rangle & \langle -- | H_0 | -+ \rangle \\ \langle ++ | H_0 | -- \rangle & \langle +- | H_0 | -- \rangle & \langle -+ | H_0 | -- \rangle & \langle -- | H_0 | -- \rangle \end{array}$$

As an example we write down the computation of the term  $\langle ++ | H_0 | ++ \rangle$  explicitly. First we need to calculate the effect of  $H_0$  on the ket  $|++\rangle = |+\rangle_1 |+\rangle_2$ . Splitting the Hamiltonian up by site this implies we need to compute

$$H_0 |+\rangle_1 |+\rangle_2 = \left( [ (g\sigma_1^x + h\sigma_1^z) |+\rangle_1 ] |+\rangle_2 \right) + \left( |+\rangle_1 [ (g\sigma_2^x + h\sigma_2^z) |+\rangle_2 ] \right). \quad (2.5)$$

Working out Eq. (2.5) results in

$$H_0 |+\rangle_1 |+\rangle_2 = 2h |+\rangle_1 |+\rangle_2 + g \left( |-\rangle_1 |+\rangle_2 + |+\rangle_1 |-\rangle_2 \right). \quad (2.6)$$

To compute the first term in the matrix representation we apply the bracket  $\langle ++| = \langle +|_1 \langle +|_2$  to Eq. (2.6)

$$\langle ++| H_0 |++\rangle = 2h \langle ++|++\rangle + g \left( \langle ++| - + \rangle + \langle ++| + - \rangle \right) = 2h.$$

The other terms of the matrix representation of the Hamiltonian are constructed in an analogous way. Using the previous results we can calculate the corresponding terms of our Hamiltonian  $H_0$

$$H_0 = \begin{pmatrix} 2h & g & g & 0 \\ g & 0 & 0 & g \\ g & 0 & 0 & g \\ 0 & g & g & -2h \end{pmatrix} \quad (2.7)$$

**$H_0$  Eigenvalues** Using the matrix representation of  $H_0$  given by Eq. (2.7) the eigenvalues of  $H_0$  can be computed. We calculate (Appendix C) the determinant

$$\begin{vmatrix} 2h - E_0 & g & g & 0 \\ g & -E_0 & 0 & g \\ g & 0 & -E_0 & g \\ 0 & g & g & -2h - E_0 \end{vmatrix} = E_0^4 - 4E_0^2(g^2 + h^2). \quad (2.8)$$

Solving the characteristic equation to find the eigenvalues of  $H_0$  we obtain

$$E_0 = 0 \quad \text{or} \quad E_0 = \pm 2\sqrt{g^2 + h^2}. \quad (2.9)$$

### 2.1.2 The complete Hamiltonian

The full Hamiltonian for two sites with an interaction term not set to zero and where the site interactions have been regrouped where possible is given by

$$H = \left( g\sigma_1^x + (h - J)\sigma_1^z \right) + \left( g\sigma_2^x + (h - J)\sigma_2^z \right) + J\sigma_1^z\sigma_2^z \quad (2.10)$$

This can be seen as the one particle Hamiltonian

$$H_1 = \begin{pmatrix} (h - J) & g \\ g & -(h - J) \end{pmatrix} \quad (2.11)$$

acting on each individual site and where subsequently the interaction term

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_{i+1}$$

acts on particle  $i$  and particle  $i+1$ . This method of decomposing the general Hamiltonian into one-site Hamiltonians will be the strategy to write the algorithm to generate the matrix representation of the Hamiltonian. In an analogous way as before the general matrix representation of Eq. (2.10) is

$$H_J = \begin{pmatrix} 2h - J & g & g & 0 \\ g & -J & 0 & g \\ g & 0 & -J & g \\ 0 & g & g & -2h + 3J \end{pmatrix}. \quad (2.12)$$

### 2.1.3 Explicit calculation of $\rho$ and $\rho_{L/2}$ for $L = 2$

To illustrate the calculation of the terms of the density matrix, suppose we randomly generated the following two spin states:

$$\begin{aligned} |s_1\rangle &= a_1 |+\rangle + b_1 |-\rangle, \\ |s_1\rangle &= a_2 |+\rangle + b_2 |-\rangle. \end{aligned}$$

The coefficients  $a_i$  and  $b_i$  are given by

$$a_{1/2} = \cos\left(\frac{\theta_{1/2}}{2}\right) \quad \text{and} \quad b_{1/2} = e^{i\phi_{1/2}} \sin\left(\frac{\theta_{1/2}}{2}\right).$$

The general state of the chain is a product state and can therefore be written as

$$|s(0)\rangle = |s_1\rangle_1 |s_2\rangle_2. \quad (2.13)$$

By definition, since  $|s(0)\rangle$  is the product of two one-particle kets, the state is not entangled and the subsystems therefore have an entanglement entropy equal to zero. The time-evolution operator  $\mathcal{U}(t, t_0)$  that transforms the state ket  $|\alpha, t_0\rangle$  to  $|\alpha, t_0; t\rangle$  is

$$\mathcal{U}(t, 0) = e^{i\hat{H}_J t}, \quad (2.14)$$

since the Hamiltonian given by Eq. (2.12) is time independent. In Eq. (2.14)  $\hbar$  has been set to 1. At a time  $t$  the state of the chain is therefore characterised by:

$$|s(t)\rangle = e^{i\hat{H}_J t} |s_1\rangle_1 |s_2\rangle_2. \quad (2.15)$$

Writing this explicitly in the orthogonal basis  $\{|++\rangle, |+-\rangle, |-+\rangle, |--\rangle\}$  we obtain:

$$|s(t)\rangle = c_1 |+\rangle_1 |+\rangle_2 + c_2 |+\rangle_1 |-\rangle_2 + c_3 |-\rangle_1 |+\rangle_2 + c_4 |-\rangle_1 |-\rangle_2 \quad (2.16)$$

The coefficients  $c_i$  can be obtained through numerical computations in Python. This is done by first explicitly computing the tensor product  $|s_1\rangle_1 \otimes |s_2\rangle_2$  and subsequently acting on the result with the matrix representation of Eq. (2.14). Using Eq. (2.16) and the definition of the density operator, we can write it explicitly

$$\begin{aligned} \hat{\rho} = & c_1 c_1^* \left( |+\rangle_1 |+\rangle_2 \langle +|_1 \langle +|_2 \right) + c_2 c_1^* \left( |+\rangle_1 |-\rangle_2 \langle +|_1 \langle +|_2 \right) + c_3 c_1^* \left( |-\rangle_1 |+\rangle_2 \langle +|_1 \langle +|_2 \right) \\ & + c_4 c_1^* \left( |-\rangle_1 |-\rangle_2 \langle +|_1 \langle +|_2 \right) + c_1 c_2^* \left( |+\rangle_1 |+\rangle_2 \langle +|_1 \langle -|_2 \right) + c_2 c_2^* \left( |+\rangle_1 |-\rangle_2 \langle +|_1 \langle -|_2 \right) \\ & + c_3 c_2^* \left( |-\rangle_1 |+\rangle_2 \langle +|_1 \langle -|_2 \right) + c_4 c_2^* \left( |-\rangle_1 |-\rangle_2 \langle +|_1 \langle -|_2 \right) + c_1 c_3^* \left( |+\rangle_1 |+\rangle_2 \langle -|_1 \langle +|_2 \right) \\ & + c_2 c_3^* \left( |+\rangle_1 |-\rangle_2 \langle -|_1 \langle +|_2 \right) + c_3 c_3^* \left( |-\rangle_1 |+\rangle_2 \langle -|_1 \langle +|_2 \right) + c_4 c_3^* \left( |-\rangle_1 |-\rangle_2 \langle -|_1 \langle +|_2 \right) \\ & + c_1 c_4^* \left( |+\rangle_1 |+\rangle_2 \langle -|_1 \langle -|_2 \right) + c_2 c_4^* \left( |+\rangle_1 |-\rangle_2 \langle -|_1 \langle -|_2 \right) + c_3 c_4^* \left( |-\rangle_1 |+\rangle_2 \langle -|_1 \langle -|_2 \right) \\ & + c_4 c_4^* \left( |-\rangle_1 |-\rangle_2 \langle -|_1 \langle -|_2 \right) \end{aligned}$$

Or in matrix form:

$$\rho = \begin{pmatrix} c_1 c_1^* & c_2 c_1^* & c_3 c_1^* & c_4 c_1^* \\ c_1 c_2^* & c_2 c_2^* & c_3 c_2^* & c_4 c_2^* \\ c_1 c_3^* & c_2 c_3^* & c_3 c_3^* & c_4 c_3^* \\ c_1 c_4^* & c_2 c_4^* & c_3 c_4^* & c_4 c_4^* \end{pmatrix}.$$

Obtaining the reduced density matrix  $\rho_1$  is done by tracing out particle 2

$$\hat{\rho}_1 = \langle + |_2 \hat{\rho} | + \rangle_2 + \langle - |_2 \hat{\rho} | - \rangle_2 ,$$

which results in

$$\begin{aligned} \hat{\rho}_1 = & c_1 c_1^* | + \rangle_1 \langle + |_1 + c_3 c_1^* | - \rangle_1 \langle + |_1 + c_1 c_3^* | + \rangle_1 \langle - |_1 + c_3 c_3^* | - \rangle_1 \langle - |_1 \\ & + c_2 c_2^* | + \rangle_1 \langle + |_1 + c_4 c_2^* | - \rangle_1 \langle + |_1 + c_2 c_4^* | + \rangle_1 \langle - |_1 + c_4 c_4^* | - \rangle_1 \langle - |_1 , \end{aligned}$$

and written in a matrix

$$\rho_1 = \begin{pmatrix} c_1 c_1^* + c_2 c_2^* & c_3 c_1^* + c_4 c_2^* \\ c_1 c_3^* + c_2 c_4^* & c_3 c_3^* + c_4 c_4^* \end{pmatrix}. \quad (2.17)$$

This explicit formula for the reduced density matrix in the two site case will be used to control the output of the algorithm that calculates the entanglement entropy.

## 2.2 Algorithm for the numerical computation

In this section the general methodology of the algorithm created to compute the entanglement entropy is discussed. The program is split into two distinct parts. The first one is responsible for generating the  $(2^L \times 2^L)$  matrix representation of the Hamiltonian, while the second part computes the entanglement entropy by evolving the randomly generated starting states to a time  $t$ , obtaining the reduced density matrix of half the chain and subsequently calculating its eigenvalues to determine the entropy with Eq. (1.26).

### 2.2.1 Generating the matrix representation of the Hamiltonian

To go through this part of the program function displayed we will suppose the number of sites to be three (this way, every feature of the Hamiltonian is discussed) but the reasoning generalizes to an arbitrary number of sites  $L$ . The function splits the computation into two distinct cases: the matrix element due to the non-interacting part of the Hamiltonian and the one due to the spin-spin interaction part of the Hamiltonian.

