

Analyzing Controllability in the 3-Qubit Array with minimal local controls.

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Declaration

Hereby, I declare on my honor that I have prepared this thesis independently. The thoughts taken over directly or indirectly from external sources are marked as such. No other sources than the references have been used. The present work has not been submitted to any other examination authority and has not yet been published.

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Chapter 1

Introduction

Nowadays, computers are used in all areas of daily life, mostly in specialized variants that are tailored to a given application purpose. Computers with increasing performance opened up new areas of application. But what if the problem that the computer is supposed to solve reaches a level of complexity such that it is either not solvable or can not be solved in a reasonable time?

Large data amounts can exhaust the computer's capacity and many arithmetic operations can take a very long processing time since they are performed one after another. One example that brings a classical computer to its limits is the factorization of integers into a product of prime numbers, the so-called prime factorization. If we set the number of digits high enough, then the prime factorization of integers will become a hard task for a computer. Even computers with very fast processing power and large capacities, so-called supercomputers, can be busy for weeks with the prime factorization of integers when the number of digits is high enough¹. The prime factorization has long ceased to be an academic task, since its fundamental use in cryptography (RSA-algorithm). Even the world's fastest supercomputers are overwhelmed with mathematical simulations motivated by practical problems such that they become a difficult task. Simulating chemical reactions, the construction of molecules, the weather system, or the stock market are just a few examples of complex systems that include large data amounts and long evaluation times, such that simulating those processes are tasks that could overwhelm the classical computer [1]. One could say, that classical computers have reached their limits. To be able to solve difficult problems that the modern worlds faces and to truly understand the behavior of complex systems, one needs new computing machines with a completely new blueprint. To be more precise, a blueprint that is not subject to the restrictions of the classical computer.

Quantum computers are built on the laws of quantum mechanics, in contrast to classical computers that are working based on electric states. It is already safe to say that quantum computers are not only faster than regular computers, quantum effects enable calculations that are impossible for classical computers [2]. Hence, quantum computers are ushering in a new era of technology, that will ultimately revolutionize our problem-solving abilities and eventually our understanding of nature, since simulating complex systems will not be a difficult problem anymore. But what are quantum computers exactly? The idea of creating computing machines using the laws of quantum mechanics

¹The RSA factoring challenge is an international challenge motivated by the firm RSA Labotary increase research in computational number theory and cryptography. The current record is the prime factorization of 200 digit numbers.

goes back to the famous physicist Richard Feynman. In a public talk in the early 1980's, he firstly speculated about how quantum states could be used as basic units of information instead of electric states. While a classical computer connects digital bits 0 and 1 through **logic gates**², quantum computers connect generalized bits, called qubits³, through **quantum logic gates**⁴. Quantum states are theoretically not restricted to a certain amount of states, it is generally possible for a qubit to have an infinite number of states⁵. If it is possible to implement every quantum logic gate, then one speaks of **universal quantum computing**. That is equivalent to saying that we can implement every possible unitary evolution.

Certain effects occur in quantum mechanics, like **superposition** and **entanglement**, that are not found in our macroscopic world. Only two states of the qubit are measurable when the qubit interacts with its environment. The interaction is a measurement of its physical properties. Those admissible states are called **eigenstates**. Generally, a qubit is in a superposition of its two eigenstates, which mathematically means any complex linear combination of its eigenstates is a possible state for a qubit[3]. While entanglement describes an invisible direct connection between two quantum objects, that acts immediately. Those quantum effects allow a quantum computing machine to perform simultaneous arithmetic operations, unlike classical computing, where calculations are performed one after another. To give a simple example of how quantum computers work differently, browsing through a huge amount of unsorted data to find a specific data point can take a very long time for a classical computer. A classical computer would go through every entry to find the data point, while a quantum computer could perform several passes simultaneously [4].

The earlier mentioned problem of prime factorization, should not be much of a problem, since in 1990 it was mathematically proven that **quantum computers** are extremely fast doing this task [5]. Since quantum computers are said to do a fast prime factorization, they can quite easily decipher encryptions, which is consequently a reason why secret services are interested in having their own quantum computer.

Not only decipher encryptions but also creating encryptions using quantum computing devices has become its field of research, named quantum cryptography [6]. Quantum computing, quantum cryptography, and generally every research area that uses quantum physics as the transmission of information can be seen as a part of **quantum information theory** [7].

However, at the time commercial quantum computers are unthinkable because they are still under development. Currently, quantum computers are not only an area of research for the academic world, major corporations like Google and IBM do research concerning quantum computers and quantum technology. Google's quantum computing research group proved that a quantum computer solved a mathematical problem considerably faster than the world's fastest supercomputer by IBM. Namely in 200 seconds instead of 10.000 years [8]. For this reason, researchers talk already about quantum supremacy, to point out the various advantages of quantum computing compared to classical computing. At the time, practicable realizations of quantum computers are restricted to an amount of a few dozen qubits. IBM has currently the highest number of qubits implemented in a computer

²Logic gates are circuits of digital electronics designed based on Boolean algebra. For instance, NOT, AND, or OR is logic gates that allow a computer to fulfill a certain task.

³The name occurs from the word quantum bit.

⁴Those are, mathematically speaking, unitary transformations.

⁵Although practically, we have to be able to measure qubit states with a certain precision, that will yield the number of states we can use.

chip. They have successfully managed to implement 65 qubits ⁶.

The implementation of qubits has become quite a competition of systems. A very promising attempt is superconducting quantum computing. Superconductors can resistance-free conduct electricity when they are extremely cooled down. The temperature that has to be reached is generally material-dependent and in a range from 1K to 90K. While Google and IBM implement qubits through superconducting circuits and manipulate their qubits via microwaves ⁷, some research centers like the University of Innsbruck has a different approach of implementing qubits. They hold ions in ion traps and manipulate the system with the use of lasers. The qubit is implemented through two states of the ion. Generally, manipulating quantum systems to create desired behaviors is an own area of research and named **quantum control theory**. It has a rich history, that was already beneficial for science and society decades before Richard Feynman shared his first thoughts on quantum computers ⁸. But with the increasing interest among many parties in quantum computing, the interest in methods of quantum control theory developed as well. It is safe to say, that many concepts of quantum control theory have applications in quantum information theory. For instance, the manipulation of qubits can be understood as a quantum control problem. Hence, one could use concepts of quantum control theory to describe the implementation of qubits.

All techniques to implement and manipulate qubits, including superconductors and ion traps, have their advantages, as well as their disadvantages. For example, while superconducting qubits allow the highest number of qubits to be implemented, their system has a high susceptibility to errors. Furthermore, it needs constant cooling to reach the temperature where the material conducts electricity without any resistance, the so-called critical temperature. Although the method of using ion traps allows precise calculations and does not need constant cooling, the method allows implementation of currently not more than 10 qubits.

Besides disadvantages that come up with the choice of implementation, some problems affect nearly every implementation of qubits, like the decoherence time and the complicated engineering. To manipulate quantum mechanical effects, the quantum computer needs to be completely isolated from its environment. The decoherence time is the time it takes for quantum effects to get lost. The quantum computer should be able to make operations as fast as possible, to avoid decoherence. Although this is a problem, where concepts of quantum control theory could be helpful, this will not be the main concern of this thesis.

In nearly every implementation of computer chips with implemented qubits, there exists a lack of space, regardless of the implementation technique. For the sake of simplicity, we consider only one example where this is the case. Consider superconducting quantum computing. In the current blueprint, each qubit is wired with an individual microwave cable. This allows manipulating each qubit via microwaves. Moreover, every qubit is wired with a cable, that causes constant cooling to reach the superconductor's critical temperature. Unfortunately, this causes a lack of space within the physical implementation and is one of the reasons why quantum computers are so difficult to physically realize.

Had not every qubit had its microwave wire, then the current blueprint could lose some of its com-

⁶The Us corporation IBM has a big community of software developers, writing quantum algorithms to steadily improve their quantum technology. The most recent version of their quantum computer has 65 Qubits, IBM estimates that within 2022 they will have a quantum computer that runs with 128 qubits.

⁷The qubit gets implemented through the state of a small superconducting circuit named Josephson-junction.

