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Simulating multi-qubit Heisenberg XY interaction entanglement

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Abstract

Quantum computation is on her way to change the fields of physics and chemistry. Within quantum computation, decoherence is one of the biggest challenges. A method to tackle decoherence is by replacing the old fashioned way of entangling with CNOT gates. Entangling multiple qubits with a single operation, reduces operation time and the number of operations. The idea has been mentioned by for example *Kandala et al.* They state a quantum processor to be more efficient utilizing the naturally available interactions possessed by the system itself.

In this thesis entanglement properties of Heisenberg XY interactions are investigated. This is done in two different ways. The first method has been set up by *Zhang et al.* for three qubits and a generalization of his method is discussed. This is proven to be an incorrect manner of solving systems with more than three qubits. The second method of solving the Schrödinger equation and the belonging differential equations for multi-qubit systems with the Heisenberg XY interaction is also discussed and simulated. This results in oscillating states for which entanglement is checked. Lastly, a boundary condition is applied to a four qubit system. This boundary condition connects the first to the last qubit as if they are positioned in a circle. Adding this boundary condition changes the evolution of the system however still creates entanglement.

Contents

Chapter 1

Introduction

Computers have revolutionized society and science. Since the first version of the classical computer, the Turing machine, computers have made steady advancement throughout the years. Computing power of these machines got its own theory in 1972 by Gordon Moore, Moores law, predicting future capabilities of these classical computing machines. Up until now Moores law has been proven to be true [1]. However, Moores law is meeting its limit due to physical limits belonging to the chip industry.

The capabilities of the computers as we know them are immense. Scientific simulations can be run in seconds, which opened new doors for science. Yet, some scientific fields run simulations not capable for these machines. The problem cannot be expressed in the means of the classical computers, bits [2]. For example, finding the prime factors for very large integers or problems where quantum mechanics play a role.

A machine to deal with this problem has been suggested in the 50's by Richard Feynman[3] and later by Paul Benioff and Yuri Manin in more detail. A processor based on the principles of quantum-mechanical phenomena such as superposition and entanglement. Using quantum mechanics within the processor allows for smarter algorithms to solve these difficult problems.

Using the quantum computer brings new challenges such as error rates and decoherence. The quantum bits, or qubits in short, used to calculate can only be used for a very short period of time. Therefore, preparing a state must take as short as possible to save time to do the actual calculation. An important aspect of preparation is creating entanglement in the system.

Kandala et al. [4] mentions an entanglement operation utilizing natural interactions present in the system. Therefore minimizing gate operations and operation times. This can play an important role in the reduction of decoherence within a quantum computer.

One of these natural existing interactions is the Heisenberg XY interaction. *K. Groenland and K Schoutens* [5] show the number of 2-qubit and single qubit gates needed for certain operations can be reduced with the help of this interaction. Furthermore, the interaction can be used to create iSWAP gates [6].

In this paper, entanglement properties of the Heisenberg XY interaction has been studied. In chapter 2, introductory information is provided. In chapter 3, a known method for three-qubit entanglement is given and generalization is tried. A simulation of this generalization is made showing inconsistency. In chapter 4, a different approaches is discussed and simulated. Moreover, for these results the presence of entanglement is checked. Lastly, in chapter 5, a conclusion of the results is given with recommendations and an outlook.

Chapter 2

Quantum computation

2.1 Schrödinger equation

The Schrödinger equation is an equation to describe the changes over time of a physical system in which quantum effects are significant. These systems are referred to as quantum (mechanical) systems. The form of the Schrödinger equation depends on the physical situation. The most general form is the time-dependent Schrödinger equation, which gives a description of a system evolving with time,

$$i\hbar\frac{\partial}{\partial t}|\Psi(\mathbf{r},t)\rangle = \hat{H}|\Psi(\mathbf{r},t)\rangle \tag{2.1}$$

where i is the imaginary unit and $\hbar$ is the reduced Planck constant which is equal to the Planck constant divided by 2π, $\frac{\partial}{\partial t}$ indicate the partial derivative with respect to time, Ψ is the wave function of the quantum system, $\mathbf{r}$ and t are the position vector and time respectively and $\hat{H}$ is the hamiltonian operator. In the systems discussed here the position vector does not play a role reducing $\Psi(\mathbf{r},t)$ to $\psi(t)$ in equation 2.1.

2.2 Qubit

Compared to the classical computers' bits, the quantum computer uses qubits. A qubit is the basic unit of quantum information. The information is described by a two state quantum-mechanical system. The quantum-mechanical system allows the qubit to be in a superposition of both states at the same time. The states are usually denoted as

$$|0\rangle = \begin{bmatrix}1\\0\end{bmatrix} \tag{2.2}$$

$$|1\rangle = \begin{bmatrix}0\\1\end{bmatrix} \tag{2.3}$$

These two basis states are said to span the two-dimensional linear vector space of the qubit and can be represented as follows,

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \tag{2.4}$$

where α and β are probability amplitudes and can be complex numbers. According to the Born rule, the probability of measuring the qubit in state $|0\rangle$ is $|\alpha|^2$ and the probability of measuring the qubit in state $|1\rangle$ is $|\beta|^2$. Because the absolute squares of the amplitudes equate to probabilities, it follows that α and β are constrained by the equation

$$\alpha^2 + \beta^2 = 1 \tag{2.5}$$

Qubit basis states can also be combined to form product basis states. The combined state is equal to the tensor product of the constituent qubits. If we take qubit 1, $\begin{bmatrix}\alpha\\ \beta\end{bmatrix}$, and qubit 2, $\begin{bmatrix}\kappa\\ \tau\end{bmatrix}$, the corresponding two-qubit state can be determined by

$$\begin{bmatrix}\alpha\\ \beta\end{bmatrix} \otimes \begin{bmatrix}\kappa\\ \tau\end{bmatrix} = \begin{bmatrix}\alpha \begin{bmatrix}\kappa\\ \tau\end{bmatrix}\\ \\ \beta \begin{bmatrix}\kappa\\ \tau\end{bmatrix}\end{bmatrix} = \begin{bmatrix}\alpha\kappa\\ \alpha\tau\\ \beta\kappa\\ \beta\tau\end{bmatrix} \tag{2.6}$$