**Non-interacting part** The Hamiltonian matrix generator is a function that takes three parameters as input: a base bra, a base ket and the total length of the chain and returns the matrix representation of the Hamiltonian. It therefore computes The goal of this function is to create the matrix representation of the Hamiltonian and

$$\langle s_i | H_0 | s_j \rangle , \quad (2.18)$$

for every base ket  $| s_{i/j} \rangle$ . In the case of a chain of three sites the basis elements could for example be  $\langle - + - |$  and  $| + + - \rangle$ . Using this input the function calculates the correlators of the one particle spin states that are present with the given bra and ket. For the bra and ket mentioned before this would be:

$$\langle - | + \rangle_1 \quad \text{and} \quad \langle + | + \rangle_2 \quad \text{and} \quad \langle - | - \rangle_3$$

where the subscript references the site number. The result of these brackets are added to the list named 'braket'. The rest of the function bases itself on this particular list.

- If the sum of the components of this list equals the number of sites then the coefficient we are calculating is located on the diagonal of our Hamiltonian. In this case, the function applies the one-site Hamiltonian Eq. (2.11) to every ‘one-site’ ket. The correlator of the resulting ket and original bra is subsequently computed. An important detail that is controlled when applying the Hamiltonian to a ‘one-site’ ket is if its located on the endpoints, since in that case the ‘one-site’ Hamiltonian is slightly different.
- If the sum of the components of the list ‘braket’ is equal to zero then the function returns 0. This follows from the fact that the correlator of any site always returns 0 since no matter how the one-particle Hamiltonian acts on a given site, the correlator will always be equal to zero.
- Lastly, if the sum of the components in the ‘braket’ list is not 0 or the length of the chain, the function checks how many one-site correlators had 0 as a result. If there are more than one then the function returns 0 as coefficient. If there is only one one-site braket that has 0 as a result, then the function applies the Hamiltonian to that given site and subsequently computes the correlator. The Hamiltonian applied depends on the location of the site.

**Interaction part** Each interaction term is of the form  $J\sigma_i^z\sigma_{i+1}^z$  which means that the coefficient due to the interaction term will be different from zero only if the input base bra and ket are the same. That is because the operator  $\sigma_i^z$  does not change the one site ket. So if the correlator before applying the interaction term is zero, it will remain zero after. The possible results for the coefficient are either  $J$  or  $-J$  depending on the ket on site  $i$  and  $i + 1$ . This comparison is done fore each consecutive pair of states.

```

48 # %% Action of the Hamiltonian
49 def hamiltonian(Hamiltonian,bra,ket):
50     coef= (bra.transpose()*(Hamiltonian*ket))[0,0]
51     return(coef)
52
53
54 # %% General Coefficient calculator
55 def coefficient_calc(Hamil,bra_L,ket_L,nr_sites):
56     braket = []
57     coefficient= []
58     zero_braket_values = []
59     for k in range(nr_sites):
60         braket.append(((bra_L[k].transpose()).dot(ket_L[k])))
61         if (bra_L[k].transpose()*ket_L[k])[0,0] == 0 :
62             zero_braket_values.append(k)
63     if sum(braket) == nr_sites:
64         coeff_bra_k_ket_k = []
65         for inx in range(nr_sites):
66             if inx == 0 or inx == (nr_sites-1):
67                 coeff_bra_k_ket_k.append(hamiltonian(Hamil[1],bra_L[inx],ket_L[inx]))
68             else:
69                 coeff_bra_k_ket_k.append(hamiltonian(Hamil[0],bra_L[inx],ket_L[inx]))
70     coefficient.append(sum(coeff_bra_k_ket_k))
71     elif sum(braket) == 0:
72         coefficient.append(0)
73     elif sum(braket) in range(1,nr_sites):
74         if len(zero_braket_values) >= 2:
75             coefficient.append(0)
76         else:
77             if zero_braket_values[0] == 0 or zero_braket_values[0] == (nr_sites-1):
78                 coefficient.append(hamiltonian(Hamil[1],bra_L[zero_braket_values[0]],ket_L[zero_braket_values[0]]))
79             else:
80                 coefficient.append(hamiltonian(Hamil[0],bra_L[zero_braket_values[0]],ket_L[zero_braket_values[0]]))
81     return(coefficient[0])
82
83
84 # %% Coding the Interaction part
85 def interaction(bra_L,ket_L,inter,nr_sites):
86     coeff_interaction = []
87     if bra_L == ket_L:
88         for k in range(nr_sites-1):
89             if ket_L[k] == bra_L[k+1]:
90                 coeff_interaction.append(inter)
91             else:
92                 coeff_interaction.append(-inter)
93     else:
94         coeff_interaction.append(0)
95     return(sum(coeff_interaction))

```

**Figure 1:** Function calculating the coefficient of the non-interacting part of the Hamiltonian.

### 2.2.2 Computing the Entanglement Entropy

**Generate random starting states and time evolution** The creation of these random starting states is done by randomly generating the parameters  $\theta_k$  and  $\phi_k$  in Eq. (2.2). After having generated the initial states we use the definition of the time evolution operator Eq.(2.14) to compute the chain state  $|s(t)\rangle$ . Computing  $\langle s(t)|$  is done by using  $\mathcal{U}(t, 0)^\dagger$ .

**Computing the density matrix** Once we have the time evolved states  $|s(t)\rangle$  and  $\langle s(t)|$  for a certain time  $t$  we are able to compute the density matrix of the operator  $|s(t)\rangle \langle s(t)|$ . This is done, naturally, in the same basis as the Hamiltonian. We therefore need to compute every element  $\langle b_i | \rho | b_j \rangle$  where  $b_i$  and  $b_j$  are the basis elements of the spin chain.

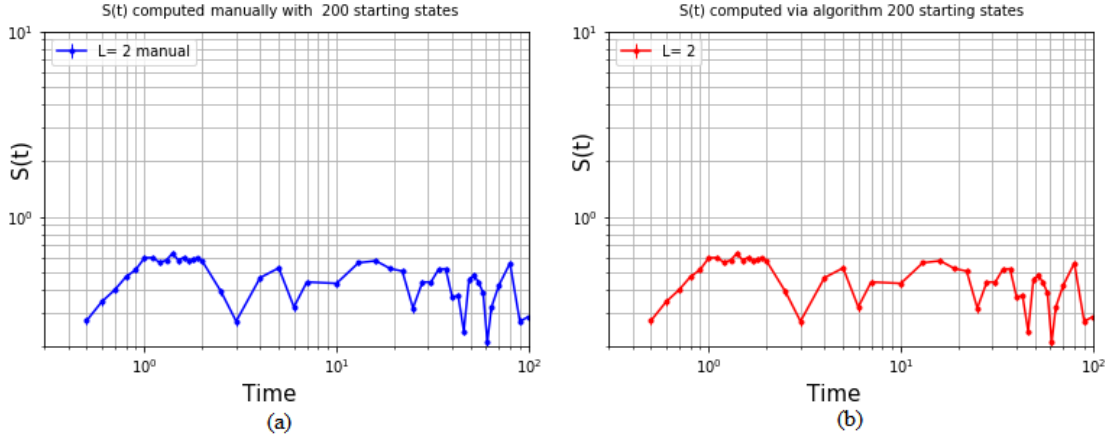
**Reduced density matrix and entanglement entropy** Eq. (1.20) was used to compute the reduced density matrix of one part of the chain. Once the reduced density matrix is obtained, the eigenvalues are calculated and Eq. (1.26) is used to obtain the entanglement entropy of the left part of the chain.

## 3 Results

### 3.1 Entanglement entropy evolution under H

#### 3.1.1 Non-integrable case

First we computed the evolution of the entanglement entropy with time for the Hamiltonian given by Eq. (2.1) in the case of two sites. This was done in order to control the algorithm that was later used to compute the entropy for a random value of the chain length  $L$ . The entanglement entropy was therefore computed with the explicit expression in terms of the density matrix coefficients which was derived in section 2.1.3. Comparing the numerical values of the entropy for both computational processes allowed to confirm that the program was working correctly. Figure 2 shows the evolution of the entropy for both processes where the same randomly generated starting states were used.



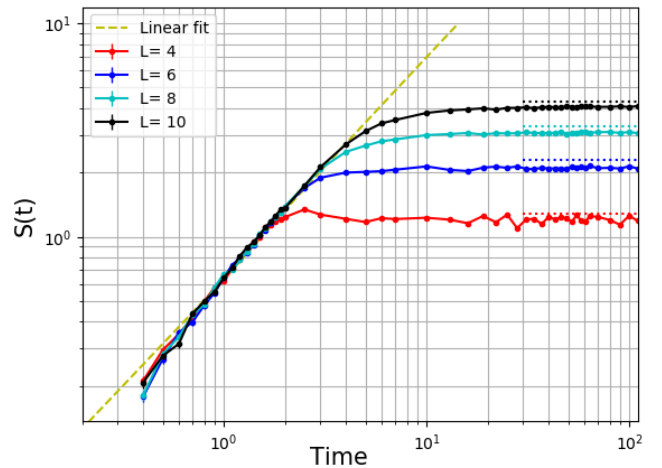
**Figure 2:** Time evolution of  $S_{EE}(L/2)$  for two sites. (a) Entanglement entropy computed with Eq. (2.17) (b) Entropy computed via the algorithm.

The error bars on the graph were computed using a standard error<sup>1</sup>

$$\sigma = \frac{s}{\sqrt{n}}. \quad (3.1)$$

The results obtained in Figure 3 correspond well with [10]. The entanglement entropy grows linearly with time until a  $t^* \approx L/2$  and afterwards saturates to an asymptotic value. In [26] it is shown that for a random pure state, which is what we would expect on average the time evolved state to behave as, in the long-time limit the average entropy is given by

$$S^R = \log_2(m) - \frac{m}{2n \ln 2} - \mathcal{O}\left(\frac{1}{mn}\right) \quad (3.2)$$



**Figure 3:** Time evolution of  $S_{EE}(L/2)$  for different chain lengths. Notice the logarithmic scale for both the x- and y-axis. The dashed line represents the average entropy given by Eq. (3.3).

<sup>1</sup>In this case  $s$  is the standard error on the sample of entanglement entropies and  $n$  the number of starting states.



where  $m$  and  $n$  are the dimensions of the respective Hilbert space of the subsystem. Since in this case  $m = n = 2^{L/2}$  we obtain that the saturation value is

$$S^R \approx \log_2(m) - \frac{1}{2 \ln 2}. \quad (3.3)$$

The linear growth and subsequent saturation to a value dependent on  $L$  is a behaviour that coincides with the results from [16] for the evolution of entanglement entropy in a block. Fitting a linear function through the dataset results in values shown in Table 1. The values obtained for the slope are perfectly in line with the linear growth rate given by [10]. We can also notice that the speed of the linear growth does not depend on the length of the chain.

**Table 1:** Values for the function  $f(t) = mt + b$  through the linear growth.

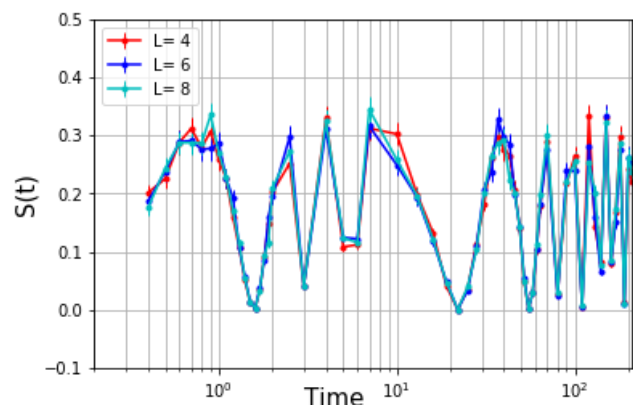
	<b>L-values</b>		
	3	6	8
<b>m</b>	0.69	0.72	0.73
<b>b</b>	-0.06	-0.08	-0.07

It is interesting to notice the particular evolution of the entanglement entropy in the case of two sites. After linearly growing in a similar fashion as the other cases, the entanglement entropy fluctuates instead of saturating. A light fluctuation can also be noticed with in the case of four sites which is a behaviour that seems to disappear for higher values of  $L$ .