⁸For example, the manipulation of nuclear spins by an electromagnetic field finds application in the medical field as MRI. Therefore, this can be considered an achievement built on the science of quantum control theory.

plexity. Hence, physical realizations of quantum computers could be done more easily. One could think, that losing microwave wires automatically means losing the ability to manipulate qubits. Following this thought, one could come up with the statement, that the physical realization of quantum computers with fewer microwave wires than qubits is practically useless since manipulating every single qubit contributes to the quantum computer's physical power. But is the assumption of this statement true?

Is it possible to manipulate all qubits arbitrarily in a superconducting-quantum computer with fewer microwave cables than qubits?

And if so, what is the minimum number of microwaves, that have to be included?

This is an important question, which will be explored in detail in the results chapter. So what does it mean to manipulate all qubits in this context? It means that any quantum logic gate in this setup is realizable. So steering any qubits initial state to an arbitrary target state is possible, with a quantum logic gate. If this is true for all qubits, one speaks of universal quantum computing. First, we will rephrase the upper question using the terms of quantum control theory. Rephrasing it will give us various advantages, for instance, we can generalize the qubit manipulation technique instead of restricting ourselves to the microwave wire technique. Ultimately, if we can read the question in terms of quantum control theory, we can use the promising concepts of quantum control theory and try to solve the upper question as a quantum control problem.

In quantum control theory, any technology used to manipulate qubits is a **local control**. Hence, the microwave wires used in superconducting quantum computing and the lasers used in ion-trap quantum computing are local controls. In quantum control theory, asking if any target state of a system is achievable is a question of **controllability**. In terms of quantum control theory, a qubit array is **controllable** if any initial state can be brought to any target state, through a unitary transformation. Universal quantum computing means that any quantum logic gate is generable in the considered qubit array. A quantum logic gate is mathematically a unitary transformation. Realizing every unitary transformation is the same as saying that, every unitary evolution of the quantum system that steers the system's initial state to any target state is possible. To conclude, **a qubit array that allows universal quantum computing is always a controllable qubit array and vice versa**. Hence, in terms of quantum control theory the upper question reads:

Can a qubit array be controllable, if the number of local controls is less than the number of qubits? And if so, what is the minimum number of local controls, such that the qubit array remains controllable?

To summarize, quantum control theory gives us terms to rephrase the problem of building quantum computers and allows us to use its concepts to solve this problem in a general way. This bachelor thesis' main concern is how to create controllable qubit networks when the number of local controls is minimal. We are not focused on the various ways to implement qubits and quantum gates. Rather, our main concern is the mathematical existence of controllable qubit arrays with minimal local controls. This work could help solve the lack of space problem within current quantum computers. Since less local controls ultimately mean more space within a quantum computer. Since we have not preferred any physical implementation, the controllable qubit arrays that were found in this thesis could theoretically be realizable for any physical implementation.

In the results chapter, the 3-qubit array was observed and analyzed. To complete the analysis of the non-trivial 3-qubit array, it was necessary to analyze the 3-qubit chain, but also the 3-qubit loop.

In the context of quantum computing, certain qubit arrays can be interpreted as a composition of 3-qubit chains and 3-qubit loops. Strategies are presented under which controllable 3-qubit arrays with a single local control could be implemented. Further, we study if controllability remains under symmetries, studied special cases when controllability was destroyed, present graphic state-transitions of the 3-qubit system, and studied controllable 3-qubit chains with minimal interactions.

Chapter 2

Foundations

2.1 Quantum Information Theory

2.1.1 Description of Quantum States

In classical mechanics, the state of any system is set by position x , velocity v and acceleration a . For instance, a mass point that moves in 3-dimensional space, has a time dependent state-function $\mathbf{r} = \mathbf{r}(\mathbf{t})$, that contains information about position, velocity and acceleration. For each fixed time $t \in \mathbb{R}_{\geq 0}$, the state of the mass point is a vector in \mathbb{R}^3 . If the initial conditions are given, one can determine the state of the mass point for all times $t \rightarrow \infty$. In quantum mechanics, there is no direct analogy to the state function of the mass point $\mathbf{r}(\mathbf{t})$ since Heisenberg's uncertainty principle prohibits the simultaneous sharp determination of position and momentum. Furthermore, one cannot give an arbitrarily precise determination of physical states like in classical mechanics, but only probabilities. Nevertheless, one can represent the state of a quantum system, although the notion of state and the notion of state-space are in quantum mechanics defined differently as in classical mechanics. A **quantum system** is any system, that obeys the laws of quantum mechanics and the state of a quantum system is a unit vector of a complex separable Hilbert space ¹.

Definition 2.1.1. (Hilbert space) Let \mathcal{H} be a vector space with an inner product $\langle \cdot, \cdot \rangle$. If \mathcal{H} is complete, then \mathcal{H} is a Hilbert space.²

A quantum system has dimension N if the corresponding Hilbert space has dimension N . In this work, only finite-dimensional quantum systems have been investigated, thus an understanding of finite-dimensional Hilbert spaces will be sufficient. In addition, we do not have to worry about separability, since finite-dimensional Hilbert spaces are always separable [9].

An important example of an finite-dimensional Hilbert space is the complex vector space \mathbb{C}^N equipped with the inner product $\langle \cdot, \cdot \rangle : \mathbb{C}^N \times \mathbb{C}^N \rightarrow \mathbb{C}, (x, y) \mapsto x^\dagger y$.

¹Separable means that, it exists a dense countable set $\{x_j\}$ in a set J which is an orthonormal basis, such that $\langle x_j, x_k \rangle = \delta_{j,k}$ holds [7].

²A vector space with inner product is called **complete**, if every Cauchy sequence $(x_n)_{n \in \mathbb{N}}$ in \mathcal{H} converges to $x \in \mathcal{H}$ with respect to the metric, that is induced by the inner product.

If the same state $|\psi\rangle \in \mathcal{H}$ is inserted into both arguments of the inner product and we take the positive square root, then we obtain a measure of the length of $|\psi\rangle$, that is said to be the norm of the state $|\psi\rangle$. It is said, that the inner product induces a norm: $\sqrt{\langle\psi, \psi\rangle} = |||\psi\rangle||$. Let \mathcal{H} be a N -dimensional complex Hilbert space. The **unit sphere** $S(\mathbb{C})^{N-1}$ contains all vectors in \mathcal{H} , that are normalized.

$$S(\mathbb{C})^{N-1} := \{|\psi\rangle \in \mathcal{H} \mid |||\psi\rangle|| = 1\}$$

If $|\psi_S\rangle \in S(\mathbb{C})^{N-1}$, then $|\psi_S\rangle$ is said to be a **unit vector** in \mathcal{H} . The state of a quantum system is represented by a unit vector in a complex Hilbert space³. Represents mean here that knowledge about the state vector gives full information about the quantum system. Consequently, any state of a quantum system can be imagined as a point on the complex unit sphere. The reason why it can be assumed that a unit vector is sufficient to describe the state of a quantum system follows directly from the Dirac-von Neumann axioms. It is an approach of deriving quantum mechanics in terms of operators⁴.

Definition 2.1.2. (Dirac- von Neumann axioms) Let \mathcal{H} be a complex Hilbert space, that is finite-dimensional or has countable infinite dimension.

1. An observable of a quantum system is defined to be a self-adjoint operator T , that acts on \mathcal{H} .
2. A state $|\psi\rangle$ of the quantum system is a unit vector in \mathcal{H} , up to scalar multiples.
3. The expectation value of an observable T for a quantum system, in state $|\psi\rangle$ is given by the inner product $\langle\psi, T\psi\rangle$

Consider a finite-dimensional complex Hilbert space \mathcal{H} , that is associated with a quantum system. Let $|\psi_S\rangle \in S(\mathbb{C})^{N-1}$. The second axiom implies that vectors that are elements of $span(|\psi_S\rangle)$ contain the same physical magnitude or the same physical information [3]. Thus, the state of a quantum system is represented not by a single state vector, but by a one-dimensional subspace of \mathcal{H} . The state of the quantum system is thus represented by $span(|\psi_S\rangle)$, which is called **ray** in this context. The second axiom derives naturally an **equivalence relation** on \mathcal{H} .

$$\text{For } |\psi\rangle, |\psi'\rangle \in \mathcal{H} : |\psi\rangle \sim |\psi'\rangle :\Leftrightarrow |\psi\rangle \in span(|\psi_S\rangle) \wedge |\psi'\rangle \in span(|\psi_S\rangle) \quad (2.1)$$

It says that any pair of vectors are equivalent if they are elements of the same ray. Unit vectors $|\psi_S\rangle \in S(\mathbb{C})^{N-1} \subset \mathcal{H}$ are chosen to be **representatives** of their ray. This equivalence relation divides the Hilbert space \mathcal{H} into overcountable infinite **equivalence classes**. Those equivalence classes are the linear spans of the unit vectors.

$$[|\psi\rangle] = [|\psi'\rangle] = [|\psi_S\rangle] = span(|\psi_S\rangle)$$

Geometrically, one could imagine that each ray is mapped to a point on a unit sphere. That is why, this equivalence relation is called **projectivization**. Applying the projectivization on \mathcal{H} gives us the **projective Hilbert space** $P(\mathcal{H})$. It is the set of all equivalence classes, in this context it is the set of all linear spans of unit vectors.