Following the operation in equation 2.6, two qubits can be represented in a four-dimensional linear vector space spanned by the following basis states

$$|00\rangle = \begin{bmatrix}1\\0\\0\\0\end{bmatrix}, |01\rangle = \begin{bmatrix}0\\1\\0\\0\end{bmatrix}, |10\rangle = \begin{bmatrix}0\\0\\1\\0\end{bmatrix}, |11\rangle = \begin{bmatrix}0\\0\\0\\1\end{bmatrix} \tag{2.7}$$

Adding probability coefficients to the basis states, the system can be expressed as a combination of the basis states. This can be represented by a matrix containing the coefficients per basis state

$$\psi = \nu_{00}|00\rangle + \nu_{01}|01\rangle + \nu_{10}|10\rangle + \nu_{11}|11\rangle = \begin{bmatrix}\nu_{00}\\ \nu_{01}\\ \nu_{10}\\ \nu_{11}\end{bmatrix} \tag{2.8}$$

Entanglement check

If multiple states are present at a certain time, the system does not necessarily have to be entangled. Entanglement can be checked by trying to write the system as tensor products. For a two-qubit system the total system is described by a tensor product of the separate qubits as can be seen in equation 2.6. If we multiply the coefficient of state $|00\rangle$, $\alpha\kappa$, with the coefficient of state $|11\rangle$, $\beta\tau$, we find a combination of all one-qubit coefficients $\alpha\beta\kappa\tau$. The same can be done multiplying the coefficients of states $|01\rangle$ and $|10\rangle$. Both multiplications give $\alpha\beta\kappa\tau$, however, they do not have to be the same. If the multiplications of the same terms do not yield the same value, then the information within the system is not confined to any of the qubits individually, but is in the correlation between the states.

2.2.1 The Bloch Sphere

The Bloch Sphere can be used to visualize the quantum state of a two-level quantum system. Equation 2.4 seems to be having four degrees of freedom. However, one degree of freedom can be eliminated by the constraint described in equation 2.5. The result can now be described by Hopf coordinates. Furthermore, the overall phase of a single qubit has no observable consequence resulting in two degrees of freedom,

$$\alpha = \cos\frac{\theta}{2}, \quad \beta = e^{i\phi}\sin\frac{\theta}{2} \tag{2.9}$$

where $e^{i\phi}$ is the relative phase. As can be seen in Figure 2.1 the parameters ϕ and θ describe a unique point on the unit sphere. In this representation the state $|0\rangle$ is mapped onto the northpole and $|1\rangle$ is mapped onto the Southpole.

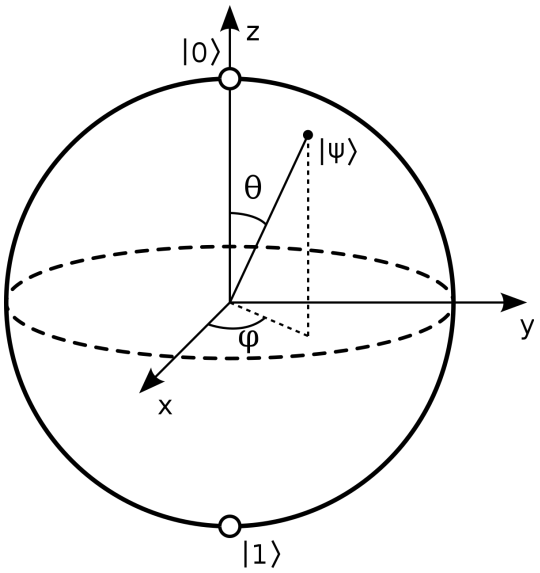

Figure 2.1: The Bloch Sphere as a visualization of a two level system, where the states $|0\rangle$ and $|1\rangle$ are assigned to the north and south pole respectively. Source: Wikipedia

2.3 Quantum gates

Where classical computing uses logic gates to process information quantum computation uses quantum gates to do the same to information within the quantum state.

A quantum logic gate is represented by a unitary matrix. A matrix U is unitary when its conjugate is also its own inverse so if $U^*U = UU^* = I$, where I is the identity matrix. The identity matrix is a representation of the gate that maps every state to itself. A quantum gate can be described by a 2^n by 2^n size matrix, where n is the number of qubits the gate must act upon. The variables that the gate acts upon, the quantum states, is a vector in 2^n complex dimensions, where n again is the number of qubits. The base vectors are the possible outcomes if the state is measured.

There are 3 Pauli gates, Pauli-X, Pauli-Y and Pauli-Z. The Pauli X gate is the equivalent of the classical NOT gate and acts on a single qubit. It maps the $|0\rangle$ state to $|1\rangle$ and state $|1\rangle$ to $|0\rangle$. This can be visualized by a rotation of π radians around the X-axis of the Bloch Sphere. The Pauli-X gate is represented by the Pauli X matrix,

$$X \; or \; \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{2.10}$$

The Pauli-Y gate maps the $|0\rangle$ state to $i|1\rangle$ and $|1\rangle$ to $i|0\rangle$. This gate can be visualized by a rotation around the Y-axis of the Bloch Sphere of π radians. The gate is represented by the Pauli-Y matrix,

$$Y \; or \; \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \tag{2.11}$$

Lastly the Pauli-Z gate leaves the state $|0\rangle$ as it is and maps $|1\rangle$ to -$|1\rangle$. It equates to a rotation of π radians around the Z axis of the Bloch Sphere. This gate can be represented by the Pauli-Z matrix,

$$Z \; or \; \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{2.12}$$

If a quantum gate applies on $m < n$ qubits in the set, we will have to extend the gate to take all n qubits. This can be done by combining the gate with an identity matrix such that their tensor product becomes a gate acting on all n qubits.

2.4 Heisenberg XY interaction

Interactions between qubits are necessary for quantum computation. The Heisenberg interactions are naturally existing interactions in spin systems. *Di Vincenzo et al.*[7] even state that the Heisenberg interaction can be universal for quantum computation.