### 3.1.2 Integrable cases

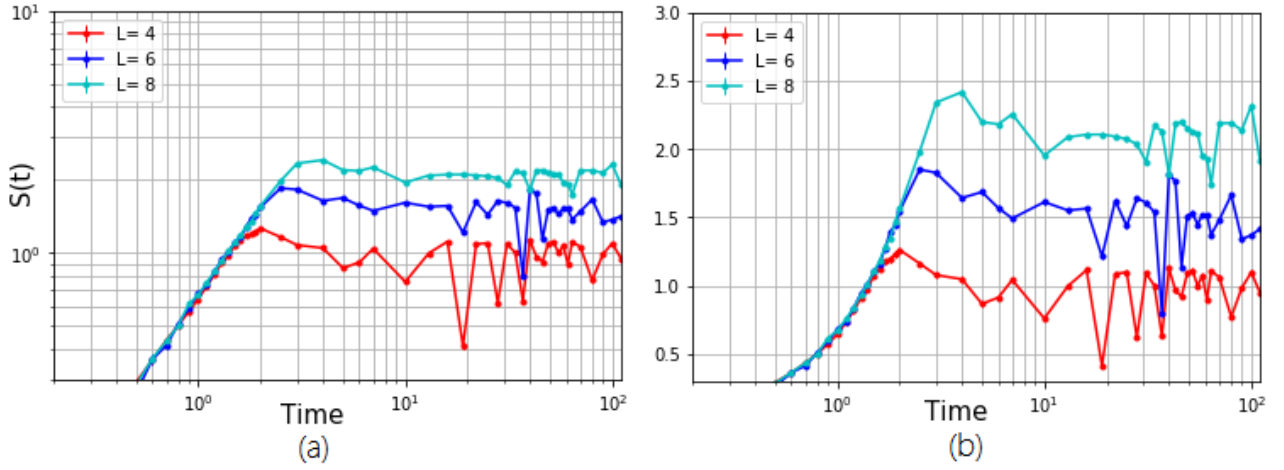
We can now study the evolution of the entanglement entropy when a change is applied to the parameters of the Hamiltonian. The changes considered were where one of the two external magnetic fields was turned off at a time  $t = 0$ . The entanglement entropy was computed in the same way as before, where random product states were generated and subsequently evolved to a time  $t$ .

**Transversal field off** First the change where the transversal field was turned off, i.e.  $g = 0$  was considered. The evolution of the entanglement entropy for this Hamiltonian can be found on Figure 4. It is peculiar to see that the evolution of the entanglement entropy does not show any dependence on the length of the chain. A possible hypothesis for this behaviour could be that is a consequence of the fact that the Hamiltonian is completely diagonal when setting  $g = 0$  since it then only depends on the spin matrix  $\sigma^z$ .



**Figure 4:** Evolution of  $S(t)$  after a change in the Hamiltonian where the transversal field was turned off (i.e.  $g = 0$ ) for different lengths of the chain  $L$ .

**Longitudinal field off** In Figure 5 the evolution for the entanglement entropy can be found in the case where the longitudinal field was turned off at  $t = 0$ . First we can notice that the entanglement entropy reaches a smaller maximum value than in the previous case. This can be seen more explicitly in Figure 6 where the evolution for the two different Hamiltonians were



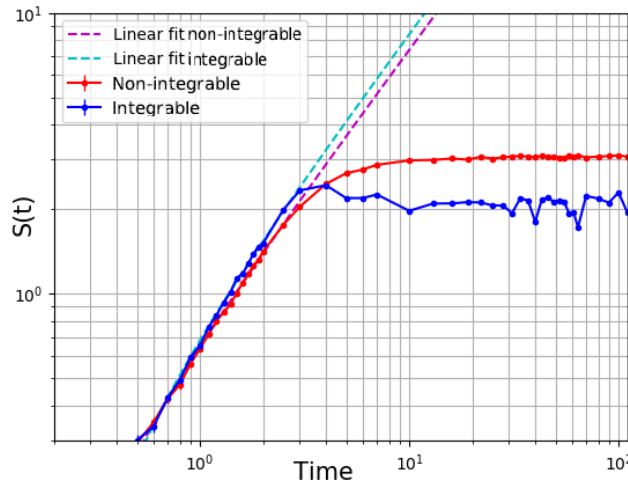
**Figure 5:** Evolution of  $S(t)$  after a change in the Hamiltonian where the longitudinal magnetic field was turned off at  $t = 0$  for different lengths of the chain  $L$ . (a) Logarithmic scale for the  $y$ -axis. (b) Linear scale for the  $y$ -axis.

computed for a chain of length  $L = 8$ . The entanglement entropy also seems to not saturate completely and instead fluctuates around the maximum value.

In Figure 5 (b) it can be seen more directly that the size of the fluctuations are not dependent on the length of the chain. To analyse if there was also a difference in the linear growth between the two systems, a linear function was fitted trough both the datasets in order to determine the slope. The linear functions determined by the parameters obtained trough the linear regression were plotted on Figure 6. The values obtained for the slopes  $m$  are

- $m_{int.} = 0.85$ .
- $m_{non-int.} = 0.74$ .

We can therefore conclude that the entanglement seems to grow slightly faster when the longitudinal field is turned off.



**Figure 6:** Comparison of the entanglement entropy evolution in the original system Eq. (2.1) (non-integrable) and the system evolved by the Hamiltonian where the longitudinal field was turned off (integrable) for  $L = 8$ .

On Figure 6 it can also be seen more explicitly that the entanglement entropy does not saturate for the integrable case but instead fluctuates.

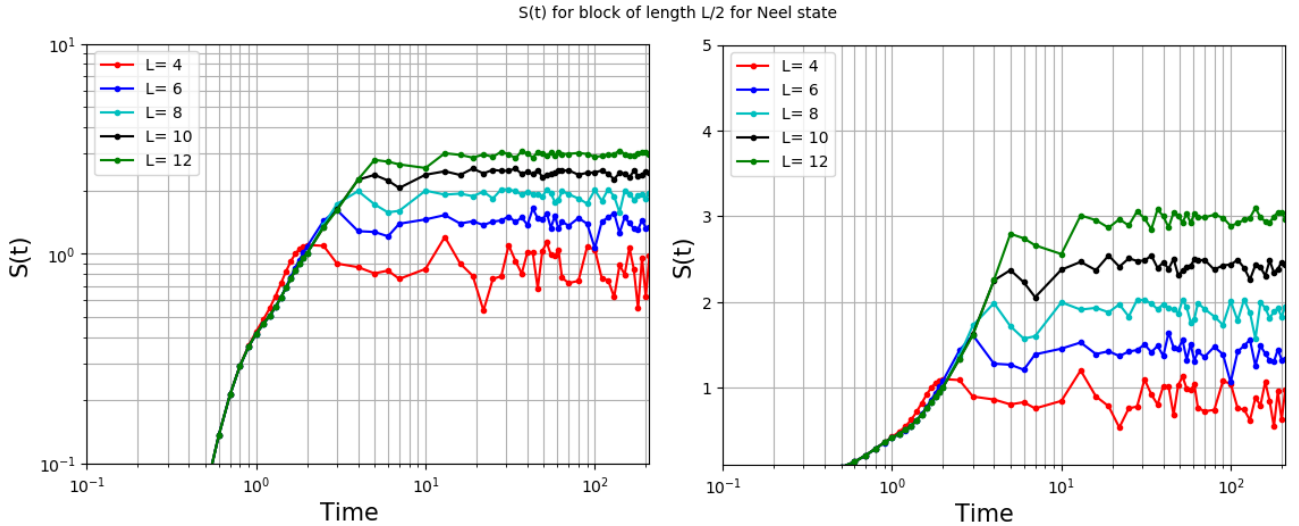
### 3.1.3 Evolution of Néel state

We can also ask how the starting states influence the evolution of the entanglement entropy. In order to try to answer this, this section will study in this part the evolution of the entropy when the system starts in the Néel state defined as

$$|s_0\rangle = |+\rangle_1 |-\rangle_2 |+\rangle_3 \dots, \quad (3.4)$$

where every other spin points in the opposite direction. The choice of having the spin on site one to be up does not influence the results obtained, since inverting the z-axis allows us to obtain the opposite Néel state. This choice of this starting state is also linked with section 3.2 where the mutual quantum information, a quantity dependent on the entanglement entropy, is computed when the system starts in the Néel state. The Hamiltonian used to evolve the Néel state is Eq. (2.1). This is also an example of a quench since the Néel state is not an eigenstate of the Hamiltonian of Eq. (2.1).

The evolution of the entanglement entropy for half of the chain can be seen in Figure 7. We can again notice the linear growth until a time  $t^* \approx L/2$  in the entropy followed by an approximate saturation to a value dependent on the length of the chain. Important to remember is the use of a log scale for both axes in Figure 7. Using a linear scale for the  $y$ -axis shows that the size of the fluctuation has a dependence on the value of the length of the block.



**Figure 7:** Time evolution of  $S_{EE}(L/2)$  for different chain lengths starting from a Néel state. Both graphs show the same entanglement entropy evolution but the right one does not have a logarithmic scale for the  $y$ -axis.

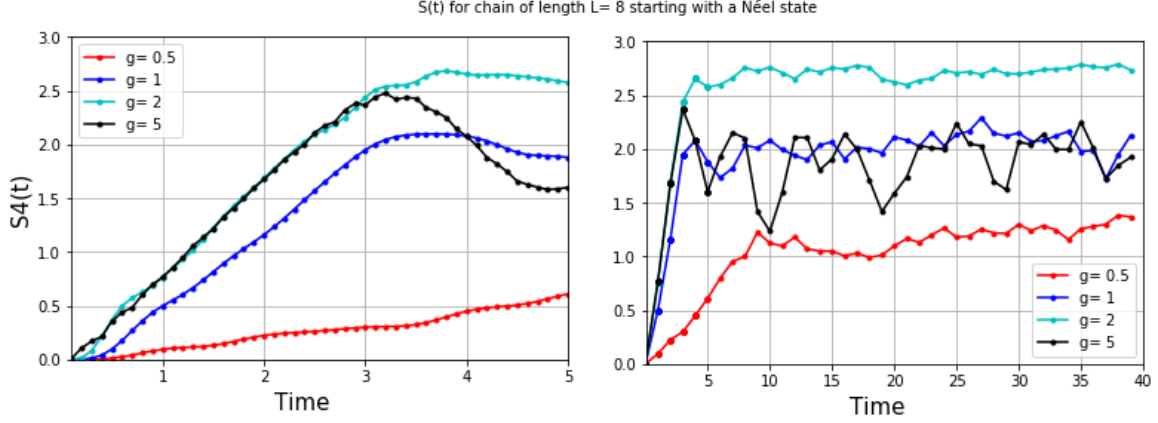
Two noticeable differences can be seen when comparing the evolution of the entanglement entropy of the Néel state to that of a random product state. First we can see that in Figure 7 the entropy saturates at a smaller value than the asymptotic value given by Eq. (3.2). Secondly, the fluctuations from this saturation value are more observable in the Néel state, especially for lower values of chain length.