³This explanation only holds for pure states, since mixed states do not have a representation as a vector in Hilbert space, which is why one uses the density operator [6].

⁴Here an operator is a continuous linear function between Hilbert spaces.

$$P(\mathcal{H}) := \mathcal{H}/\sim := \{\text{span}(|\psi_S\rangle) \mid |\psi_S\rangle \in S(\mathbb{C})^{N-1}\}. \quad (2.2)$$

Therefore, the 2. Dirac- von Neumann axiom is understandable as:

All states that are elements of the same ray in Hilbert space \mathcal{H} contain the same physical information. A representative of a ray is a unit vector.

So we see that the Dirac-von Neumann axioms imply the projectivization of the Hilbert space. Indeed, all states which lie on the same ray are physically equivalent, but to select unit vectors as representatives allow an illustration and thinking aid. As an important remark, the following should be mentioned:

The unit norm constraint does not completely determine $|\psi\rangle$ within the ray, since $|\psi\rangle$ could be multiplied by any λ with absolute value 1 and retain its normalization. Such a λ can be written as $\lambda = e^{i\phi}$ with $\phi \in [0, 2\pi)$ called the **phase**.

2.1.2 Representation of a Qubit and the Bloch sphere

In classical information theory, the bit is the basic unit of information, which is physically realized by a two-state device. The bit is saved in the system, which has exactly 2 states, represented by 0 and 1. The system is in either one of those states. In **quantum information theory** the state $|\psi\rangle$ of a finite-dimensional quantum system encodes information. Conventionally, one uses quantum mechanical two-state systems, named qubits as an implementation of information. The qubit is the quantum-mechanical analog of the classical bit, but the qubit is of a very different nature than the classical bit. In the following, we will explain certain important properties of the qubit in more detail. First of all, we start from the definition of a qubit.

Definition 2.1.3. (Qubit)

A 2-dimensional quantum system with two arbitrarily manipulable eigenstates is a qubit. For the Hilbert space associated to the qubit holds,

$$\mathcal{H} = \mathbb{C}^2, \quad \text{with inner product} \quad \langle x, y \rangle = x^\dagger y \in \mathbb{C}, \quad \forall |x\rangle, |y\rangle \in \mathbb{C}^2. \quad (2.3)$$

The state of a qubit is represented by a unit vector $|\psi\rangle \in S(\mathbb{C})^1$.

Formally, there are 7 conditions that a quantum mechanical two-state system has to fulfill, to be a qubit [10]. But since the physical implementation of qubits is not the subject of this work, the introduction of those criteria is not necessary. The electron spin or the nuclear spin are examples of qubits. In such a case, the spin can have two states, spin-down, and spin-up. Through radiation one could manipulate the state of the spin arbitrarily. As a counterexample consider a quantum mechanical harmonic oscillator. Firstly, it has more than two eigenstates, and secondly, it is impossible to manipulate just two eigenstates, since the harmonic oscillator has equidistant energy levels. A qubit can be in one of its eigenstates, but also in a **superposition** of its eigenstates. A superposition is the most general state for a qubit. This means that the qubit is in a complex linear combination of its eigenstates. Inspired by the state representation of the classical bit, the eigenstates of the qubit

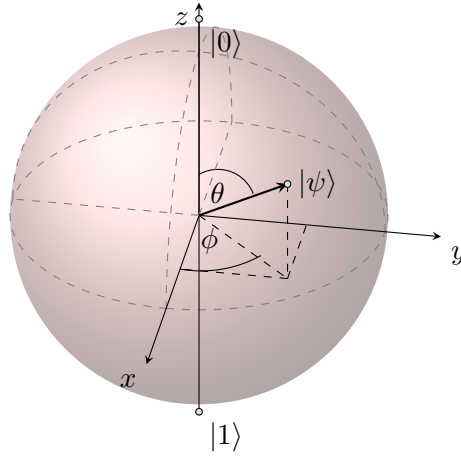


Figure 2.1: The Bloch sphere represents the qubit's state $|\psi\rangle$ on the surface with azimuth angle ϕ and polar angle Θ . Note that the qubit's eigenstates $|0\rangle$ and $|1\rangle$ are oriented in opposite directions on the z -axis.

are usually written as $|0\rangle$ and $|1\rangle$. The qubit is in a superposition, which means the qubit's state is:

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle, \quad \alpha, \beta \in \mathbb{C}. \quad (2.4)$$

The complex numbers α, β are called **probability amplitudes**, which fulfill the relation ⁵

$$|\alpha|^2 + |\beta|^2 = 1.$$

Generally, the qubit is in a superposition of the eigenstates. However, by measuring the energy of the system one obtains an eigenvalue λ of the associated Hamiltonian H , while the qubit collapses into the eigenstate, which corresponds to the eigenvalue λ . The system is then in the eigenstate $|0\rangle$ or in the eigenstate $|1\rangle$. The coefficient $|\alpha|^2$ is the probability to measure the eigenstate $|0\rangle$ and equally $|\beta|^2$ is the probability to measure the eigenstate $|1\rangle$, therefore it is natural to call α and β probability amplitudes. This circumstance is completely different from the possible states of a classical bit. Linear combinations of the classical states 0 and 1 do not describe a possible state and do not make sense physically.

The Bloch sphere

Since a qubit's state is represented by equation (2.4), one could assume that it takes 4 real numbers to illustrate the qubit's state. This follows from $\alpha, \beta \in \mathbb{C}$:

$$\alpha = \text{Re}(\alpha) + i\text{Im}(\alpha)$$

$$\beta = \text{Re}(\beta) + i\text{Im}(\beta)$$

However, the **Bloch sphere** is a graphic visualization of the qubit's state $|\psi\rangle$, that only needs 2 real numbers. Formally, the qubit's state and the represented state in the Bloch sphere are

⁵Normalization constraint according to the second axiom in 2.1.2.

mathematically not equal. However, they share the same physical information. In the derivation of the Bloch sphere, restrictions are made that affect the state vector. However, the restrictions leave the physical information of the state vector invariant. We chose the state vector to be a unit vector since states on the same ray are physically equivalent and one chooses unit vectors conventionally as representatives. A unit vector is uniquely determined except for a complex factor λ that leaves its norm the same. We call such a complex factor a **global phase** and it has the form $\lambda = e^{i\phi}$ with $\phi \in [0, 2\pi)$ ⁶. Hence, one can multiply the unit vector by any global phase and the physical information of the unit vector remains the same. Suppose $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ is the state of the qubit, that we want to represent on the Bloch sphere. Note that, any complex number z can be written in its polar form: $z = r(\cos(\phi) + i\sin(\phi))$ with $\phi = \arctan(\frac{\text{Im}(z)}{\text{Re}(z)})$. Using Euler's identity, it follows: $z = re^{i\phi}$. Consequently, one can rewrite the qubit's state:

$$|\psi\rangle = r_\alpha e^{i\phi_\alpha} |0\rangle + r_\beta e^{i\phi_\beta} |1\rangle, \text{ with } r_\alpha, r_\beta \in [0, 1] \text{ and } r_\alpha^2 + r_\beta^2 = 1 \quad (2.5)$$

Multiplying the state $|\psi\rangle$ with a scalar $\lambda \in \mathbb{C}$, different from zero, does not change the physical state, since quantum states with equal directions are equivalent to the unit vector. Setting $\lambda = e^{-i\phi_\alpha}$, one obtains the state $|\psi'\rangle = \lambda|\psi\rangle = r_\alpha|0\rangle + r_\beta e^{i(-\phi_\alpha + \phi_\beta)}|1\rangle$. Then it follows, that

$$|\psi\rangle \Leftrightarrow |\psi'\rangle.$$

From equation (2.5) follows $r_\alpha = \cos(\frac{\Theta}{2})$, $r_\beta = \sin(\frac{\Theta}{2})$, $\Theta \in [0, \pi]$. Hence, the representation of the state on the Bloch sphere is given by:

$$|\psi'\rangle = \cos(\frac{\Theta}{2})|0\rangle + \sin(\frac{\Theta}{2})e^{i\phi'}|1\rangle, \text{ with } \phi' = -\phi_\alpha + \phi_\beta, \quad \phi' \in [0, 2\pi). \quad (2.6)$$

We interpret the equation 2.6 in the following way: Θ can be understood as a polar angle and ϕ as an azimuth angle, describing a point on a unit sphere. Since scaling does not matter, the state $|\psi\rangle$ has a equivalent state $|\psi'\rangle$ with $\| |\psi'\rangle \| = 1$. Hence, the state of a qubit can be imagined as a point on the unit sphere's surface, with angles ϕ and Θ . Consequently, 2 real numbers ϕ and Θ are sufficient to describe and to visualize the qubit's state. Note that, the qubit reaches its eigenstates $|0\rangle, |1\rangle$ if $|\psi\rangle$ points in either one of the directions of the z-axis.