The Heisenberg interaction Hamiltonian is given by

$$\hat{H}^n = \frac{1}{2}\sum_{j=1}^{n}(J_x\sigma_x^j\sigma_x^{j+1} + J_y\sigma_y^j\sigma_y^{j+1} + J_z\sigma_z^j\sigma_z^{j+1} + h\sigma_z^j) \tag{2.13}$$

where J_x, J_y and J_z are coupling constants and σ_x^j, σ_y^j and σ_z^j are the Pauli matrices defined in equation 2.10 till 2.12 acting on qubit j. The h on the right indicates the external magnetic fields.

It has been simulated by *Zhang et al.*[8] that the Heisenberg XY nearest-neighbor interaction can be used to entangle a system of three qubits which will be discussed in the next chapter. Furthermore *K. Koteswara Rao and A. Kumar*[9] analyzed this simulation and the entanglement within the system. Showing entanglement measurements and describing the entanglement dynamics.

The nearest-neighbor Heisenberg XY interaction can be found by setting the J_z coupling constant and h to "0" and equalling $J_x = J_y$ in equation 2.13. This results in a 2D system without interaction of external magnetic fields,

$$\hat{H}_{XY}^n = \frac{1}{2}J\sum_{j=1}^{n-1}(\sigma_x^j\sigma_x^{j+1} + \sigma_y^j\sigma_y^{j+1}) \tag{2.14}$$

This type of interaction can as stated by *N. Schuch and J. Siewert* [6] be used for quantum dot spins coupled by a cavity [10], for Josephson charge qubits coupled by Josephson junctions [11], and for nuclear spins interacting via a two-dimensional electron gas [12].
An extreme example of strong natural interaction can be found with Rydberg atoms. Coherent control of these interactions combined with their relatively long lifetime makes them a suitable candidate to realize a quantum computer[13]. Therefore the applications of these atoms are also being studied at the TU/e within the Coherence and Quantum Technology group.

These hamiltonians can easily be expressed in matrix terms as they are build by the Pauli-matrices. For $n = 3$ the Heisenberg XY nearest-neighbor interaction given above in equation 2.14 can be defined by a matrix as

$$\hat{H}_{XY}^3 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{1} & 0 & 0 & \mathbf{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 \\ 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbf{1} & 0 & 0 & \mathbf{1} & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \tag{2.15}$$

For $n = 4$ the matrix defined by equation 2.14 is as follows

$$\hat{H}^4_{XY} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{1} & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbf{1} & 0 & 0 & \mathbf{1} & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & \mathbf{1} & 0 & 0 & \mathbf{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & \mathbf{1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \tag{2.16}$$

Chapter 3

Multi-qubit entanglement with Heisenberg XY interaction by Zhang et al.

3.1 3 qubit XY interaction

For 3 qubits as discussed by *Zhang et al.* the neighboring Heisenberg interaction is given by

$$\hat{H}^3_{XY} = \frac{1}{2}J(\sigma^1_x\sigma^2_x + \sigma^1_y\sigma^2_y + \sigma^2_x\sigma^3_x + \sigma^2_y\sigma^3_y) \tag{3.1}$$

where $\sigma^i_{x/y}$ are Pauli matrices acting on qubit i. The evolution caused by this hamiltonian can be expressed as

$$U(t) = e^{-i\hat{H}^3_{XY}t/\hbar} \tag{3.2}$$

here t is the time for the system to evolve and $\hbar$ is the reduced Planck constant. After which they introduce two operators $A = (\sigma^1_x\sigma^2_x + \sigma^2_y\sigma^3_y)/2$ and $B = (\sigma^1_y\sigma^2_y + \sigma^2_x\sigma^3_x)/2$ so $U(t)$ can be written as $U_A(t)\, U_B(t)$, where

$$U_A(t) = e^{-iJtA/\hbar} \equiv e^{-iJt(\sigma^1_x\sigma^2_x+\sigma^2_y\sigma^3_y)/2\hbar} \tag{3.3}$$

$$U_B(t) = e^{-iJtB/\hbar} \equiv e^{-iJt(\sigma^1_y\sigma^2_y+\sigma^2_x\sigma^3_x)/2\hbar} \tag{3.4}$$

Then they define three operators to solve $U_A(t)$ which can be viewed as three components of an angular momentum vector L^A because they satisfy the corresponding angular momentum commutation relations. Using these operators $U_A(t)$ can be written as

$$U_A(t) = e^{-iJt(L^A_x+L^A_y)/\hbar} = e^{-i(\sqrt{2}Jt/\hbar)L^A\cdot\mathbf{n}} \tag{3.5}$$

Where $\mathbf{n}$ is a unit vector defined by $(1/\sqrt{2}, 1/\sqrt{2}, 0)$ and denotes the rotation axis of $U_A(t)$. Applying a rotation around an arbitrary axis can be described as

$$e^{i\theta M} = \cos\theta I - i\sin\theta M \tag{3.6}$$

if M satisfies the relation $M^2 = I$. For our operator A described by equation 3.3 a rotation around the $\mathbf{n}$ axis will result in

$$U_A(t) = \cos\left(\frac{Jt}{\hbar\sqrt{2}}\right)I - \frac{i}{\sqrt{2}}\sin\left(\frac{Jt}{\hbar\sqrt{2}}\right)(\sigma^1_x\sigma^2_x + \sigma^2_y\sigma^3_y) \tag{3.7}$$

as $[(\sigma_x^1\sigma_x^2 + \sigma_y^2\sigma_y^3)/\sqrt{2}]^2 = 1$. The same steps can be taken for B, this will result in

$$U_B(t) = \cos\left(\frac{Jt}{\hbar\sqrt{2}}\right)I - \frac{i}{\sqrt{2}}\sin\left(\frac{Jt}{\hbar\sqrt{2}}\right)(\sigma_y^1\sigma_y^2 + \sigma_x^2\sigma_x^3) \tag{3.8}$$

After multiplication of $U_A(t)$ and $U_B(t)$ in the forms of equations 3.7 and 3.8 we obtain the following matrix