### 3.1.4 Evolution of Néel state for different values of the coupling constant $g$

Instead of completely turning off one of the magnetic fields we will consider the case where the values of the different parameters are changed and study the effect on the entanglement entropy evolution. The parameter that was tweaked was the transversal field  $g$ , motivated by the study done in [16] where quenches of different transversal field strengths were studied for

the Ising model. A value that was not used was  $g = 0$ . This is because the Hamiltonian without transverse magnetic field consists only of  $\sigma_i^z$  Pauli matrices and will therefore not flip the spins and the starting Neel states is then an eigenstate of the Hamiltonian. Since it is a product of single particle state and therefore not entangled the entropy will remain zero.

The evolution of the entanglement entropy can be found in Figure 8. The linear growth seems to last longer for some values and shorter for others than the time  $t \approx L/2$  characteristic of the previous situations. The linear growth is then, for some parameter values, followed by a saturation. It can be noticed that this saturation value is clearly dependent on the field strength value.



**Figure 8:** Evolution of  $S_\ell(t)$  with  $\ell = 4$  for the Néel state after where different values of the transversal field  $g$  are used in the Hamiltonian. Both graphs show the same entanglement entropy but for different time ranges.

### 3.2 Evolution of quantum mutual information after a quench

An important question in quantum many-body physics is how the mutual information encoded in the initial state, Eq. (1.63) spreads following a quench in the system. In [11] it is argued that evidence for scrambling, a scenario where the information gets dispersed globally, is the scaling of the mutual information between two intervals of fixed length as a function of the distance between them. At intermediate times the mutual information shows a well defined peak whose features depend on if the system is integrable or not. In this last part we therefore study the evolution of the quantum information of the Neel state under unitary time evolution in line with the studies done by P. Calabrese and V. Alba in [11]. After confirming the results obtained by Calabrese the evolution of mutual information is analysed in a system described by Hamiltonian used in the previous section.

The mutual information, given by Eq. (1.63), is computed for two intervals of length  $\ell = 2$  placed at the end of the spin chain. By increasing the length of the chain  $L$  we can study the scrambling of the mutual information for an increasing distance  $d (= L - 4)$  between the two intervals.

Before using the Hamiltonian described by Eq. (2.1) to evolve the chain described by the Neel state we first considered the one used in [11], namely

$$H_2 = \sum_{i=1}^L \left[ \frac{1}{2} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + \Delta S_i^z S_{i+1}^z \right] + h_x \sum_{i=1}^L S_i^x, \quad (3.5)$$

in order to corroborate the results obtained in [11] and asses the reliability of our further results. Here  $S^{\pm,z,x}$  are spin-1/2 operators, which in terms of Pauli spin matrices are written

as<sup>2</sup> [19]

$$S_i^\pm = \sigma_i^\pm \equiv \frac{\sigma_i^x \pm i\sigma_i^y}{2}, \quad S_i^z = \frac{\sigma_i^z}{2} \quad \text{and} \quad S_i^x = \frac{\sigma_i^x}{2}. \quad (3.6)$$

### 3.2.1 Time evolution under $H_2$

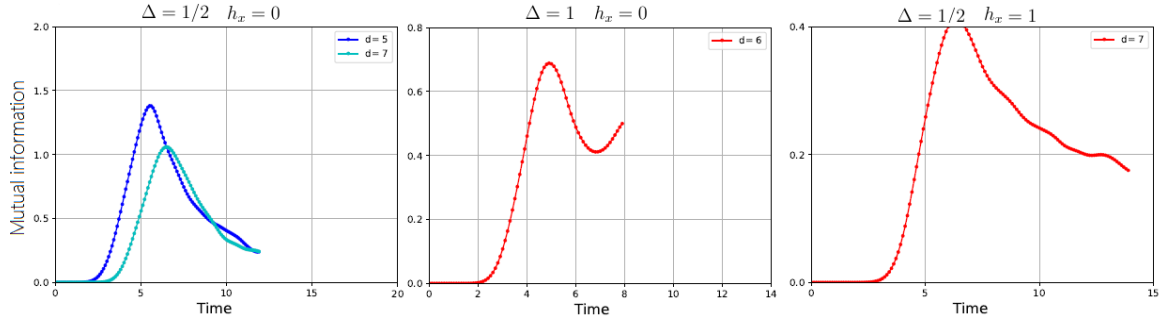
First we write Eq. (3.5) in terms of the Pauli matrices

$$H_2 = \sum_{i=1}^L \left[ \frac{1}{2} (\sigma_i^+ \sigma_{i+1}^- + \sigma_i^- \sigma_{i+1}^+) + \frac{\Delta}{4} \sigma_i^z \sigma_{i+1}^z \right] + \frac{h_x}{2} \sum_{i=1}^L \sigma_i^x. \quad (3.7)$$

If the parameter  $h_x$  is set to 0 and the product  $(\sigma_i^+ \sigma_{i+1}^- + \sigma_i^- \sigma_{i+1}^+)$  is rewritten in terms of  $\sigma^x$  and  $\sigma^y$  we obtain

$$H_2 = \sum_{i=1}^L \frac{1}{4} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z), \quad (3.8)$$

which correspond to the XXZ model Hamiltonian [7]. The XXZ model can be solved analytically through the Bethe Ansatz technique [15]. The time evolution given by the Hamiltonian with  $h_x = 0$  therefore corresponds to integrable dynamics. Since the Hamiltonian used previously is non-integrable it is useful to analyse the results obtained in [11] for non-integrable models, by setting, for example,  $\Delta = 1/2$  and  $h_x = 1$ . The results obtained for the evolution of the mutual information can be found on Figure 9. These correspond exactly to the ones obtained in [11]. It should be noted that the entanglement entropy was computed in [11] with the natural logarithm  $\ln$  instead of  $\log_2$  which was used in section 3.1. The values appearing in Figure 9 were therefore also computed with the natural logarithm. The mutual information shows a clear peak which decreases in height for an increasing distance  $d$  which corresponds exactly to the behaviour in [11] for the Hamiltonian and parameter values considered.



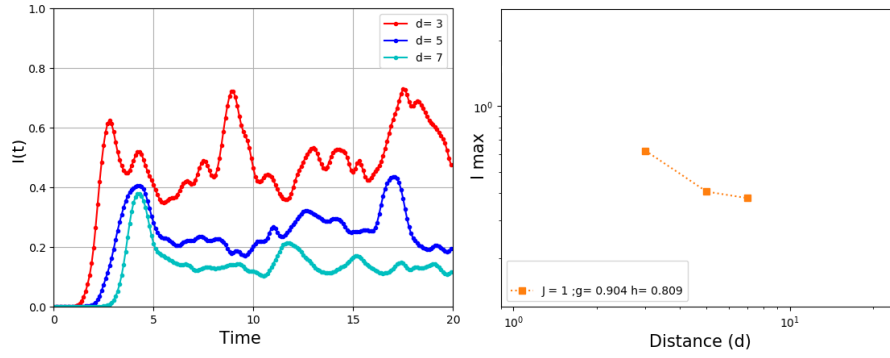
**Figure 9:** Evolution of the mutual information after a quench of the Néel state with  $H_2$  for different values of the parameters  $\Delta$  and  $h_x$  and chain lengths. Increasing the chain length results in a larger distance  $d$  between the two intervals of length  $\ell = 2$ .

### 3.2.2 Time evolution under $H$

Since the reliability of the algorithm used has been proven we can now examine the time evolution of the mutual information in the case where the unitary time evolution of the Néel state is determined by Eq. (2.1). The results of the evolution can be found on Figure 10.

---

<sup>2</sup>The Pauli matrix  $\sigma^y$  is defined as follows:  $\sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$  [19].



**Figure 10:** (a): Time evolution of the mutual information after a quench of the Néel state with  $H$  given by Eq. (2.1). (b) Maximum value of the mutual information in function of the distance  $d$  between the two intervals of length  $\ell$ .

The height of mutual information peak does decrease with a larger distance  $d$  between the intervals. On the other hand it can be noticed that the exponential decrease, theorised for large  $d$  in [11] for non-integrable models, does not seem to appear. In order to confirm if this is a general behaviour computations of the mutual information for greater values of the distance  $d$  would be required. It would also be interesting to see if this behaviour is present for other parameter values.

## 4 Conclusion

During this work an introduction to the study of entanglement entropy was presented. After an overview of the density matrix formalism to study quantum systems, the entanglement entropy of a system was defined as  $S = -\rho \log_2 \rho$ . Through the analysis of the Ising model it was shown that for specific systems of spin chains it is possible to compute the entanglement entropy of the ground state analytically. In a first part of this work the time evolution of the entanglement entropy in a non-integrable model was studied. To achieve this an algorithm was developed and the VUB cluster ‘Hydra’ was used to execute the computations. The results obtained agreed perfectly with the ones in [10]. Subsequently, the parameters of the Hamiltonian were changed to obtain an integrable model and analyse the difference in the entropy evolution. The influence of the starting state on the time evolution was also analysed by considering a different starting state. Lastly, the evolution of mutual information was studied for different systems as an introduction to the study of information spreading in quantum many-body systems.

# Appendix

## A. Spectrum of the Ising Hamiltonian

### A.1. Relations between Pauli matrices and Fermi operators.

**Pauli matrix  $\sigma_l^z$ :** We start by writing out the expression  $2a_l^\dagger a_l - 1$  explicitly obtained from [21]:

$$\begin{aligned} 2a_l^\dagger a_l - 1 &= 2 \left( \sigma_1^z \otimes \dots \otimes \sigma_{l-1}^z \otimes \sigma_l^+ \otimes \mathbb{1}_{l+1} \otimes \dots \otimes \mathbb{1}_n \right) \left( \sigma_1^z \otimes \dots \otimes \sigma_{l-1}^z \otimes \sigma_l^- \otimes \mathbb{1}_{l+1} \otimes \dots \otimes \mathbb{1}_n \right) - 1 \\ &= 2 \left( \mathbb{1}_1 \otimes \dots \otimes \mathbb{1}_{l-1} \otimes \sigma_l^+ \sigma_l^- \otimes \mathbb{1}_{l+1} \otimes \dots \otimes \mathbb{1}_n \right) - 1. \end{aligned} \quad (4.1)$$

Computing the product  $\sigma_l^+ \sigma_l^-$  explicitly results in:

$$\sigma_l^+ \sigma_l^- = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}_l \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_l = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}_l. \quad (4.2)$$

Combining Eq.(4.1) and Eq. (4.2) results<sup>3</sup> in

$$\begin{aligned} 2a_l^\dagger a_l - 1 &= \left( \mathbb{1}_1 \otimes \dots \otimes \mathbb{1}_{l-1} \otimes \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix}_l - \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - l \otimes \mathbb{1}_{l+1} \otimes \dots \otimes \mathbb{1}_n \right) \\ &= \left( \mathbb{1}_1 \otimes \dots \otimes \mathbb{1}_{l-1} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_l \otimes \mathbb{1}_{l+1} \otimes \dots \otimes \mathbb{1}_n \right). \end{aligned} \quad (4.3)$$

The matrix on site  $l$  is just the Pauli matrix  $\sigma^z$  which confirms that  $2a_l^\dagger a_l - 1 = \sigma_l^z$ .