2.1.3 Quantum Dynamics as Information Processing

From the first axiom of the Dirac-von Neumann axioms 2.1.2 we know, that physical observables are self-adjoint operators. Throughout this thesis, the Hilbert spaces associated with quantum systems will be finite-dimensional. Consequently, the observables will be matrices, since they can be considered as transformations between finite-dimensional spaces. From this follows that the operators under consideration are Hermitian matrices.

Corollary 2.1.4. *(Observable on finite-dimensional Hilbert space) Let \mathcal{H} be a complex finite-dimensional Hilbert space associated with a quantum system. An observable T of the quantum system is a Hermitian matrix A , that acts on \mathcal{H} .*

⁶The global phase is a phase of a state, in a quantum system that can have multiple states.

Proof. Let \mathcal{H} be a finite-dimensional complex Hilbert space. According to definition 2.1.2, an observable is generally represented by a self-adjoint operator $T: \mathcal{H} \rightarrow \mathcal{H}$. T is defined to fulfill $\langle Tx, y \rangle = \langle x, Ty \rangle$ for any $x, y \in \mathcal{H}$. Let $\dim(\mathcal{H}) = N$, consequently the operator T has a transformation matrix A . From self adjointness follows: $\langle Ax, y \rangle = (Ax)^\dagger y = x^\dagger A^\dagger y = x^\dagger Ay = \langle x, Ay \rangle$, therefore A is a Hermitian matrix. \square

Consider an N -dimensional quantum system with associated Hilbert space \mathcal{H} . The energy of the quantum system is an important observable and corresponds to the operator H , that is called **Hamiltonian**. The Hamiltonian contains information, necessary for determining the state of the quantum system at any arbitrary time t . It can be time-independent or, as in the case of quantum control systems, time-dependent, i.e., $H = H(t)$. The state $|\psi(t)\rangle$ of the quantum system evolves with respect to the **time-dependent Schrödinger Equation**.

$$-i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle \quad (2.7)$$

With reduced planck's unit \hbar ⁷. Let $|\psi\rangle = |\psi(0)\rangle$ be the initial state of the quantum system. Since there exists a probability that the quantum system is in any state of Hilbert space, the arbitrarily chosen state $|\psi(t)\rangle$ is a possible final state. Generally, any state $|\psi(t)\rangle$ in Hilbert space is achievable, through a **unitary operator** $U(t)$ acting on the initial state $|\psi(0)\rangle$:

$$U(t) |\psi(0)\rangle = |\psi(t)\rangle \quad (2.8)$$

In the considered case, where $\dim(\mathcal{H}) = N$ the unitary operator is a unitary matrix. Unitary matrices fulfill $U^{-1} = U^\dagger$, hence $UU^\dagger = \mathbb{1}_N$. Furthermore, the set of all $N \times N$ unitary matrices form an multiplicative group referred as $U(N)$. In the chapter on Lie algebras and Lie groups 2.3.2, the multiplicative group $U(N)$ will be discussed in more detail. It is important to remark that, $U(t)$ contains information, about the time evolution of the quantum system and is not representing an physical observable⁸. Since $U(t)$ is a unitary matrix, the norm of the state stays the same throughout the time evolution:

$$\|U(t) |\psi(0)\rangle\| = \|\psi(t)\|.$$

If one inserts equation (2.8) into the time-dependent Schrödinger equation (2.7), one can derive a differential equation, that contains information about the dynamics of the quantum system, but in terms of linear operators:

$$\begin{aligned} -i\hbar \frac{d}{dt} U(t) |\psi(0)\rangle &= H(t) U(t) |\psi(0)\rangle \\ (-i\hbar \frac{d}{dt} U(t) - H(t) U(t)) |\psi(0)\rangle &= 0 \end{aligned}$$

By setting $\hbar = 1$ and considering the term within the bracket, one derives the **time-dependent Schrödinger Operator Equation**:

$$\dot{U} = -iH(t)U(t), \quad U(0) = \mathbb{1}_N \quad (2.9)$$

⁷plancks unit : $h = 6.62607015e - 34 Js$ and reduced plancks unit: $\hbar = \frac{h}{2\pi}$.

⁸Unitary evolution is time evolution for quantum systems.

Where $U(t)$ is the solution for (2.9). Due $H(t)$ is a Hermitian matrix, $-iH(t)$ is a skew-Hermitian matrix and $U(t)$ is a unitary matrix for all times t . Equation (2.9) will become relevant for quantum control theory, presented in section 2.2.1.

Example 2.1.5. (Measurement and Dynamics of a Qubit) Consider a qubit with constant Hamiltonian:

$$H_0 = \hbar\sigma_y = \begin{pmatrix} 0 & -i\hbar \\ i\hbar & 0 \end{pmatrix}.$$

Measuring the energy of the system one obtains the eigenvalues of H , these are $\lambda_0 = \hbar, \lambda_1 = -\hbar$. We will refer to a qubit's eigenvalues as **level spacing** since they can be interpreted as the system's different energy levels. While one measures an eigenvalue, the qubit collapses to one of its eigenstates:

$$|0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -i \\ 1 \end{pmatrix}, \quad |1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 1 \end{pmatrix}.$$

A basis given by $\{|0\rangle, |1\rangle\}$. In order to determine the unitary evolution of the qubit, the time-dependent Schrödinger equation is setted. One finds a system of two coupled linear differential equations of second order.

$$\frac{d}{dt} |\psi(t)\rangle = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} |\psi(t)\rangle$$

The solution of this system can be given analytically:

$$|\psi(t)\rangle = \begin{pmatrix} \cos(t) & \sin(t) \\ -\sin(t) & \cos(t) \end{pmatrix} |\psi(0)\rangle$$

For $t = \frac{\pi}{2}$ one obtains:

$$|\psi(\pi/2)\rangle = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} |\psi(0)\rangle.$$

This dynamics performs the logic operation **NOT**. It inverts the state which is transferred from $|1\rangle$ to $|0\rangle$, and from $|0\rangle$ to $-|1\rangle$. Note that, the minus sign is a global phase. Physically, $-|1\rangle$ is equivalent to $|1\rangle$.

2.1.4 Quantum Gates

Consider a qubit, that is in the state $|\psi\rangle$. A **quantum gate** or **quantum logic gate** is a unitary transformation U that transforms the state $|\psi\rangle$ to the state $U|\psi\rangle$. They are called this way, because of their crucial role in quantum information theory, which is analog to classical logic gates⁹. Quantum gates describe changes between the qubit's state within a time $t \in [0, T]$. As the quantum systems, that is described according to equation (2.9), does a unitary evolution during the time interval $[0, T]$, the information captured by the initial state $|\psi(0)\rangle$ obtains

$$|\psi(T)\rangle = U(T) |\psi(0)\rangle.$$

Therefore, it can be seen, that $U(T)$ performs a logical operation on the initial state. Quantum gates, that are important throughout this thesis are **1-qubit gates**. A 1-qubit gate is a unitary

⁹The name may suggest a false fact, since those are not real physical devices, but time-manipulable interactions between qubits.

transformation, that changes the state of a single qubit. Therefore 1-qubit gates are local gates¹⁰. As a significant example for 1-qubit gates consider the **Pauli matrices**:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (2.10)$$

The notion of **Universal set** is important. It describes the property of a subset S of the unitary group, that can generate every single unitary transformation, through the multiplication of elements in S . Another important notion for this thesis is **Universal quantum computing**. Consider a system that contains N qubits. Ultimately it depends on the system if certain quantum logic gates are realizable or not.