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \cos(x)^2 & -\frac{\sin(2x)\,i}{\sqrt{2}} & 0 & -\sin(x)^2 & 0 & 0 & 0 \\ 0 & -\frac{\sin(2x)\,i}{\sqrt{2}} & \cos(2x) & 0 & -\frac{\sin(2x)\,i}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \cos(x)^2 & 0 & -\frac{\sin(2x)\,i}{\sqrt{2}} & -\sin(x)^2 & 0 \\ 0 & -\sin(x)^2 & -\frac{\sin(2x)\,i}{\sqrt{2}} & 0 & \cos(x)^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sin(2x)\,i}{\sqrt{2}} & 0 & \cos(2x) & -\frac{\sin(2x)\,i}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & -\sin(x)^2 & 0 & -\frac{\sin(2x)\,i}{\sqrt{2}} & \cos(x)^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \tag{3.9}$$

3.2 Multi-qubit XY interaction

To generalize the solution given in equation 3.9 to a solution for more than three qubits, the general Heisenberg XY interaction hamiltonian of a system is given by 2.14. For this Hamiltonian it seems impossible to find operators to split the Hamiltonian to small parts as has been done by *Zhang et al.* The σ_x and σ_y operator pairs in the middle must be shared with both neighbors while the interaction with the first and last qubit are not shared. The middle terms are given by

$$(\sigma_y^{j-1}\sigma_y^j + \sigma_x^j\sigma_x^{j+1})/4 \text{ and } (\sigma_x^j\sigma_x^{j+1} + \sigma_y^{j+1}\sigma_y^{j+2})/4 \tag{3.10}$$

which share the $\sigma_x^j\sigma_x^{j+1}$ term. This needs to be compensated by dividing by 4 to end with the factor $\frac{1}{2}$ in front of equation 2.14. Whereas the terms in the beginning and the end of the spin chain do not have to be shared, as can bee seen

$$(\sigma_y^1\sigma_y^2 + \sigma_x^2\sigma_x^3)/4 \text{ and } (\sigma_x^1\sigma_x^2 + \sigma_y^2\sigma_y^3)/4 \tag{3.11}$$

This results in a shortage of the $\sigma_{x/y}^1\sigma_{x/y}^2$ terms since the $\sigma_{x/y}^2\sigma_{x/y}^3$ terms need the factor $\frac{1}{4}$ as mentioned already. It is clear that a boundary condition must be set to add the missing terms. This can be done by placing the spins in a circle instead of a straight line. Hereby we give the first and last spin of the former system the ability to interact with each other. The Hamiltonian will therefore change to

$$\hat{H}_{XY}^n = \frac{1}{2}J\sum_{j=1}^{n}(\sigma_x^j\sigma_x^{j+1} + \sigma_y^j\sigma_y^{j+1}) \tag{3.12}$$

where $\sigma_{x/y}^{n+1} = \sigma_{x/y}^1$. This results in $2n$ operators to work out. Hereby $U(t)$ can be written as $U_A(t)\ U_B(t)\ldots U_{2n}(t)$ where the operators A up until $2n$ are described in equations 3.10 and 3.11. For all operators A to $2n$ it is possible to define 3 operators L_x^i, L_y^i and L_z^i which satisfy the angular momentum commutation relations. By defining the operations as

$$U_j(t) = e^{-i(\frac{Jt}{2\hbar})(\sigma_x^j\sigma_x^{j+1} + \sigma_y^k\sigma_y^l)/2} \tag{3.13}$$

where only $\sigma_y^k\sigma_y^l = \sigma_y^{j-1}\sigma_y^j$ and $\sigma_y^k\sigma_y^l = \sigma_y^{j+1}\sigma_y^{j+2}$ are allowed, one can follow the steps taken by *Zhang et al.* with a small change in front of the Pauli terms. This will result in a change of the angle as defined in equation 3.6. Which will develop into a combination of operations in line with

$$\begin{aligned} U_{j+}(t) &= \cos\left(\frac{Jt}{2\hbar\sqrt{2}}\right)I - \frac{i}{\sqrt{2}}\sin\left(\frac{Jt}{2\hbar\sqrt{2}}\right)(\sigma_x^j\sigma_x^{j+1} + \sigma_y^{j+1}\sigma_y^{j+2}) \\ U_{j-}(t) &= \cos\left(\frac{Jt}{2\hbar\sqrt{2}}\right)I - \frac{i}{\sqrt{2}}\sin\left(\frac{Jt}{2\hbar\sqrt{2}}\right)(\sigma_x^j\sigma_x^{j+1} + \sigma_y^{j-1}\sigma_y^j) \end{aligned} \tag{3.14}$$

By multiplying all allowed terms described in equation 3.14, $U(t)$ can be found

$$U(t) = \prod_{j=1}^{n} U_{j+}(t)\, U_{j-}(t) \tag{3.15}$$

As one can notice, the operators defined in the beginning by equation 3.10 do not commute with all other operators. This results in multiple evolutions for one hamiltonian as will be shown in the next section. Therefore, the steps taken by *Zhang et al.* are only applicable to systems of 3 qubits and can not be used for larger systems.

3.3 4 qubit simulation by Zhang plan

For a system of 4 qubits in a circle, the hamiltonian of the Heisenberg XY interaction is given by

$$\hat{H}_{XY}^4 = \frac{1}{2}J(\sigma_x^1\sigma_x^2 + \sigma_y^1\sigma_y^2 + \sigma_x^2\sigma_x^3 + \sigma_y^2\sigma_y^3 + \sigma_x^3\sigma_x^4 + \sigma_y^3\sigma_y^4 + \sigma_x^4\sigma_x^1 + \sigma_y^4\sigma_y^1) \tag{3.16}$$

The time evolution of three different multiplication orders is visualized in figure 3.1. For all three evolutions the input state $\psi = \frac{1}{\sqrt{2}}(|0001\rangle + |0011\rangle)$ is taken. The multiplication orders of the figures are:

$$\begin{aligned} &\textit{Figure } 3.1a : U_{1+}(t)\, U_{1-}(t)\, U_{2+}(t)\, U_{2-}(t)\, U_{3+}(t)\, U_{3-}(t)\, U_{4+}(t)\, U_{4-}(t), \\ &\textit{Figure } 3.1b : U_{2+}(t)\, U_{2-}(t)\, U_{4+}(t)\, U_{4-}(t)\, U_{3+}(t)\, U_{3-}(t)\, U_{1+}(t)\, U_{1-}(t), \\ &\textit{Figure } 3.1c : U_{3+}(t)\, U_{3-}(t)\, U_{2+}(t)\, U_{2-}(t)\, U_{1+}(t)\, U_{1-}(t)\, U_{4+}(t)\, U_{4-}(t) \end{aligned} \tag{3.17}$$

Here the x-axis is given as a unit of time where x is equal to $\frac{Jt}{2\hbar\sqrt{2}}$. On the y-axis the probability of the different states are plotted.