**Pauli matrix  $\sigma_l^x \sigma_{l+1}^x$ :** This computation follows the same procedure as the previous. The expression  $(a_l^\dagger - a_l)(a_{l+1}^\dagger + a_{l+1})$  obtained again from [21] is written out.

$$\begin{aligned} (a_l^\dagger - a_l)(a_{l+1}^\dagger + a_{l+1}) &= \left[ (\sigma_1^z \otimes \dots \otimes \sigma_{l-1}^z \otimes \sigma_l^+ \otimes \mathbb{1}_{l+1} \otimes \dots \otimes \mathbb{1}_n) - (\sigma_1^z \otimes \dots \otimes \sigma_{l-1}^z \otimes \sigma_l^- \otimes \mathbb{1}_{l+1} \otimes \dots \otimes \mathbb{1}_n) \right] \\ &\quad \left[ (\sigma_1^z \otimes \dots \otimes \sigma_l^z \otimes \sigma_{l+1}^+ \otimes \mathbb{1}_{l+2} \otimes \dots \otimes \mathbb{1}_n) + (\sigma_1^z \otimes \dots \otimes \sigma_l^z \otimes \sigma_{l+1}^- \otimes \mathbb{1}_{l+2} \otimes \dots \otimes \mathbb{1}_n) \right] \\ &= \left[ (\sigma_1^z \otimes \dots \otimes \sigma_{l-1}^z \otimes \sigma_l^+ - \sigma_l^- \otimes \mathbb{1}_{l+1} \otimes \dots \otimes \mathbb{1}_n) \right] \left[ (\sigma_1^z \otimes \dots \otimes \sigma_l^z \otimes \sigma_{l+1}^+ + \sigma_{l+1}^- \otimes \mathbb{1}_{l+2} \otimes \dots \otimes \mathbb{1}_n) \right] \\ &= (\mathbb{1}_1 \otimes \dots \otimes \mathbb{1}_{l-1} \otimes (\sigma_l^+ - \sigma_l^-) \sigma_l^z \otimes \sigma_{l+1}^+ + \sigma_{l+1}^- \otimes \dots \otimes \mathbb{1}_n) \end{aligned} \quad (4.4)$$

We now write out the products and sums appearing on site  $l$  and  $l+1$ .

$$\begin{aligned} (\sigma_l^+ - \sigma_l^-) \sigma_l^z &= \left[ \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}_l - \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_l \right] \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_l \\ &= \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}_l = -\sigma_l^x \end{aligned} \quad (4.5)$$

$$\begin{aligned} (\sigma_{l+1}^+ + \sigma_{l+1}^-) &= \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}_{l+1} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_{l+1} \\ &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_{l+1} = \sigma_{l+1}^x \end{aligned} \quad (4.6)$$

Combining the previous three equations confirms the relation:

$$\sigma_l^x \sigma_{l+1}^x = -(a_l^\dagger - a_l)(a_{l+1}^\dagger + a_{l+1}). \quad (4.7)$$

---

<sup>3</sup>The 1 in Eq. (4.1) is to be seen as  $\otimes_{i=0}^n \mathbb{1}_i$

## A.2. Ising Hamiltonian in terms of Fourier transformed fermion operators

To write the Ising Hamiltonian in function of the Fourier transformed operators we will split it in three different sections and rewrite each section apart for clarity.

$$H_I = -\frac{1}{2} \sum_{l=0}^{N-1} \left[ \underbrace{(a_l a_{l+1}^\dagger + a_{l+1} a_l^\dagger)}_{(a)} + \underbrace{a_l a_{l+1} + a_{l+1}^\dagger a_l^\dagger}_{(b)} - 2\lambda \underbrace{(a_l a_l^\dagger - \frac{1}{2})}_{(c)} \right] \quad (4.8)$$

$$(4.9)$$

From the definition of the transformed operators, Eq. (1.54), we find the inverse relation

$$c_j = \frac{1}{\sqrt{N}} \sum_{k=-(N-1)/2}^{(N-1)/2} d_k e^{i \frac{2\pi}{N} k j}. \quad (4.10)$$

**Section (a)** We start by replacing the operators  $a_l$  in the Hamiltonian with the Fourier transformed ones

$$(a) = \sum_{j=-(N-1)/2}^{(N-1)/2} \left[ \left( \frac{1}{N} \sum_{k_1=-(N-1)/2}^{(N-1)/2} \sum_{k_2=-(N-1)/2}^{(N-1)/2} d_{k_1} d_{k_2}^\dagger e^{i \frac{2\pi}{N} k_1 j} e^{-i \frac{2\pi}{N} k_2 (j+1)} \right) + \left( \frac{1}{N} \sum_{k_3=-(N-1)/2}^{(N-1)/2} \sum_{k_4=-(N-1)/2}^{(N-1)/2} d_{k_3} d_{k_4}^\dagger e^{i \frac{2\pi}{N} k_3 (j+1)} e^{-i \frac{2\pi}{N} k_4 j} \right) \right] \quad (4.11)$$

Next we can rearrange the summations

$$(a) = \left( \frac{1}{N} \sum_{k_1=-(N-1)/2}^{(N-1)/2} \sum_{k_2=-(N-1)/2}^{(N-1)/2} d_{k_1} d_{k_2}^\dagger e^{-i \frac{2\pi}{N} k_2} \sum_{j=-(N-1)/2}^{(N-1)/2} e^{i \frac{2\pi}{N} (k_1 - k_2) j} \right) + \left( \frac{1}{N} \sum_{k_3=-(N-1)/2}^{(N-1)/2} \sum_{k_4=-(N-1)/2}^{(N-1)/2} d_{k_3} d_{k_4}^\dagger e^{i \frac{2\pi}{N} k_3} \sum_{j=-(N-1)/2}^{(N-1)/2} e^{-i \frac{2\pi}{N} (k_3 - k_4) j} \right). \quad (4.12)$$

To continue we should notice that

$$\begin{aligned} \sum_{j=-(N-1)/2}^{(N-1)/2} e^{i \frac{2\pi}{N} (k_1 - k_2) j} &= e^{-i \frac{2\pi}{N} \frac{(N-1)}{2} (k_1 - k_2)} \sum_{j=0}^{(N-1)} e^{i \frac{2\pi}{N} (k_1 - k_2) j} \\ &= \begin{cases} 0 & k_1 \neq k_2 \\ 1 \sum_{l=0}^{(N-1)} 1 = N & k_1 = k_2 \end{cases} \\ &= \delta_{k_1, k_2} N \end{aligned} \quad (4.13)$$

since  $(k_1 - k_2) \in \{(N-1), \dots, -1, 1, \dots, (N-1)\}$  if  $k_1 \neq k_2$ . In an analogous way we find that

$$\sum_{j=-(N-1)/2}^{(N-1)/2} e^{i \frac{2\pi}{N} (k_3 - k_4) j} = \delta_{k_3, k_4} N. \quad (4.14)$$



Eq. (4.13) therefore becomes

$$\begin{aligned}
(a) &= \left( \sum_{k_1, k_2 = -(N-1)/2}^{(N-1)/2} d_{k_1} d_{k_2}^\dagger e^{-i \frac{2\pi}{N} k_2} \delta_{k_1, k_2} \right) + \left( \sum_{k_3, k_4 = -(N-1)/2}^{(N-1)/2} d_{k_3} d_{k_4}^\dagger e^{i \frac{2\pi}{N} k_3} \delta_{k_3, k_4} \right) \\
&= \sum_{k_1 = -(N-1)/2}^{(N-1)/2} d_{k_1} d_{k_1}^\dagger e^{-i \frac{2\pi}{N} k_1} + \sum_{k_3 = -(N-1)/2}^{(N-1)/2} d_{k_3} d_{k_3}^\dagger e^{i \frac{2\pi}{N} k_3} \\
&= 2 \sum_{k_1 = -(N-1)/2}^{(N-1)/2} d_k d_k^\dagger \cos \left( \frac{2\pi k}{N} \right). \tag{4.15}
\end{aligned}$$

**Section (b)** Again, we first replace the operators  $a_l$  with their Fourier transform

$$\begin{aligned}
(b) &= \sum_{j = \frac{-(N-1)}{2}}^{\frac{N-1}{2}} \left( \frac{1}{N} \sum_{k_1 = \frac{-(N-1)}{2}}^{\frac{N-1}{2}} \sum_{k_2 = \frac{-(N-1)}{2}}^{\frac{N-1}{2}} d_{k_1} d_{k_2} e^{i \frac{2\pi}{N} k_1 j} e^{i \frac{2\pi}{N} k_2 (j+1)} \right) \\
&+ \left( \frac{1}{N} \sum_{k_3 = \frac{-(N-1)}{2}}^{\frac{N-1}{2}} \sum_{k_4 = \frac{-(N-1)}{2}}^{\frac{N-1}{2}} d_{k_3}^\dagger d_{k_4}^\dagger e^{-i \frac{2\pi}{N} k_3 (j+1)} e^{-i \frac{2\pi}{N} k_4 j} \right) \\
&= \left( \frac{1}{N} \sum_{k_1 = \frac{-(N-1)}{2}}^{\frac{N-1}{2}} \sum_{k_2 = \frac{-(N-1)}{2}}^{\frac{N-1}{2}} d_{k_1} d_{-k_2} e^{-i \frac{2\pi}{N} k_2} \sum_{j = \frac{-(N-1)}{2}}^{\frac{N-1}{2}} e^{i \frac{2\pi}{N} (k_1 - k_2) j} \right) \\
&+ \left( \frac{1}{N} \sum_{k_3 = \frac{-(N-1)}{2}}^{\frac{N-1}{2}} \sum_{k_4 = \frac{-(N-1)}{2}}^{\frac{N-1}{2}} d_{-k_3}^\dagger d_{k_4}^\dagger e^{i \frac{2\pi}{N} k_3} \sum_{j = \frac{-(N-1)}{2}}^{\frac{N-1}{2}} e^{-i \frac{2\pi}{N} (k_3 - k_4) j} \right) \tag{4.16}
\end{aligned}$$

where in the second equality we replaced  $k_2$  and  $k_3$  with  $-k_2$  and  $-k_3$  thereby inverting the summation. Using the same reasoning as in Eq. (4.13) and the relation  $\{d_l^\dagger, d_m^\dagger\} = 0$  this expression simplifies to

$$\begin{aligned}
(b) &= \sum_{k_1 = \frac{-(N-1)}{2}}^{\frac{N-1}{2}} d_{k_1} d_{-k_1} e^{-i \frac{2\pi}{N} k_1} + \sum_{k_3 = \frac{-(N-1)}{2}}^{\frac{N-1}{2}} d_{-k_3}^\dagger d_{k_3}^\dagger e^{i \frac{2\pi}{N} k_3} \\
&= \sum_{k = \frac{-(N-1)}{2}}^{\frac{N-1}{2}} d_k d_{-k} e^{-i \frac{2\pi}{N} k} - \sum_{k = \frac{-(N-1)}{2}}^{\frac{N-1}{2}} d_k^\dagger d_{-k}^\dagger e^{i \frac{2\pi}{N} k} \\
&= - \sum_{k = \frac{-(N-1)}{2}}^{\frac{N-1}{2}} \left( d_k d_{-k} + d_k^\dagger d_{-k}^\dagger \right) i \sin \left( \frac{2\pi k}{N} \right) + \sum_{k = \frac{-(N-1)}{2}}^{\frac{N-1}{2}} \left( d_k d_{-k} - d_k^\dagger d_{-k}^\dagger \right) \cos \left( \frac{2\pi k}{N} \right) \tag{4.17}
\end{aligned}$$