Consider a system of N qubits, that is described by the equation 2.9. If the system allows that, every $U \in U(2^N)$ or every $U \in SU(2^N)$ to be generated, then **universal quantum computing** is possible.

In the chapter 2.3, we will introduce concepts and different notions of controllability. Ultimately, it is a way of determining if universal quantum computing is possible or not.

2.1.5 Representation of Qubit Arrays

Composite Systems

Consider two quantum systems \sum_1 and \sum_2 associated to the Hilbert spaces \mathcal{H}_1 and \mathcal{H}_2 . Both quantum systems can be understood as subsystems of a larger quantum system, which is said to be the **composite system**. The state-space of the composite system is the tensor product of the associated Hilbert spaces \mathcal{H}_1 , and \mathcal{H}_2 . The state of the composite system is described by a unit vector that is an element of the tensor product space $\mathcal{H}_1 \otimes \mathcal{H}_2$.

Definition 2.1.6. (Tensor product of Hilbert spaces) Let \mathcal{H}_1 with inner product $\langle \cdot, \cdot \rangle_1$, and \mathcal{H}_2 with inner product $\langle \cdot, \cdot \rangle_2$ be Hilbert spaces. The tensor product space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ is a Hilbert space, if for states $|\psi_1\rangle, |\phi_1\rangle \in \mathcal{H}_1$ and $|\psi_2\rangle, |\phi_2\rangle \in \mathcal{H}_2$, an inner product is induced on \mathcal{H} by

$$\langle \phi_1 \otimes \phi_2, \psi_1 \otimes \psi_2 \rangle = \langle \psi_1, \phi_1 \rangle_1 \langle \psi_2, \phi_2 \rangle_2.$$

The dimension of \mathcal{H} is the product of the dimensions of \mathcal{H}_1 and \mathcal{H}_2 :

$$\dim(\mathcal{H}) = \dim(\mathcal{H}_1) \cdot \dim(\mathcal{H}_2). \quad (2.11)$$

Analogously, one can construct a Hilbert space \mathcal{H} by taking the tensor product of N Hilbert spaces \mathcal{H}_i in the same manner:

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \dots \otimes \mathcal{H}_N = \otimes_{i=1}^N \mathcal{H}_i, \text{ with } \dim(\mathcal{H}) = \prod_{i=1}^N \dim(\mathcal{H}_i) \quad (2.12)$$

The Hilbert space (2.12) corresponds to the composite system that is built of N quantum systems. Tensor product of Hilbert spaces will be referred as **tensor spaces** from now on. Let \mathcal{H}_1 and \mathcal{H}_2 be

¹⁰There are also non-local gates, i.e., unitary transformations affecting more qubits at the same time. For instance, those could be obtained by Kronecker products of Pauli matrices.

Hilbert spaces. Consider a composite system with associated tensor space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. A clear definition is needed, if an operator A that is defined on \mathcal{H} only acts on a subspace $\mathcal{H}_{1,2}$ and leaves the other invariant.

Definition 2.1.7. (Extension of an Operator on tensor space) Let $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ be a tensor space and I be the Identity operator, $I : \mathcal{H}_i \rightarrow \mathcal{H}_i, x \rightarrow x$, with $i \in \{1, 2\}$. An operator $A : \mathcal{H}_1 \rightarrow \mathcal{H}_1, x \rightarrow Ax$ has an extension on \mathcal{H} , that is, $A \otimes I : \mathcal{H}_1 \otimes \mathcal{H}_2 \rightarrow \mathcal{H}_1 \otimes \mathcal{H}_2$, $(x, y) \mapsto (Ax \otimes y)$.

In this thesis index notation is used, to clarify on which Hilbert space the operator A is acting on. Therefore $A^1 = A^1 \otimes I$ describes A acting on the first Hilbert space \mathcal{H}_1 . The principle of definition 2.1.7 can likewise be extended in a Tensor space consisting of N Hilbert spaces. Considering composite systems, it is needed to testify actions of linear operators on tensor products of Hilbert spaces.

Definition 2.1.8. (Tensor Product of Linear Operators) Let $A : \mathcal{H}_1 \rightarrow \mathcal{V}_1, |\psi_1\rangle \rightarrow A|\psi_1\rangle$ and $B : \mathcal{H}_2 \rightarrow \mathcal{V}_2, |\psi_2\rangle \rightarrow B|\psi_2\rangle$ be linear operators between Hilbert spaces. The tensor product of linear operators A and B is defined as:

$$A \otimes B : \mathcal{H}_1 \otimes \mathcal{H}_2 \rightarrow \mathcal{V}_1 \otimes \mathcal{V}_2, (|\psi_1\rangle, |\psi_2\rangle) \rightarrow A|\psi_1\rangle \otimes B|\psi_2\rangle. \quad (2.13)$$

The tensor product of linear operators is a linear operator. If the linear operators are defined on finite-dimensional Hilbert spaces, the tensor product of linear operators is a tensor product of their transformation matrices. In this special case, it will be called **Kronecker product** as we will see in the following.

N-qubit Array

A **qubit array** is a system or network that only consists of qubits. In principle, qubit arrays are important whenever more than one qubit is needed to do meaningful work within a quantum computer. However, mathematically the geometrical arrangement in space does not matter at all. Only the number of qubits and the number of interactions are significant. In this thesis, we are mainly concerned with two types of 3-qubit arrays, which are shown in the figure 2.2.

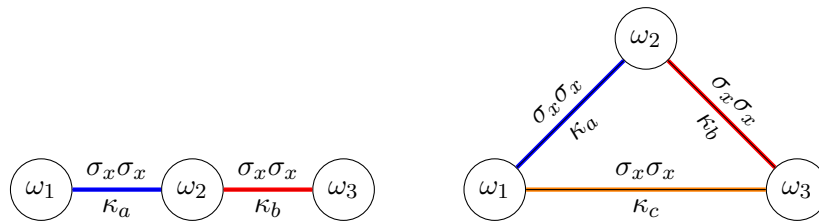


Figure 2.2: **On the right side:** The 3-qubit chain with nearest-neighbour interactions $\sigma_x^1 \sigma_x^2$ and $\sigma_x^2 \sigma_x^3$. The blue edge corresponds to κ_a and the red edge to κ_b , to indicate that they are generally different. The level-spacing ω_α of the qubits is written within the nodes, it represents that the system has no degeneracy. **On the left side:** a third connecting line is needed to represent the coupling of the first and the third qubit. By analogy the colour orange was chosen, to represent that κ_c is generally different as κ_a or κ_b .

Let $N \in \mathbb{N}$ be the number of qubits, that form a N -qubit array. Each qubit q_i has an associated Hilbert space \mathcal{H}_i , for $1 \leq i \leq N$. According to equation (2.3) for every Hilbert space \mathcal{H}_i holds, $\mathcal{H}_i = \mathbb{C}^2$. Therefore, $\dim(\mathcal{H}_i) = \dim(\mathbb{C}^2) = 2$ holds. According to equation (2.12), the state space of the N -qubit array, is the tensor product of every single Hilbert space, that is $\mathcal{H} = \otimes_{i=1}^N \mathbb{C}^2 = \mathbb{C}^{2^N}$ with $\dim(\mathcal{H}) = 2^N$.

Corollary 2.1.9. (*Kronecker product*) Let \mathbb{K} be a field, $A \in \mathbb{K}^{(m,m)}$ and $B \in \mathbb{K}^{(n,n)}$, then the mapping

$$\otimes : \mathbb{K}^{(m,m)} \times \mathbb{K}^{(n,n)} \rightarrow \mathbb{K}^{(mn,mn)}, (A, B) \rightarrow A \otimes B := \begin{pmatrix} a_{11}B & \dots & a_{1n}B \\ \vdots & & \vdots \\ a_{m1}B & \dots & a_{mn}B \end{pmatrix},$$

is the Kronecker product of A and B .

In analogy to the expansion of the Tensor product of Hilbert spaces, the Kronecker product can be expanded in the same manner, by taking the Kronecker product of N matrices $\otimes_{i=1}^N A_i$ [11].