As can be seen in the legend of figure 3.1 all the present states through time contain the same number of 1's and 0's as the input state. It has been known that the Heisenberg XY interaction can be used to perform Swap operations [14].

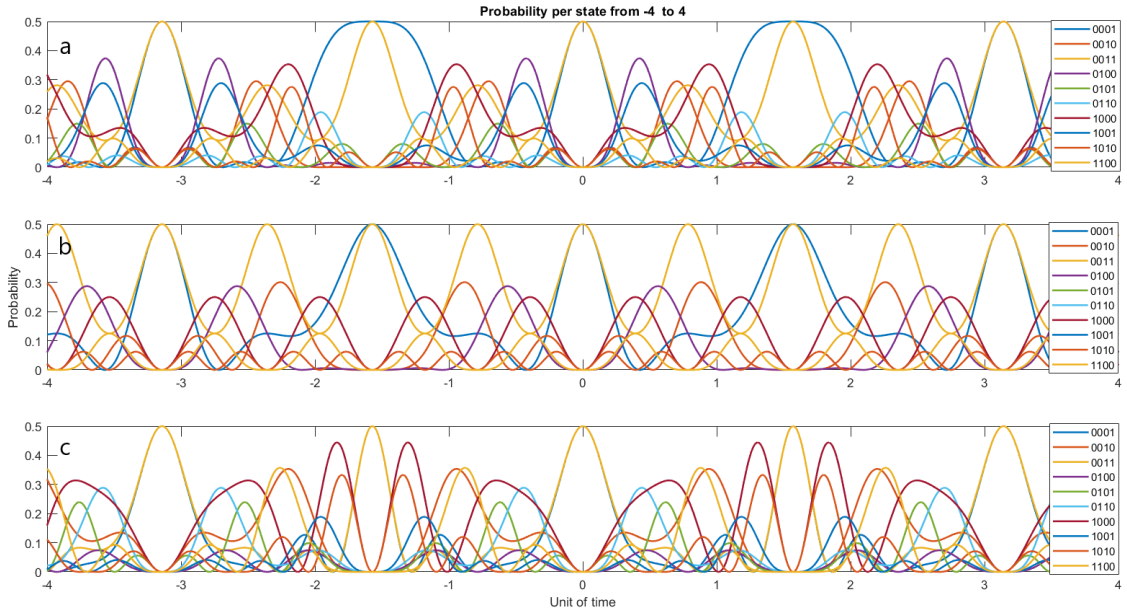

Figure 3.1: The evolution of the same four qubit hamiltonian as described by equation 3.16, with input state $|\psi\rangle = \frac{1}{\sqrt{2}}(|0001\rangle + |0011\rangle)$ for 3 different multiplication orders described by equation 3.17

Chapter 4

Multi-qubit entanglement with Heisenberg XY interaction by solving the Schrödinger equation

The system can also be evaluated by the Schrödinger equation shown in equation 2.1. For $\hat{H}$ the hamiltonian described by equation 2.14 or equation 3.12 must be taken. The matrix form of the hamiltonian is given in equation 2.15 and equation 2.16 for 3 and 4 qubits respectively.

By substituting $\hat{H}$ and ψ into the Schrödinger equation in matrix form, where the matrix for ψ is described by equation 2.8, a set of 2^n linked differential equation can be found. Solving these differential equation results in the time evolution of the system described by the hamiltonian. This can be done for any number of qubits.

Solving these differential equations can best be done by Mathematica. The scripts used to solve these differential equations can be found in the appendix. In order to export the answers from Mathematica to MATLAB one must use the "ToMatlab"[15] program developed by *Harri Ojanen* in 1999. Adjusting some of the outdated MATLAB operations to newer versions allows for perfect transfer of information.

The solutions to the differential equation need to be evaluated as they are not immediately values of the operator $U(t)$. The manner of organizing the information imported from Mathematica can be found in the Appendix.

4.1 Validation of solving via differential equations

A simple check of the model can be done by comparing the results for three qubits with results generated by the matrix provided by *Zhang et al.* This comparison is shown in figure 4.1. As can clearly be seen, the system evolves the same. Therefore we can conclude the evolution resulted by solving the Schrödinger equation to be correct.