Using the process described in [28] we can eliminate the term with the cosine by splitting the sum

$$\begin{aligned}
&= \sum_{k>0}^{\frac{N-1}{2}} \left( d_k d_{-k} - d_k^\dagger d_{-k}^\dagger \right) \cos \left( \frac{2\pi k}{N} \right) + \sum_{k<0}^{\frac{-(N-1)}{2}} \left( d_k d_{-k} - d_k^\dagger d_{-k}^\dagger \right) \cos \left( \frac{2\pi k}{N} \right) \\
&= \sum_{k>0}^{\frac{N-1}{2}} \left( d_k d_{-k} - d_k^\dagger d_{-k}^\dagger \right) \cos \left( \frac{2\pi k}{N} \right) + \sum_{k>0}^{\frac{(N-1)}{2}} \left( d_{-k} d_k - d_{-k}^\dagger d_k^\dagger \right) \cos \left( \frac{2\pi(-k)}{N} \right) \\
&= \sum_{k>0}^{\frac{N-1}{2}} \left( d_k d_{-k} - d_k^\dagger d_{-k}^\dagger \right) \cos \left( \frac{2\pi k}{N} \right) + \sum_{k>0}^{\frac{(N-1)}{2}} \left( -d_k d_{-k} + d_k^\dagger d_{-k}^\dagger \right) \cos \left( \frac{2\pi(k)}{N} \right), = 0 \quad (4.18)
\end{aligned}$$

and for  $k = 0$ , using the commutation relation  $\{d_k, d_k\} = 0$ , we notice that

$$d_0 d_0 - d_0^\dagger d_0^\dagger = 0. \quad (4.19)$$

So we conclude that

$$(b) = - \sum_{k=\frac{-(N-1)}{2}}^{\frac{N-1}{2}} \left( d_k d_{-k} + d_k^\dagger d_{-k}^\dagger \right) i \sin \left( \frac{2\pi k}{N} \right) \quad (4.20)$$

**Section (c)** The computation for part (c) of the Hamiltonian is completely analogous to the one for section (a). We obtain that

$$(c) = \sum_{k=\frac{-(N-1)}{2}}^{\frac{N-1}{2}} d_k d_k^\dagger \quad (4.21)$$

Combining Eq. (4.15),(4.17) and (4.21) we obtain exactly Eq. (1.56).

### A.3. Commutation relations of the Bogoliubov operators

We start from the definition of the operator and its complex conjugate

$$\begin{aligned}
\gamma_k &= u_k d_k - i v_k d_{-k}^\dagger \\
\gamma_k^\dagger &= u_k d_k^\dagger + i v_k d_{-k}
\end{aligned} \quad (4.22)$$

The first relation to control is  $\{\gamma_{k_1}, \gamma_{k_2}^\dagger\}$ . We use the definitions Eq. (4.22) of the new operators explicitly and subsequently use the linearity of the commutation relations.

$$\begin{aligned}
\{\gamma_{k_1}, \gamma_{k_2}^\dagger\} &= \left\{ u_{k_1} d_{k_1} - i v_{k_1} d_{-k_1}^\dagger, u_{k_2} d_{k_2}^\dagger + i v_{k_2} d_{-k_2} \right\} \\
&= \left\{ u_{k_1} d_{k_1}, u_{k_2} d_{k_2}^\dagger \right\} + \left\{ u_{k_1} d_{k_1}, i v_{k_2} d_{-k_2}^\dagger \right\} + \left\{ i v_{k_1} d_{-k_1}^\dagger, u_{k_2} d_{k_2}^\dagger \right\} + \left\{ -i v_{k_1} d_{-k_1}^\dagger, i v_{k_2} d_{-k_2} \right\} \\
&= u_{k_1} u_{k_2} \left\{ d_{k_1}, d_{k_2}^\dagger \right\} + u_{k_1} i v_{k_2} \left\{ d_{k_1}, d_{-k_2}^\dagger \right\} + i v_{k_1} u_{k_2} \left\{ d_{-k_1}^\dagger, d_{k_2}^\dagger \right\} + v_{k_1} v_{k_2} \left\{ d_{-k_1}^\dagger, d_{-k_2} \right\} \\
&= u_{k_1} u_{k_2} \delta_{k_1, k_2} + v_{k_1} v_{k_2} \delta_{-k_1, -k_2} \\
&= 0 \text{ ( for } k_1 \neq k_2 \text{ )} \quad (4.23)
\end{aligned}$$

where in the last equation the commutation relations of  $d_k$  where used. For  $k_1 = k_2$  Eq.(4.23), using the definition of the transformation, becomes

$$\begin{aligned}\{\gamma_{k_1}, \gamma_{k_1}^\dagger\} &= u_{k_1}^2 + v_{k_1}^2 \\ &= 1\end{aligned}\quad (4.24)$$

The new operators therefore satisfy  $\{\gamma_{k_1}, \gamma_{k_2}^\dagger\} = \delta_{k_1, k_2}$  as expected. The second commutation relation, namely  $\{\gamma_{k_1}^\dagger, \gamma_{k_2}^\dagger\}$ , follows the same procedure and the explicit computation is given below.

$$\begin{aligned}\{\gamma_{k_1}^\dagger, \gamma_{k_2}^\dagger\} &= \{u_{k_1} d_{k_1}^\dagger + i v_{k_1} d_{-k_1}, u_{k_2} d_{k_2}^\dagger + i v_{k_2} d_{-k_2}\} \\ &= u_{k_1} u_{k_2} \{d_{k_1}^\dagger, d_{k_2}^\dagger\} + i u_{k_1} v_{k_2} \{d_{k_1}^\dagger, d_{-k_2}\} + i v_{k_1} u_{k_2} \{d_{-k_1}, d_{k_2}^\dagger\} - v_{k_1} v_{k_2} \{d_{-k_1}, d_{-k_2}\} \\ &= i (u_{k_1} v_{k_2} \delta_{k_1, -k_2} + v_{k_1} u_{k_2} \delta_{-k_1, k_2}) \\ &= \begin{cases} 0 & k_1 \neq -k_2 \\ i(u_{-k_2} v_{k_2} + v_{-k_2} u_{k_2}) = i(u_{k_2} v_{k_2} - v_{k_2} u_{k_2}) = 0 & k_1 = -k_2 \end{cases}\end{aligned}\quad (4.25)$$

The relation  $\{\gamma_{k_1}^\dagger, \gamma_{k_2}^\dagger\} = \{\gamma_{k_1}, \gamma_{k_2}\} = 0$  is therefore also satisfied by the new operators.

#### A.4. Diagonalisation of the Ising Hamiltonian

The Hamiltonian given by Eq. (1.56) written in function of the operators  $\gamma_k$  is

$$\begin{aligned}H_I &= \sum_{k=-\frac{(N-1)}{2}}^{\frac{N-1}{2}} \left( \lambda - \cos\left(\frac{2\pi k}{N}\right) \right) (u_k \gamma_k + i v_k \gamma_{-k}^\dagger) (u_k \gamma_k^\dagger - i v_k \gamma_{-k}) \\ &\quad + \frac{i}{2} \sin\left(\frac{2\pi k}{N}\right) \left[ (u_k \gamma_k + i v_k \gamma_{-k}^\dagger) (u_k \gamma_{-k} - i v_k \gamma_k^\dagger) + (u_k \gamma_k^\dagger - i v_k \gamma_{-k}) (u_k \gamma_{-k}^\dagger + i v_k \gamma_k) - \frac{\lambda}{2} \right] \\ &= \sum_{k=-\frac{(N-1)}{2}}^{\frac{N-1}{2}} \left[ \left( \lambda - \cos\left(\frac{2\pi k}{N}\right) \right) (u_k^2 \gamma_k \gamma_k^\dagger + i u_k v_k (-\gamma_k \gamma_{-k} + \gamma_{-k}^\dagger \gamma_k^\dagger) + v_k^2 \gamma_{-k}^\dagger \gamma_{-k}) \right. \\ &\quad \left. + \frac{i}{2} \sin\left(\frac{2\pi N}{k}\right) (2 i u_k v_k (\gamma_{-k}^\dagger \gamma_{-k} - \gamma_k \gamma_k^\dagger) + (v_k^2 - u_k^2) (\gamma_{-k}^\dagger \gamma_k^\dagger + \gamma_{-k} \gamma_k)) - \frac{\lambda}{2} \right].\end{aligned}\quad (4.26)$$

First we consider the term

$$\begin{aligned}&\left( \lambda - \cos\left(\frac{2\pi k}{N}\right) \right) (i u_k v_k (-\gamma_k \gamma_{-k} + \gamma_{-k}^\dagger \gamma_k^\dagger)) + \frac{i}{2} \sin\left(\frac{2\pi k}{N}\right) (v_k^2 - u_k^2) (\gamma_k \gamma_{-k} + \gamma_{-k}^\dagger \gamma_k^\dagger) \\ &= (\gamma_k \gamma_{-k} + \gamma_{-k}^\dagger \gamma_k^\dagger) \left( (\lambda - \cos(\alpha_k)) i u_k v_k + \frac{i}{2} \sin\left(\frac{2\pi k}{N}\right) (v_k^2 - u_k^2) \right)\end{aligned}\quad (4.27)$$

of Eq. (4.26). For simplicity we set  $\alpha_k \equiv \frac{2\pi k}{N}$  and chose for the constant

$$\cos(\theta_k) \equiv \frac{-\lambda + \cos(\alpha_k)}{\sqrt{\beta_k}}\quad (4.28)$$

where  $\beta_k \equiv \sqrt{(\lambda - \cos(\alpha_k))^2 + \sin^2(\alpha_k)}$ . Using the fact [27] that  $2 \cos(2x) = 2 \cos^2(x) - 1$  we obtain that

$$u_k^2 = \frac{1}{2} + \frac{(\lambda - \cos(\alpha_k))}{2\sqrt{\beta_k}} \quad (4.29)$$

$$v_k^2 = \frac{1}{2} - \frac{(\lambda - \cos(\alpha_k))}{2\sqrt{\beta_k}}. \quad (4.30)$$