Let $\mathcal{H} = \mathbb{C}^{2^N}$ be the Hilbert space associated with an N -qubit array. Let σ_i be a arbitrary Pauli matrix. Consider the extension of σ_i on \mathbb{C}^{2^N} , that is, σ_i^α . The operator σ_i^α is a **local operator** on \mathbb{C}^{2^N} , that only acts on the Hilbert space \mathcal{H}_α and leaves the other $N-1$ Hilbert spaces invariant. Physically, the local operator σ_i^α only acts on the qubit with index α . In section 2.2.2 we will extend the notion of a local operator to the notion of local control. A Kronecker product of N matrices, that contains k Pauli matrices $\sigma_1, \sigma_2, \dots, \sigma_k$ and $N - k$ identity matrices is called **Pauli interaction** and a special type of a **global operators**¹¹. Physically, it can be interpreted as coupling k qubits in an N -qubit array. For instance, if one affects a single qubit by a local control. Then the other $k - 1$ qubits are also affected, while the other $N - k$ qubits are left invariant. The following Pauli interactions will be important in the further course of the bachelor thesis.

Definition 2.1.10. (Two-qubit interaction) Let $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \dots \otimes \mathcal{H}_N$ be a Hilbert space associated to a N -qubit System. Let $\alpha, \alpha' \leq N$ and without loss of generality let $\alpha < \alpha'$. A **two-qubit interaction** is a Kronecker product of N matrices with the form,

$$\sigma_i^\alpha \sigma_j^{\alpha'} = \mathbb{1}^1 \otimes \mathbb{1}^2 \otimes \dots \otimes \mathbb{1}^{n-1} \otimes \sigma_i^\alpha \otimes \mathbb{1}^{\alpha+1} \otimes \dots \otimes \sigma_j^{\alpha'} \otimes \mathbb{1}^{\alpha'+1} \otimes \dots \otimes \mathbb{1}^N. \quad (2.14)$$

With Pauli matrix σ_i on the position α , Pauli matrix σ_j on the position α' and identity matrices $\mathbb{1} = \mathbb{1}_2$ elsewhere.

Physically, the two-qubit interaction is a coupling between the qubits with index α and α' ¹². An important special case of the two-qubit interaction, is the **nearest-neighbour interaction**, where only adjacent qubits are coupling. Let $n < N$,

$$\sigma_i^\alpha \sigma_j^{\alpha+1} = \mathbb{1}^1 \otimes \mathbb{1}^2 \otimes \dots \otimes \mathbb{1}^{\alpha-1} \otimes \sigma_i^\alpha \otimes \sigma_j^{\alpha+1} \otimes \mathbb{1}^{\alpha+2} \otimes \dots \otimes \mathbb{1}^N. \quad (2.15)$$

In the following, we discuss examples of 3-qubit arrays in which the nearest-neighbour interaction describes couplings between qubits. Furthermore, the notion of nearest-neighbour interaction will

¹¹Local operators are local gates. Global operators are non-local gates.

¹²In some sources the two-qubit interaction is referred as two-body interaction.

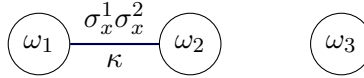


Figure 2.3: Shown is a 3-qubit system. The nodes represent the qubits. Here, $\omega_1, \omega_2, \omega_3$ means all considered qubits have different level-spacings, i.e., no energy degeneracy. Furthermore, the edges represent interactions between the qubits. The first and the second qubit couple via nearest-neighbour interaction $\kappa \sigma_x^1 \sigma_x^2$, while $\kappa \in \mathbb{R}$ is a **strenght coefficient** that describes the strength of the coupling. The third qubit is decoupled since there exists no two-qubit interaction between the third -and any other qubit.

become important in section 2.2.2, where it will be used for the N-qubit chain and the N-qubit loop. In a system consisting of N qubits, qubits can also exist which do not interact with any other qubits. Consider a N-qubit array that contains N-qubits, q_1, q_2, \dots, q_N . It has a **decoupled** qubit q_n , if there is no two-qubit interaction, that connects q_n with another qubit $q_i, i \neq n, 1 \leq i \leq N$. A trivial example would be a system of two decoupled qubits. A more meaningful example is the 3-qubit system with only one two-qubit interaction and a single decoupled qubit, shown in the figure 2.3.

Example 2.1.11. (3-qubit chain) Consider the Hamiltonian:

$$H_0 = \sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \kappa_a \sigma_x^1 \sigma_x^2 + \kappa_b \sigma_x^2 \sigma_x^3, \quad \text{with } \omega_\alpha, \kappa_a, \kappa_b \in \mathbb{R} \setminus \{0\}.$$

H_0 describes a time-independent, non-degenerate 3-qubit chain with nearest-neighbour interactions $\kappa_a \sigma_x^1 \sigma_x^2 + \kappa_b \sigma_x^2 \sigma_x^3$. The system is illustrated in figure 2.2. It is an important qubit array, that was investigated in the results chapter 4.1.

Another important 3-qubit array is the **3-qubit loop**. It is a 3-qubit chain, with an additional **loop interaction**. The loop interaction lets the first and the third qubit couple via an two-qubit interaction of the form $\kappa_c \sigma_x^1 \sigma_x^3$ with $\kappa_c \in \mathbb{R} \setminus \{0\}$.

Example 2.1.12. (3-qubit loop) Consider the 3-qubit chain from the previous example with an additional loop interaction $\sigma_x^1 \sigma_x^3$, which means the first and the third qubit are linked through two-qubit interaction. The Hamiltonian that describes the 3-qubit loop, has then an additional loop term.

$$H_{0,Lp} = \underbrace{H_0}_{\text{chain}} + \underbrace{\kappa_c \sigma_x^1 \sigma_x^3}_{\text{loop-interaction}} = \sum_{\alpha}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \kappa_a \sigma_x^1 \sigma_x^2 + \kappa_b \sigma_x^2 \sigma_x^3 + \kappa_c \sigma_x^1 \sigma_x^3, \quad \text{with } \omega_\alpha, \kappa_{a,b,c} \in \mathbb{R} \setminus \{0\}.$$

Considering the left side of figure 2.2 one can recognize a triangle, that emerged by connecting the nodes through edges. Since the diagram shows not only a connected graph, but a closed graph it justifies the name 3 qubit loop.

2.2 Quantum Control Theory

Quantum control theory mainly focuses on how to efficiently manipulate quantum systems to create desired behaviors [12]. It developed through decades of research in nuclear magnetic resonance and electron paramagnetic resonance. In several cases, one uses electric fields, magnetic fields, or lasers to manipulate the unitary evolution of a quantum system. The technologies used to manipulate the behavior of the quantum system are called **controls**. If the dynamics of a quantum system, depends on one or more controls, it is said to be a **quantum control system**. The famous Stern-Gerlach experiment can be understood as a quantum control experiment, where the trajectory of a particle-ray was influenced by a magnetic field. The implementation of qubits, for instance, superconducting circuits that are manipulated by microwave radiation or ion-traps, where laser-pulses manipulate ions, are understandable as quantum control systems. The example 2.2.1 is an example of a quantum control system. Since the second qubit is periodically affected by an electromagnetic field, the quantum system is influenced to do certain behaviors.

Example 2.2.1. (Two-Qubit System manipulated by periodic Electromagnetic Field)

The Hamiltonian that is associated with the two-qubit system, that is manipulated by an electromagnetic field has the form:

$$H(u(t)) = \sum_{\alpha=1}^2 \frac{\omega_{\alpha}}{2} \sigma_z^{\alpha} + \sigma_x^1 \sigma_x^2 + A \cos(t) \sigma_y^2. \quad (2.16)$$

The two-qubit system is a composite system, where each qubit has Hilbert space $\mathcal{H}_1 = \mathcal{H}_2 = \mathbb{C}^2$. According to definition 2.1.6 the state space that corresponds to the system is the tensor space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 = \mathbb{C}^4$ with $\dim(\mathcal{H}) = 4$. The drift-Hamiltonian $\sum_{\alpha=1}^2 \frac{\omega_{\alpha}}{2} \sigma_z^{\alpha}$ describes the level-spacing of the single qubits $\pm \frac{\omega_1}{2}$, $\pm \frac{\omega_2}{2}$ of the undisturbed system. The interaction between both qubits is described by the Kronecker product $\sigma_x^1 \sigma_x^2$, while the second qubit gets manipulated by an extern electromagnetic field via the operator $A \cos(t) \sigma_y^2$.