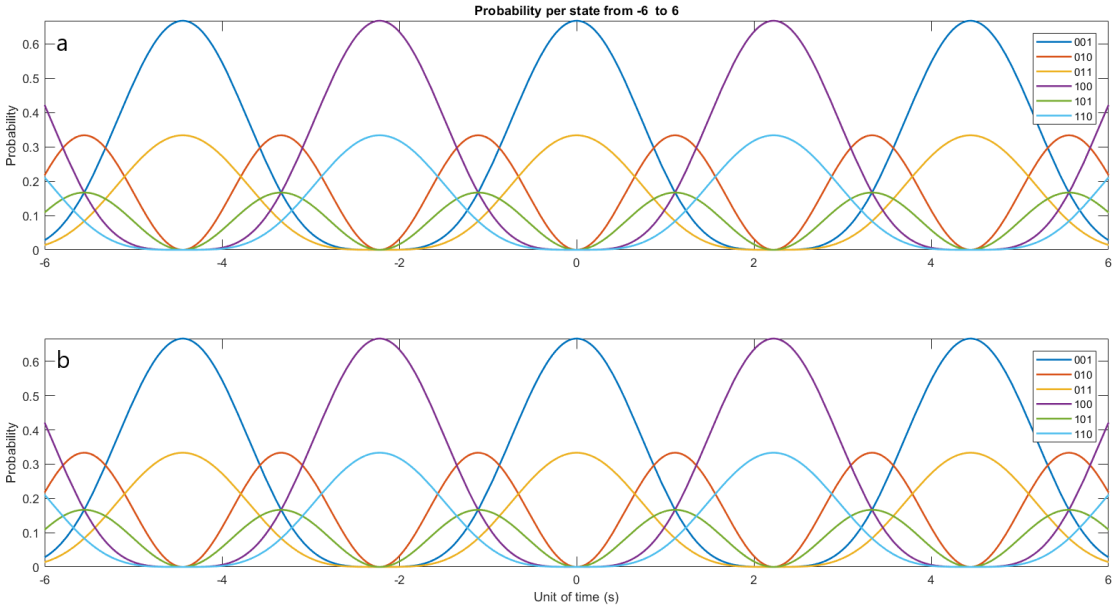

Figure 4.1: The evolution of a three qubit system with input state $|\psi\rangle = \sqrt{\frac{2}{3}}|001\rangle + \sqrt{\frac{1}{3}}|011\rangle$ through time for solutions to a.) the Schrödinger equation and b.) the matrix provided by Zhang.

4.2 Multi-qubit evolution simulations

The procedure described above can be followed for more than three qubits. However, it must be mentioned that the complexity of the system grows exponentially. The amount of differential equations and the complexity of these equations rise by raising the number of qubits in the system. This results in tremendous calculating times. Therefore, systems up until 5 qubits are investigated.

For three, four and five qubits the differential equations have been defined and solved. For solving the differential equations the coupling constant, J, and the reduced Planck constant, $\hbar$, have both been set to 1. The evolutions caused by the hamiltonian described in equation 2.14 for $n = 3$, $n = 4$ and $n = 5$ have been plotted in figure 4.2. The evolutions start with the input states $|\psi\rangle = \frac{1}{\sqrt{2}}(|001\rangle + |011\rangle)$ for $n = 3$, $|\psi\rangle = \frac{1}{\sqrt{2}}(|0001\rangle + |0011\rangle)$ for $n = 4$ and $|\psi\rangle = \frac{1}{\sqrt{2}}(|00001\rangle + |00011\rangle)$ for $n = 5$.

As with the evolution build via the Zhang method, these evolutions have the same states present in time. The evolutions visualized in figure 4.2 only contain states with the same numbers of 1's and 0's as the initial state. In the case of figure 4.2 these are states containing one or two 1's.

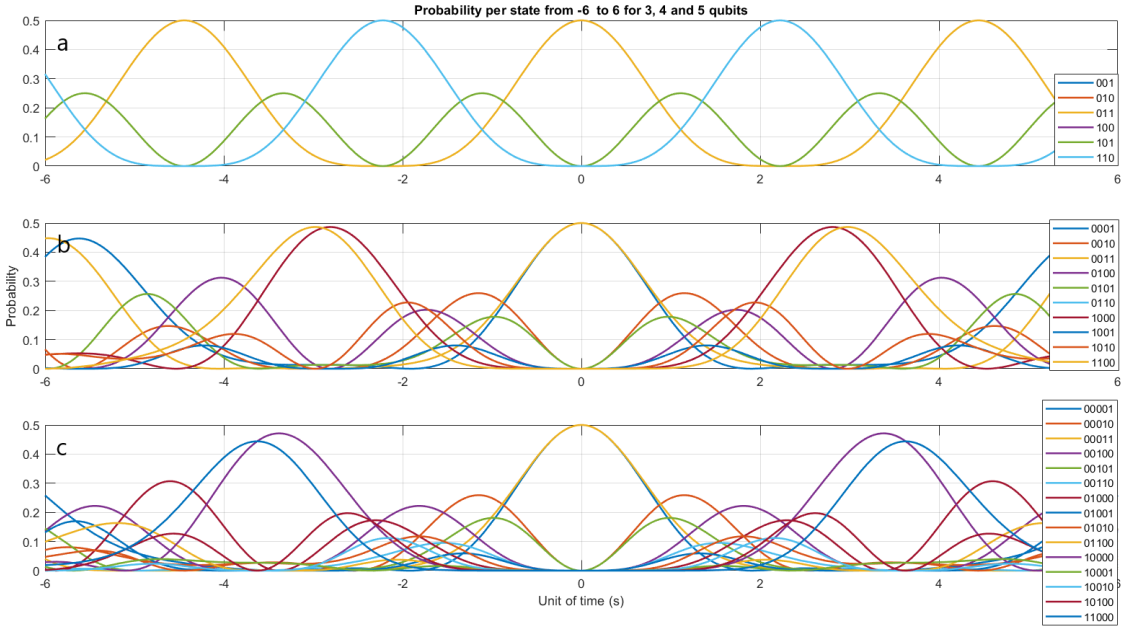

Figure 4.2: The evolution of a three(a), four(b) and five(c) qubit hamiltonian as defined by equation 2.14 through time, where the systems have the input states $|\psi\rangle = \frac{1}{\sqrt{2}}(|001\rangle + |011\rangle)$ for $n = 3$, $|\psi\rangle = \frac{1}{\sqrt{2}}(|0001\rangle + |0011\rangle)$ for $n = 4$ and $|\psi\rangle = \frac{1}{\sqrt{2}}(|00001\rangle + |00011\rangle)$ for $n = 5$.

4.2.1 System entanglement

As can clearly be seen, in all evolutions a time can be set for which more states are present than the number of initial states. However, this does not necessarily mean these states are entangled. The procedure to check for entanglement has been described in chapter 2.2. This has been done for all evolutions, for the four qubit system the results can be seen below in table 4.1 for $t = 1.5$.