Therefore the non-operator part of Eq. (4.27) reduces to

$$\begin{aligned} & (\lambda - \cos(\alpha_k)) \sqrt{\left(\frac{1}{2} - \frac{(\lambda + \cos(\alpha_k))}{2\sqrt{\beta_k}}\right) \left(\frac{1}{2} - \frac{(\lambda + \cos(\alpha_k))}{2\sqrt{\beta_k}}\right) - \frac{i}{2} \sin(\alpha_k) \frac{(\lambda - \cos(\alpha_k))}{\sqrt{\beta_k}}} \\ &= (\lambda - \cos(\alpha_k)) \sqrt{\left(\frac{1}{4} - \frac{(\lambda - \cos(\alpha_k))^2}{4\beta_k}\right) - \frac{i}{2} \sin(\alpha_k) \frac{(\lambda - \cos(\alpha_k))}{\sqrt{\beta_k}}} \\ &= (\lambda - \cos(\alpha_k)) \frac{i \sin(\alpha_k)}{2 \sqrt{\beta_k}} - \frac{i}{2} \sin(\alpha_k) \frac{(\lambda - \cos(\alpha_k))}{\sqrt{\beta_k}} = 0. \end{aligned} \quad (4.31)$$

The other term of Eq. (4.26) is

$$\begin{aligned} & (\lambda - \cos(\alpha_k)) \left( u_k^2 \gamma_k \gamma_k^\dagger + v_k^2 \gamma_{-k}^\dagger \gamma_{-k} \right) - \sin(\alpha_k) u_k v_k \left( \gamma_{-k}^\dagger \gamma_{-k} - \gamma_k \gamma_k^\dagger \right) \\ &= [(\lambda - \cos(\alpha_k)) v_k^2 - \sin(\alpha_k) u_k v_k] \gamma_{-k}^\dagger \gamma_{-k} + [(\lambda - \cos(\alpha_k)) v_k^2 + \sin(\alpha_k) u_k v_k] \gamma_k \gamma_k^\dagger \\ &= \left[ \frac{(\lambda - \cos(\alpha_k))}{2} - \frac{\sqrt{\beta_k}}{2} \right] (1 - \gamma_{-k} \gamma_{-k}^\dagger) + \left[ \frac{(\lambda - \cos(\alpha_k))}{2} + \frac{\sqrt{\beta_k}}{2} \right] \gamma_k \gamma_k^\dagger. \end{aligned} \quad (4.32)$$

The Hamiltonian therefore becomes

$$\begin{aligned} H_I &= \sum_{k=\frac{-(N-1)}{2}}^{\frac{N-1}{2}} \left[ \frac{(\lambda - \cos(\alpha_k))}{2} - \frac{\sqrt{\beta_k}}{2} \right] (1 - \gamma_{-k} \gamma_{-k}^\dagger) + \left[ \frac{(\lambda - \cos(\alpha_k))}{2} + \frac{\sqrt{\beta_k}}{2} \right] \gamma_k \gamma_k^\dagger - \frac{\lambda}{2} \\ &= \sum_{k=\frac{-(N-1)}{2}}^{\frac{N-1}{2}} \left[ -\frac{(\cos(\alpha_k))}{2} - \frac{\sqrt{\beta_k}}{2} \right] + \left[ \frac{(\lambda - \cos(\alpha_k))}{2} \right] (\gamma_k \gamma_k^\dagger - \gamma_{-k} \gamma_{-k}^\dagger) + \frac{\sqrt{\beta_k}}{2} (\gamma_k \gamma_k^\dagger + \gamma_{-k} \gamma_{-k}^\dagger) \\ &= \sum_{k=\frac{-(N-1)}{2}}^{\frac{N-1}{2}} \left[ \sqrt{\beta_k} \left( \gamma_k \gamma_k^\dagger - \frac{1}{2} \right) - \frac{\cos(\alpha_k)}{2} \right] \end{aligned} \quad (4.33)$$

## B. Coefficients for the particle in a box quench

The integral

$$\int_0^L \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}\right) \sqrt{\frac{2}{L'}} \sin\left(\frac{n'\pi}{L'}\right) dx = \frac{2}{\sqrt{LL'}} \int_0^L \sin\left(\frac{\pi}{L}\right) \sin\left(\frac{n'\pi}{L'}\right) dx \quad (4.34)$$

can be solved by using the goniometric formula :  $2 \sin(\alpha) \sin(\beta) = \cos(\alpha - \beta) - \cos(\alpha + \beta)$  ([27]). Using this equality we can compute the integral from Eq.(4.34) as follows

$$\begin{aligned}
& \frac{2}{\sqrt{LL'}} \left( \frac{1}{2} \int_0^L \left[ \cos \left( \frac{\pi x}{L} - \frac{n' \pi x}{L'} \right) - \cos \left( \frac{\pi x}{L} + \frac{n' \pi x}{L'} \right) \right] dx \right) \\
&= \frac{1}{\sqrt{LL'}} \left[ \sin \left( \frac{\pi x}{L} - \frac{n' \pi x}{L'} \right) \frac{1}{\frac{\pi}{L} - \frac{n' \pi}{L'}} - \sin \left( \frac{\pi x}{L} + \frac{n' \pi x}{L'} \right) \frac{1}{\frac{\pi}{L} + \frac{n' \pi}{L'}} \right] \Bigg|_0^L \\
&= \frac{1}{\sqrt{LL'}} \left[ \sin \left( \pi - \frac{n' \pi L}{L'} \right) \frac{LL'}{\pi(L' - n'L)} - \sin \left( \pi + \frac{n' \pi L}{L'} \right) \frac{LL'}{\pi(L' + n'L)} \right] \\
&= \frac{\sqrt{LL'}}{\pi} \left[ \sin \left( \pi - \frac{n' \pi L}{L'} \right) \frac{1}{(L' - n'L)} - \sin \left( \pi + \frac{n' \pi L}{L'} \right) \frac{1}{(L' + n'L)} \right] \quad (4.35)
\end{aligned}$$

Making use of the fact that  $\sin(\pi - x) = \sin(x)$  and  $\sin(\pi + x) = -\sin(x)$  the expression above can be simplified to obtain

$$\begin{aligned}
&= \frac{\sqrt{LL'}}{\pi} \left[ \sin \left( \frac{n' \pi L}{L'} \right) \frac{1}{(L' - n'L)} + \sin \left( \frac{n' \pi L}{L'} \right) \frac{1}{(L' + n'L)} \right] \\
&= \frac{\sqrt{LL'}}{\pi(L^2 - n'^2 L^2)} \left[ \sin \left( \frac{n' \pi L}{L'} \right) (L' + n'L) + \sin \left( \frac{n' \pi L}{L'} \right) (L' - n'L) \right] \\
&= \frac{\sqrt{LL'}}{\pi(L^2 - n'^2 L^2)} \left[ 2 \sin \left( \frac{n' \pi L}{L'} \right) L' \right]. \quad (4.36)
\end{aligned}$$

Eq. (4.36) is exactly the expression given for the coefficients  $a_{n'}$ .

## C. Diagonalisation of the non-interacting Hamiltonian

Performing the elementary row operation  $1 - 4$  and  $2 - 3$  on the determinant given by Eq. (2.8)

$$\begin{vmatrix} 2h - \lambda & 0 & 0 & 2h + \lambda \\ g & -\lambda & 0 & g \\ g & 0 & -\lambda & g \\ 0 & g & g & -2h - \lambda \end{vmatrix} = 0$$

We obtain the following expression for the determinant

$$\begin{aligned}
& (2h - \lambda) \left[ -\lambda(2h\lambda + \lambda^2 - g^2) + \lambda g^2 \right] - (2h + \lambda) [\lambda g^2 + \lambda g^2] = 0 \\
& \Leftrightarrow (-4h^2 \lambda^2 - 2h\lambda^3 + 4h\lambda g^2 + 2h\lambda^3 + \lambda^4 - 2\lambda^2 g^2) - 4h\lambda g^2 - 2\lambda^2 g^2 = 0 \\
& \Leftrightarrow -4h^2 \lambda^2 + \lambda^4 - 4\lambda^2 g^2 = 0 \\
& \Leftrightarrow \lambda^2 (\lambda^2 - 4(h^2 + g^2)) = 0
\end{aligned}$$

Solving this equation for  $\lambda$  results in

$$\begin{aligned}
& \lambda^2 = 0 \quad \text{or} \quad \lambda^2 = 4(h^2 + g^2) \\
& \Leftrightarrow \lambda = 0 \quad \text{or} \quad \lambda = \pm 2\sqrt{(h^2 + g^2)}. \quad (4.37)
\end{aligned}$$

## D. Computation of the partial trace

To prove the equivalence between the definition given by Eq.(1.18) and the sum

$$Tr_B(\rho) = \sum_{j=1}^{d_A} (\mathbb{1}_A \otimes \langle b_j |) \rho (\mathbb{1}_A \otimes |b_j\rangle), \quad (4.38)$$

for the partial trace over subsystem B of a composite system AB we first need to rewrite the operator  $\hat{\rho}$  as

$$\hat{\rho} = (\mathbb{1}_A \otimes \mathbb{1}_B) \hat{\rho} (\mathbb{1}_A \otimes \mathbb{1}_B), \quad (4.39)$$

where  $\mathbb{1}_A$  and  $\mathbb{1}_B$  are the identity matrices on respectively on subsystem A and B. Let  $\{|a_j\rangle\}$  be a basis for  $\mathcal{H}_A$  and  $\{|b_k\rangle\}$  a basis for  $\mathcal{H}_B$  then we can rewrite the expression as

$$\hat{\rho} = \left( \sum_j^{d_a} |a_j\rangle \langle a_j| \otimes \sum_k^{d_b} |b_k\rangle \langle b_k| \right) \hat{\rho} \left( \sum_l^{d_a} |a_l\rangle \langle a_l| \otimes \sum_m^{d_b} |b_m\rangle \langle b_m| \right), \quad (4.40)$$

where we used the completeness relation [12]. We can now rewrite Eq. (4.40) further using the property  $(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$  from [20] of the Kronecker product.

$$\begin{aligned} \hat{\rho} &= \sum_{j,l}^{d_a} \sum_{k,m}^{d_b} \left[ |a_j\rangle \langle a_j| \otimes |b_k\rangle \langle b_k| \right] \hat{\rho} \left[ |a_l\rangle \langle a_l| \otimes |b_m\rangle \langle b_m| \right] \\ &= \sum_{j,l}^{d_a} \sum_{k,m}^{d_b} \left[ (|a_j\rangle \otimes |b_k\rangle \langle a_j| \otimes \langle b_k|) \right] \hat{\rho} \left[ (|a_l\rangle \otimes |b_m\rangle \langle a_l| \otimes \langle b_m|) \right] \\ &= \sum_{j,l}^{d_a} \sum_{k,m}^{d_b} \left( \left[ \langle a_j| \otimes \langle b_k| \hat{\rho} |a_l\rangle \otimes |b_m\rangle \right] (|a_j\rangle \otimes |b_k\rangle \langle a_l| \otimes \langle b_m|) \right) \\ &= \sum_{j,l}^{d_a} \sum_{k,m}^{d_b} \left( \left[ \langle a_j| \otimes \langle b_k| \hat{\rho} |a_l\rangle \otimes |b_m\rangle \right] |a_j\rangle \langle a_l| \otimes |b_k\rangle \langle b_m| \right). \end{aligned} \quad (4.41)$$