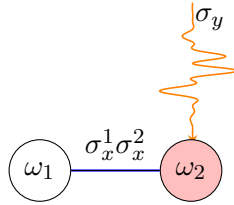


Figure 2.4: This two-qubit system is manipulated by the local control $A \cos(t) \sigma_x^2$. More precisely, the time-dependent electromagnetic field $A \cos(t)$ acts on the second qubit via the local operator σ_x^2 .

2.2.1 Quantum Control Systems

In this work, we have been mainly concerned with a class of quantum control systems modeled by a time-dependent Hamiltonian $H = H(t)$. That is:

$$H(t) = H_0 + \sum_{i=1}^N u_i(t) H_i(t).$$

The time-independent Hamiltonian H_0 describes the undisturbed quantum system. The control functions $u_i(t)$, that contain information about the dynamics of the external system are modeled by piecewise continuous functions. The control-Hamiltonian $\sum_{i=1}^N u_i(t) H_i(t)$, contains information about the unitary evolution of the control, that affects the quantum system. The complete Hamiltonian $H(t)$ models the energy exchange with the external system, that is the control.

All quantum control systems have a mathematical feature in common:

Quantum control systems are modelled by **bilinear control systems**.

This fact is useful because the unitary evolution of bilinear systems can be determined. More precisely, the unitary evolution is determined by an element of unitary matrices or an element of special unitary matrices, as we will see later in the chapter 2.3.3. To give an appropriate mathematical description of quantum control systems, we will introduce a sufficient amount about **classical control theory**, that is needed for further descriptions. **Linear systems** are mathematical models for sufficiently well-isolated parts of nature¹³. Linear systems are deterministic and have internal state functions. The system dynamics is describable and solutions of the system's state equation follow the superposition principle.¹⁴ Linear systems are imaginable through the **black box model**. There is an input, which is called the state of the system and there is an output, that is measurable for the observer. Let V be a vector space, with $\dim(V) = N$ and $U \subset V$ be a subspace, with $\dim(U) = M$. A **linear control system** is a linear matrix differential equation

$$\dot{x} = A(t)x(t) + B(t)u(t) \quad (2.17)$$

with continuous time $t \in \mathbb{R}_{\geq 0}$, continuous state operators $A(t) \in \mathbb{K}^{NxN}$ and $B(t) \in \mathbb{K}^{NxM}$, internal state $x(t) \in V$ and control $u(t) \in U$. Quantum control systems are generally not modeled by linear control systems, but from **bilinear control system**. A bilinear control system is a bilinear matrix differential equation

$$\dot{x} = \left(A(t) + \sum_{i=1}^M B_i(t)u_i(t) \right) x(t). \quad (2.18)$$

Note, that a state $x(t)$ behaving according to equation (2.18) is not an element of a linear vector space, but an **affine vector space**. For the linear vector space V and a translation vector $u \in U$, exists a affine subspace of the form:

$$u + V := \{u + x | x \in V\}$$

¹³Since all appearing functions are linear, it is reasonable to call those mathematical models, linear systems.

¹⁴One could add that there are physical states that are observable but do not give information about the underlying physics, additionally there are always weak interactions with the environment.

Eventually, it is the goal to find an accurate model for quantum control systems, therefore it is to clarify why bilinear control systems are suitable in modeling quantum control systems. Firstly, it is needed to find an equation of motion in terms of operators, similar to equation (2.9). Therefore, the following statement is helpful, because it links the equation of motion for vector states with the equation of motion for matrix states and uses terms of bilinear control.

The unitary operator $U(t)$ obeys the same equation of motion as the state vector $x(t)$.

$$\dot{U} = \left(A(t) + \sum_{i=1}^M B_i u_i(t) \right) U(t), \quad U(0) = \mathbb{1}_N \quad (2.19)$$

Consider a N-dimensional quantum system with time-independent Hamiltonian H_0 , that is manipulated by M controls. The emerging system is a Quantum control systems with Hamiltonian:

$$H(u(t)) = \frac{-i}{\hbar} \left(H_0 + \sum_{k=1}^{M \leq N} H_k u_k(t) \right).$$

H_0 is the undisturbed Hamiltonian and $\sum_{k=1}^N H_k u_k$ the control-Hamiltonian. Firstly, setting the bilinear equation of motion for states (2.18):

$$\frac{d}{dt} |\psi(t)\rangle = \frac{-i}{\hbar} \left(H_0 + \sum_{k=1}^{M \leq N} H_k u_k \right) |\psi(t)\rangle.$$

Hence, one obtains the equation of motion for quantum control systems for quantum states $|\psi(t)\rangle$ in the associated Hilbert space \mathcal{H} . Replacing the quantum state $|\psi(t)\rangle$ with the unitary evolution operator according to equation 2.19.

$$\dot{U} = \frac{-i}{\hbar} \left(H_0 + \sum_{k=1}^{M \leq N} H_k u_k \right) U(t), \quad U(0) = \mathbb{1}_N \quad (2.20)$$

The solution of equation (2.20) is a unitary matrix and varies in the Lie group $U(N)$ for $t \in \mathbb{R}_{\geq 0}$. The unitary matrix $U(t)$ can be considered as the state of the system at the time t. If $U(t)$ reaches all possible $U \in U(N)$, then the system is controllable as we will see in chapter 2.3.

2.2.2 Controlling Qubit Arrays

In this section, it will be shown how to control qubits using local controls. Consider the Hamiltonian in equation (2.20). When controlling qubits is the desired goal, it takes a special form that is going to be discussed in the following.

Definition 2.2.2. (Local Control) Let $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \dots \otimes \mathcal{H}_N$ be a Hilbert space associated to a N-qubit system. Let $u(t)$ be a control function and $1 \leq \alpha \leq N$. A **local control** is the product of $u(t)$ and a linear combination of local operators $\sigma_{i,j,k}^\alpha$ that act on the same Hilbert space \mathcal{H}^α .

$$u(t)(\kappa_i \sigma_i^\alpha + \kappa_j \sigma_j^\alpha + \kappa_k \sigma_k^\alpha), \quad \text{with} \quad \kappa_i, \kappa_j, \kappa_k \in \mathbb{R}. \quad (2.21)$$

Consider example 2.2.1, it has a local control $A\cos(t)\sigma_y^2$. In the results chapter, we will mainly concern 3-qubit arrays with a local control is $u(t)\sigma_x^2$. We will refer to this type of local control as σ_x -control on the second qubit.

Now we will introduce how to describe N -qubit arrays mathematically. For N qubits are many different arrangements imaginable. Generally, any graph containing nodes and edges can be understood as a qubit array. The nodes represent the qubits and the edges represent the two-qubit interactions. Let $N, M \in \mathbb{N}$. A generic **N -qubit array** with M local controls, $M \leq N$, is described by the following Hamiltonian $H(u(t))$. It has three parts of that it is composed.

$$H(u(t)) = \underbrace{\sum_{\alpha=1}^N \frac{\omega_\alpha}{2} \sigma_z^\alpha}_{\text{drift}} + \underbrace{\sum_{\alpha', \alpha=1}^N \sum_{i,j=1, i \neq j}^3 \kappa_{(i,j)}^{\alpha, \alpha'} \sigma_i^\alpha \sigma_j^{\alpha'}}_{\text{interaction}} + \underbrace{\sum_{\alpha=1}^M \sum_{k=1}^3 u_k^\alpha(t) \sigma_k^\alpha}_{\text{control}} \quad (2.22)$$

The first part, is said to be the **drift-Hamiltonian**. The drift Hamiltonian describes the level-spacing of the qubits, when the qubit is not affected. That is, when the qubits do not interact with each other and they are not under control. The second part, is the **interaction-Hamiltonian**. The interaction Hamiltonian describes all interactions that exist between the qubits. The addition of the drift-Hamiltonian and the interaction-Hamiltonian is a time-independent Hamiltonian and will be referred as H_0 . The systems **control-Hamiltonian** describes all local controls acting on all qubits. One could arrange N qubits with nearest-neighbour interactions in a line, what is called a **N -qubit chain** and an important type of a qubit array. To manipulate an N -qubit array, it must be equipped with local controls.