For a four qubit system, first the states need to be defined as a tensor product of the separate qubit states,

$$|\psi\rangle = (\alpha|0\rangle + \beta|1\rangle) \otimes (\gamma|0\rangle + \delta|1\rangle) \otimes (\epsilon|0\rangle + \theta|1\rangle) \otimes (\kappa|0\rangle + \lambda|1\rangle) \tag{4.1}$$

By multiplying coefficients of a state with the state where all 0's become 1's and 1's are 0's, we always find a multiplication of all the coefficients "$\alpha\beta\gamma\delta\epsilon\theta\kappa\lambda$". Evidently, from table 4.1 can be concluded that there is indeed entanglement in the system at $t = 1.5s$ as the values are not equal.

state multiplication	total coefficients	value
$\|0000\rangle \times \|1111\rangle$	$\alpha\beta\gamma\delta\epsilon\theta\kappa\lambda$	0
$\|0001\rangle \times \|1110\rangle$	$\alpha\beta\gamma\delta\epsilon\theta\kappa\lambda$	0
$\|0010\rangle \times \|1101\rangle$	$\alpha\beta\gamma\delta\epsilon\theta\kappa\lambda$	0
$\|0011\rangle \times \|1100\rangle$	$\alpha\beta\gamma\delta\epsilon\theta\kappa\lambda$	0.04505
$\|0100\rangle \times \|1011\rangle$	$\alpha\beta\gamma\delta\epsilon\theta\kappa\lambda$	0
$\|0101\rangle \times \|1010\rangle$	$\alpha\beta\gamma\delta\epsilon\theta\kappa\lambda$	0.1233
$\|0110\rangle \times \|1001\rangle$	$\alpha\beta\gamma\delta\epsilon\theta\kappa\lambda$	0.07821
$\|0111\rangle \times \|1000\rangle$	$\alpha\beta\gamma\delta\epsilon\theta\kappa\lambda$	0

Table 4.1: Entanglement check for a four qubit system

This has been done for multiple initial states and multiple system sizes. It can be concluded that entanglement is only created if the input contains multiple states which cover a certain presence of 1's. If the system contains five qubits and the input state is defined as $|\psi\rangle = \frac{1}{\sqrt{2}}(|00001\rangle + |00011\rangle)$, there will never be states containing three or four 1's present. Following the entanglement check, every present state will be multiplied with 0 resulting in $\alpha\beta\gamma\delta\epsilon\theta\kappa\lambda\phi\zeta$ being zero in every case. Therefore, the input must contain $a \geq \frac{n}{2}$ number of states with different numbers of 1's.

4.2.2 Evolution time

The time for the system to evolve to entangled states can be observed from figure 4.2. It can be seen that the time increases with the number of qubits. Furthermore, the system is mirrored around $t = 0s$ which can be explained as all terms contain combinations of sinuses and cosines. The periodicity of the evolution depends on the amount of the qubits. For three qubits a period can clearly be defined as can be found underneath in figure 4.3. For four qubits, this is more complicated. The states oscillate with a certain period. However, the evolution does not perfectly repeat itself as can be seen in figure 4.4.

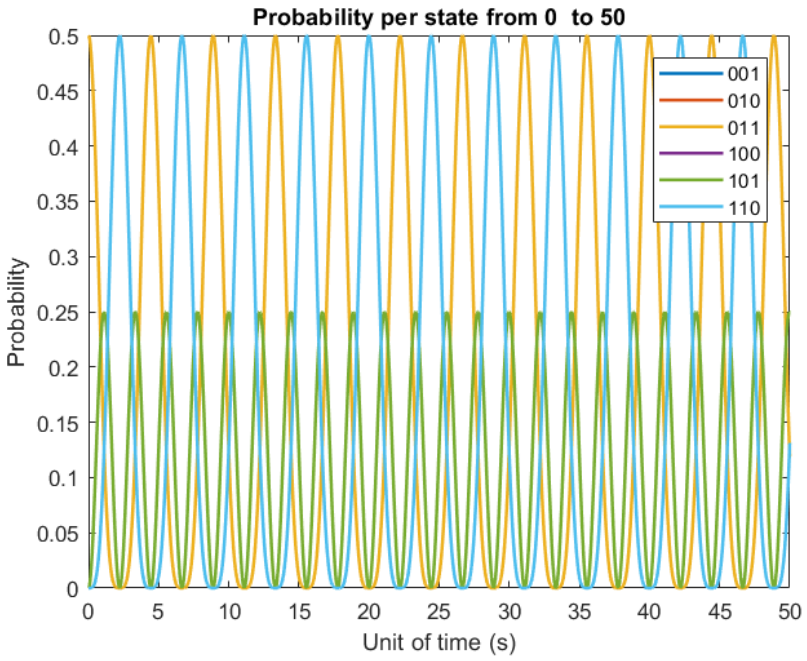

Figure 4.3: The evolution of a three qubit hamiltonian described by equation 2.14 with initial state $\psi = \frac{1}{\sqrt{2}}(|001\rangle + |011\rangle)$ over a longer period of time.