We can now apply the definition Eq. (1.18) to  $\hat{\rho}$  given by the expression Eq. (4.41)

$$Tr_B(\hat{\rho}) = Tr_B \left( \sum_{j,l}^{d_a} \sum_{k,m}^{d_b} \left( \left[ \langle a_j| \otimes \langle b_k| \hat{\rho} |a_l\rangle \otimes |b_m\rangle \right] |a_j\rangle \langle a_l| \otimes |b_k\rangle \langle b_m| \right) \right), \quad (4.42)$$

which using the linearity of the trace function is equal to

$$\begin{aligned} Tr_B(\hat{\rho}) &= \sum_{j,l}^{d_a} \sum_{k,m}^{d_b} \left[ \langle a_j| \otimes \langle b_k| \hat{\rho} |a_l\rangle \otimes |b_m\rangle \right] Tr_B \left( |a_j\rangle \langle a_l| \otimes |b_k\rangle \langle b_m| \right) \\ &= \sum_{j,l}^{d_a} \sum_{k,m}^{d_b} \left[ \langle a_j| \otimes \langle b_k| \hat{\rho} |a_l\rangle \otimes |b_m\rangle \right] |a_j\rangle \langle a_l| \underbrace{Tr_B \left( |b_k\rangle \langle b_m| \right)}_{=\delta_{km}} \\ &= \sum_{j,l}^{d_a} \sum_k^{d_b} \left[ \langle a_j| \otimes \langle b_k| \hat{\rho} |a_l\rangle \otimes |b_m\rangle \right] |a_j\rangle \langle a_l|. \end{aligned} \quad (4.43)$$

To carry out the last modifications we first need to prove that for any vectors  $|a\rangle, |a'\rangle \in \mathcal{H}_A$  and  $|b\rangle \in \mathcal{H}_B$  the relation

$$(|a\rangle \otimes |b\rangle) \langle a'| = |a\rangle \langle a'| \otimes |b\rangle. \quad (4.44)$$

Since all the vectors are finite dimensional this can be checked by explicitly writing out the matrix product. Taking the conjugate transpose of the above equality we can also obtain

$$|a'\rangle (\langle a| \otimes \langle b|) = |a'\rangle \langle a| \otimes \langle b| \quad (4.45)$$

Using these relations we can rewrite Eq.(4.43)

$$\begin{aligned} \hat{\rho} &= \sum_{j,l}^{d_a} \sum_k^{d_b} |a_j\rangle \left[ \langle a_j| \otimes \langle b_k| \hat{\rho} |a_l\rangle \otimes |b_m\rangle \right] \langle a_l| \\ &= \sum_k^{d_b} \sum_{j,l}^{d_a} \left[ \left( |a_j\rangle \langle a_j| \otimes \langle b_k| \right) \hat{\rho} \left( |a_l\rangle \langle a_l| \otimes |b_m\rangle \right) \right] \\ &= \sum_k^{d_b} \left[ \left( \sum_j^{d_a} |a_j\rangle \langle a_j| \otimes \langle b_k| \right) \hat{\rho} \left( \sum_l^{d_a} |a_l\rangle \langle a_l| \otimes |b_m\rangle \right) \right] \\ &= \sum_{j=1}^{d_A} (\mathbb{1}_A \otimes \langle b_j|) \hat{\rho} (\mathbb{1}_A \otimes |b_j\rangle), \end{aligned} \quad (4.46)$$

where we used the completeness relations in the last equation.

## E. Schmidt decomposition theorem

The derivation of the theorem follows the reasoning from [30]. Consider an arbitrary pure state  $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ . Let the set  $\{|j_A\rangle | 1 \leq j \leq d_A = \dim(\mathcal{H}_A)\}$  be an orthonormal basis for  $\mathcal{H}_A$  and the set  $\{|k_B\rangle | 1 \leq k \leq d_B = \dim(\mathcal{H}_B)\}$  an orthonormal basis for  $\mathcal{H}_B$ . It follows [29] that the set  $\{|i_A\rangle \otimes |i_B\rangle | 1 \leq i \leq d_A, 1 \leq j \leq d_B\}$  will be an orthonormal basis for  $\mathcal{H}_A \otimes \mathcal{H}_B$  and we can therefore write

$$|\psi\rangle = \sum_{j=1}^{d_A} \sum_{k=1}^{d_B} \alpha_{jk} |j_A\rangle |k_B\rangle, \quad (4.47)$$

where  $\alpha_{jk} \in \mathbb{C}$ . We can then write the coefficients out in a matrix  $A$  as follows

$$[A]_{jk} = \alpha_{jk}. \quad (4.48)$$

The matrix  $A$  is therefore of size  $d_A \times d_B$ . We can now use the singular value decomposition of a complex that states it is possible to write the matrix  $A$  as

$$A = U \Lambda V, \quad (4.49)$$

where  $U$  is a  $d_A \times d_A$  unitary matrix,  $V$  a  $d_B \times d_B$  unitary matrix and  $\Lambda$  a  $d_A \times d_B$  rectangular diagonal matrix with  $d \leq \min\{d_A, d_B\}$  real ‘diagonal’ elements. The product  $U\Lambda$  written in terms of the coefficient is

$$\begin{aligned} [U\Lambda]_{ji} &= \sum_{l=1}^{d_a} u_{jl} \Lambda_{li} \\ &= \sum_{l=1}^d u_{jl} \delta_{lm} \Lambda_{ii} = u_{ji} \Lambda_{ii}. \end{aligned} \quad (4.50)$$

Eq. (4.49) becomes

$$\begin{aligned}\alpha_{jk} &= \sum_{i=1}^{d_b} (U\Lambda)_{ji} v_{ik} \\ &= \sum_{i=1}^d u_{ji} \Lambda_{ii} v_{ik}.\end{aligned}\tag{4.51}$$

Replacing the coefficient  $\alpha_{jk}$  in Eq. (4.47):

$$\begin{aligned}|\psi\rangle &= \sum_{j=1}^{d_A} \sum_{k=1}^{d_B} \left( \sum_{i=1}^d u_{ji} \Lambda_{ii} v_{ik} \right) |j_A\rangle |k_B\rangle \\ &= \sum_{i=1}^d \Lambda_{ii} \left( \sum_{j=1}^{d_A} u_{ji} |j_A\rangle \right) \otimes \left( \sum_{k=1}^{d_B} v_{ik} |k_B\rangle \right)\end{aligned}\tag{4.52}$$

By defining the states  $|i_A\rangle := \sum_{j=1}^{d_A} u_{ji} |j_A\rangle$  and  $|i_B\rangle := \sum_{k=1}^{d_B} v_{ik} |k_B\rangle$ , which are orthogonal since  $U$  and  $V$  where unitary matrices and the states  $|j_A\rangle$  and  $|k_B\rangle$  were an orthonormal basis, we obtain the desired result:

$$|\psi\rangle = \sum_{i=1}^d \Lambda_{ii} |i_A\rangle \otimes |i_B\rangle.\tag{4.53}$$



## References

- [1] E. Schrödinger, Mathematical Proceedings Of The Cambridge Philosophical Society 32, 446 (1936).
- [2] J. Latorre, E. Rico and G. Vidal, Quantum Information & Computation 4, 48 (2004).
- [3] S. Sachdev, Quantum Phase Transitions (Cambridge University Press, Cambridge, 2011).
- [4] T. J. Osborne and M. A. Nielsen, Quantum Inf. Process. 1, 45 (2002).
- [5] Y. Chen, P. Zanardi, Z. D. Wang, and F. C. Zhang, 2006, New J. Phys. 8, 97 (2006).
- [6] A. Osterloh, L. Amico, G. Falci and R. Fazio, Nature 416, 608 (2002).
- [7] M. Nielsen and I. Chuang, Quantum Computation And Quantum Information (Cambridge University Press, Cambridge, 2018).
- [8] J. Ren, P. Xu, H. Yong, L. Zhang, S. Liao, J. Yin, W. Liu, W. Cai, M. Yang, L. Li, K. Yang, X. Han, Y. Yao, J. Li, H. Wu, S. Wan, L. Liu, D. Liu, Y. Kuang, Z. He, P. Shang, C. Guo, R. Zheng, K. Tian, Z. Zhu, N. Liu, C. Lu, R. Shu, Y. Chen, C. Peng, J. Wang and J. Pan, Nature 549, 70 (2017).
- [9] X. Ma, T. Herbst, T. Scheidl, D. Wang, S. Kropatschek, W. Naylor, B. Wittmann, A. Mech, J. Kofler, E. Anisimova, V. Makarov, T. Jennewein, R. Ursin and A. Zeilinger, Nature 489, 269 (2012).
- [10] H. Kim and D. A. Huse, Phys. Rev. Lett. 111, 127205 (2013).
- [11] V. Alba and P. Calabrese, Proceedings Of The National Academy Of Sciences 114, 7947 (2017).
- [12] J. Sakurai and S. Tuan, Modern Quantum Mechanics (Addison-Wesley Longman, Reading, Mass., 1994).
- [13] J. Maziero, International Journal Of Modern Physics C 28, 1750005 (2017).
- [14] R. Coldea, D. Tennant, E. Wheeler, E. Wawrzynska, D. Prabhakaran, M. Telling, K. Habicht, P. Smeibidl and K. Kiefer, Science 327, 177 (2010).
- [15] J. Latorre and A. Riera, Journal Of Physics A: Mathematical And Theoretical 42, 50 (2009).
- [16] P. Calabrese , and J. Cardy, Journal of Statistical Mechanics: Theory and Experiment 0504, 04010 (2005).
- [17] E. Lieb, T. Schultz and D. Mattis, Annals Of Physics 16, 407 (1961).
- [18] S. Suzuki, J. Inoue and B. Chakrabarti, Quantum Ising Phases And Transitions In Transverse Ising Models (Springer, Berlin, 2013).
- [19] D. Griffiths, Introduction To Quantum Mechanics (Pearson Prentice Hall, Upper Saddle River, 2005).
- [20] R. Horn and C. Johnson, Matrix Analysis (Cambridge Univ. Press, Cambridge, 1999), pp. 242-244.
- [21] M. Nielsen. "The Fermionic canonical commutation relations and the Jordan-Wigner transform." School of Physical Sciences The University of Queensland (2005)

- [22] M. Fagotti and P. Calabrese, Physical Review A 78, 010306 (2008).
- [23] P. Calabrese, F. Essler and M. Fagotti, Journal Of Statistical Mechanics: Theory And Experiment, P07016 (2012).
- [24] P. Calabrese, F. Essler and M. Fagotti, Physical Review Letters 106, 227203 (2011).
- [25] <https://hpc.vub.be/hydra.php> (2019).
- [26] D. Page, Phys. Rev. Lett. 71, 1291 (1993).
- [27] S. Caenepeel, Analyse: Afleiden, Integreren, Wiskundige Software, Formularium Analyse (2017).
- [28] S. Suzuki, J. Inoue and B. Chakrabarti, Quantum Ising Phases And Transitions In Transverse Ising Models (Springer, Berlin, 2013).
- [29] Prof. E. Jespers, Ring- en Modultheorie (VUB, 2018-2019)
- [30] M. Wilde, Quantum Information Theory, 2nd ed. (Cambridge University press, Cambridge, 2017), pp. 98-99.