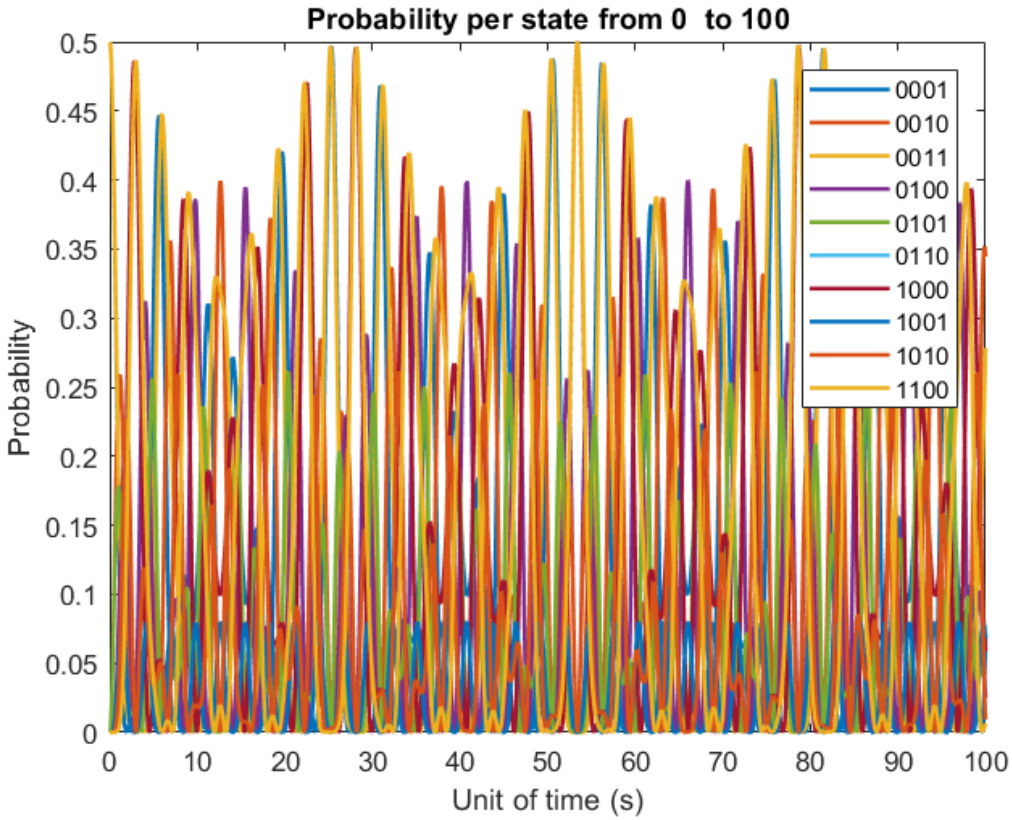

Figure 4.4: The evolution of a four qubit hamiltonian described by equation 2.14 with initial state $\psi = \frac{1}{\sqrt{2}}(|0001\rangle + |0011\rangle)$ over a longer period of time.

4.3 Circular boundary condition

For finding solutions via the Zhang way, a circular boundary conditions was introduced. This changed the hamiltonian from equation 2.14 to equation 3.12. For four qubits the evolution caused by equation 3.16 is plotted and can be compared in figure 4.5, with the evolution caused by the hamiltonian without the circular boundary.

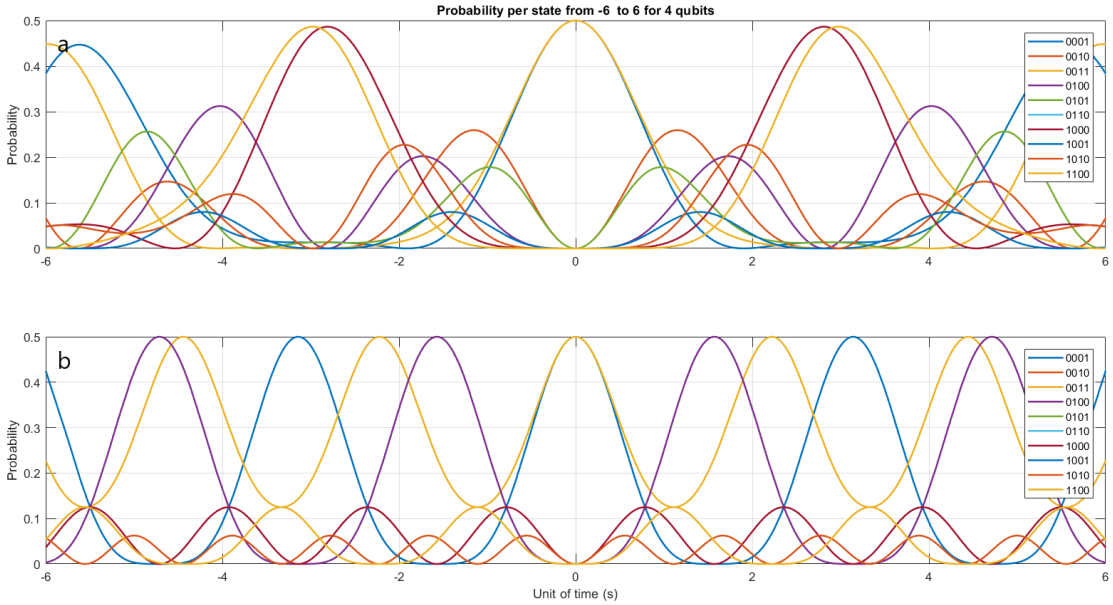

Figure 4.5: The evolution of a four qubit system with input state $\psi = \frac{1}{\sqrt{2}}(|0001\rangle + |0011\rangle)$ through time for a.) a straight system where the hamiltonian is described by equation 2.14 and b.) a circular system where the hamiltonian can be described by equation 3.16.

Clearly, the boundary condition changes the way the system behaves through time. The system has been checked for entangled and different results were found than stated in table 4.1. Still, the presence of entanglement can be confirmed.

Chapter 5

Conclusions and outlook

5.1 Conclusions

The goal of this paper was to develop a model to simulate multi-qubit entanglement generated by the Heisenberg XY interaction. This has been tried by following two different methods. First, by generalizing the three qubit entanglement found by *Zhang et al.* This theory can not be generalized to systems containing more than three qubits due to not commutable operators which have to be defined. The second methond is by solving the Schrödinger equation for the Heisenberg XY hamiltonian. The evolution of states through time caused by this hamiltonian is plotted for three, four and five qubits. These simulations clearly show that only states with the same number of 1's and 0's as the initial state can be present at all times. Furthermore, the entanglement of the system is checked by trying to write the solution as tensor products. This showed the presence of entanglement for certain times. Lastly, an extra boundary condition is tested. The boundary condition states that the qubits lie in a circle providing contact between the first and last qubit in the system. Applying the boundary condition resulted in different scenarios while still creating entanglement.

5.2 Outlook

To realize quantum supremacy, a lot still has to be done. Luckily, records in the field of quantum mechanics are being broken monthly. Personally, I am convinced multi-qubit entanglement will be the standard in a few years. The theory of creating entanglement with the help of the Heisenberg XY interaction entanglement investigated in this paper still needs extra work. The level of entanglement must be investigated by for example expressing the concurrence of the system through time. This way the efficiency of the system can be tested and one can search for the maximally entangled states. Furthermore, comparisons with other methods of creating entanglement can be made. The theory can truly be useful if it proves to be better than the ordinary CNOT-gate entanglement. Additionally, the practical implementation of this theory must be worked out. A theory is only the start, the use of this theory within a real quantum computer must be thought through to find the added value of this paper. Lastly, error must be added to the simulations. This can be done by adding offsets in some steps within the calculation. Error plays a crucial role within quantum computation and remains one of the biggest challenges we face.

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Appendix A

Codes

A.1 Matlab

Codes can be provided on request : l.p.v.rijn@student.tue.nl

A.2 Mathematica

Codes can be provided on request : l.p.v.rijn@student.tue.nl