Definition 2.2.3. (N -qubit Chain with M local controls)

Let $N, M \in \mathbb{N}$ and $M \leq N$. A System of N qubits, is a N -qubit Chain, if the qubits only interact through nearest-neighbour interaction. The generic Hamiltonian associated to a N -qubit chain:

$$H(u(t)) = \sum_{\alpha=1}^N \frac{\omega_\alpha}{2} \sigma_z^\alpha + \sum_{\alpha=1}^N \sum_{i,j=1, i \neq j}^3 \kappa_{(i,j)}^{\alpha, \alpha+1} \sigma_i^\alpha \sigma_j^{\alpha+1} + \sum_{\alpha=1}^M \sum_{k=1}^3 u_k^\alpha(t) \sigma_k^\alpha \quad (2.23)$$

With $\omega_\alpha, \kappa_{(i,j)}^{\alpha, \alpha+1} \in \mathbb{R} \setminus \{0\}$.

The coefficients have physical meaning, that is going to be listed:

1. ω_α describes the level spacing of the qubit with index α .
2. $\kappa_{(i,j)}^{\alpha, \alpha+1}$ is the strength or **strength coefficient** of the coupling between the qubit α and qubit $\alpha + 1$ mediated via the operator $\sigma_i^\alpha \sigma_j^{\alpha+1}$.
3. $u_k(t)^\alpha$ is a control-function acting on the qubit α , through the operator σ_k^α .

One could take an N -qubit chain with M local controls and couple the first-and the N' th qubit via two-qubit interaction. This important qubit array is referred to as **N -qubit loop** with M local controls.

Definition 2.2.4. (N -qubit Loop with M local controls)

An N -qubit Loop is a N -qubit chain, with an additional two-qubit interaction, which connects the first and the N 'th qubit. Let $H(u(t))$ be the generic Hamiltonian of an N -qubit chain with M local controls, then a generic N -qubit Loop is described by the Hamiltonian

$$H_{Lp}(u(t)) = H(u(t)) + \sum_{i,j=1, i \neq j}^3 \kappa_{(i,j)}^{1,N} \sigma_i^1 \sigma_j^N \quad (2.24)$$

Terms of the structure $\sum_{i,j=1, i \neq j}^3 \kappa_{(i,j)}^{1,N} \sigma_i^1 \sigma_j^N$ will be referred as being **loop interactions** or **loop terms**.

Consider the example 2.1.11 for a 3-qubit chain and example 2.1.12 for a 3-qubit loop. If the desired goal is to control the qubit arrays, then one could equip the systems with local controls of the form $u(t)\sigma_i^\alpha, i \in \{x, y, z\}, \alpha \in 1, 2, 3$. Degenerate energy levels of the drift-Hamiltonian, that is, $\omega_\alpha = \omega$ or all equal strenght coefficients $\kappa_{i,j} = \kappa$ are referred as **symmetries**. The next comment is a bit of anticipation of the next chapter, but is very appropriate at this point [13]:

Symmetries can make quantum systems uncontrollable. Therefore, it is advantageous to avoid symmetries whenever possible.

If $\omega_\alpha = \omega = \kappa_{i,j} = \kappa \neq 0$ is true for a qubit array, it will be referred as **maximized symmetry**.

2.3 Controllability of Quantum Systems

Controllability describes the ability to move a system around, in its entire configuration space using only certain admissible manipulations¹⁵. Consider the 2-qubit system as in example 2.2.1. The Hamiltonian of this 2-qubit system obeys the bilinear equation of motion (2.20). Roughly speaking, if the state $U(t)$ reaches every element of the Lie group $U(4)$, then the 2-qubit system would be controllable (As we will see in this chapter). There are multiple forms of controllability. Some notions are equivalent, like pure state controllability and state-to-state controllability. Other notions are stronger than others as **operator controllability**. In this thesis, the operator controllability of certain 3-qubit arrays was examined, see chapter 4.5. Generally, there are many approaches studying the controllability of a quantum system. However, in this thesis, we are going to consider two different methods, that are presented in the method chapter. The first way uses concepts of Lie theory, while the second way uses concepts of graph theory [7], [14].

2.3.1 Notions of Controllability

Definition 2.3.1. (State-to-State Controllability) Let \mathcal{H} be a finite-dimensional Hilbert space, associated to a quantum system. If any final time $T > 0$ and control function $u(t)$ exist, such that $u(t)$ is able to steer the system from $|\psi(0)\rangle$ to any arbitrary target state $|\psi(T)\rangle$, then the quantum system is said to be **state-to-state controllable**.

$$\exists u(t), T \text{ such that } |\psi\rangle_0 = |\psi(0)\rangle, \text{ then } |\psi\rangle_1 = |\psi(T)\rangle. \quad (2.25)$$

¹⁵The exact definition varies slightly within the framework or the type of models applied.

Controllability means in that case, that every state $|\psi\rangle$ in the Hilbert space \mathcal{H} is achievable, by manipulating the control function $u(t)$. Physically, manipulating a quantum system could be effectively done by laser pulses [14]. According to the equation 2.8, a state transition with final state $|\psi(T)\rangle$ is achievable, through a unitary transformation that acts on the initial state $|\psi\rangle_0$. Hence, we can rephrase the definition 2.3.1 and formulate it in terms of unitary operators. Furthermore, we emphasize the fact that quantum mechanical states are normalized unit vectors, so they are elements of the unit sphere.

Definition 2.3.2. (Pure State Controllability) A N-dimensional quantum system is **pure state controllable**, if for **any** pair of elements on the complex unit sphere $|\psi\rangle_0, |\psi\rangle_1 \in S(\mathbb{C})^{N-1}$ exists a unitary matrix U in the Lie group $\mathbf{e}^{\mathcal{L}}$, connected to the quantum system, such that the following equation holds ¹⁶:

$$|\psi\rangle_1 = U |\psi\rangle_0. \quad (2.26)$$

The Lie group connected to a quantum system is going to be explained in more detail in the theorem 2.3.12. For now, it is only important, that the reachable set of unitary operators U in the bilinear equation of motion (2.20) forms a Lie group.

Definition 2.3.3. (Operator Controllability) An N-dimensional quantum control system, that unitary evolution obeys to the bilinear equation of motion (2.20), is said to be **operator controllable**, if all matrices $U(t)$ that can be obtained, is the group of unitary matrices $U(N)$ or the group of special unitary matrices $SU(N)$.

Physically, if a quantum system is operator controllable, it exists an admissible control $u(t)$, that drives the state U into every other desired unitary (or special unitary) state. The difference between achieving $U(N)$ and $SU(N)$ is in the global phase¹⁷.

- Achieving $U(N) \Leftrightarrow$ Controlling the global phase and all local phases.
- Achieving $SU(N) \Leftrightarrow$ Controlling all local phases.

Operator controllability is sufficient but not necessary for pure-state-controllability. If an N-dimensional quantum system with associated Hilbert space \mathcal{H} is operator controllable, then any unitary-or special unitary transformation is admissible. Hence, it can take any initial state $|\psi(0)\rangle$ into any final state $|\psi(t)\rangle$, by a unitary transformation. It is a much stricter requirement than pure state controllability because it requires simultaneous control of all N^2 entries of the evolution operator $U(t)$. In comparison, moving any state to any other state, as in pure state controllability, requires controlling only one row or one column of the $N \times N$ evolution operator $U(t)$.

¹⁶The unit-norm constraint does not completely determine a state $|\psi\rangle$ within the ray. Hence, if we can steer $|\psi\rangle$ to any target state, then we can also steer equivalent states $\mathbf{e}^{i\phi} |\psi\rangle$ to any target state. This is referred as equivalent state controllability [7].

¹⁷Conventionally, one uses the term operator controllable for both, meaning for the unitary case and for the special unitary case as well, while pointing out differences wherever appropriate. In some cases, authors refer to operator controllability in the unitary case as complete controllability [15].

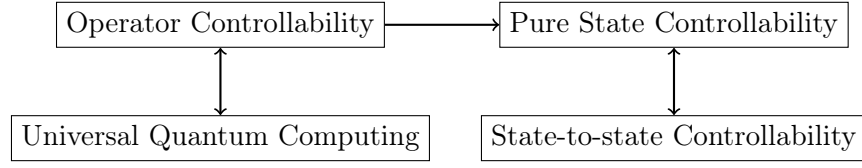


Figure 2.5: Universal quantum computing is equivalent to Operator controllability of a **qubit array**. While operator controllability implies pure state controllability. Pure state controllability is equivalent to state-to-state controllability since we only consider quantum systems.

If an N -qubit array is operator controllable, then every unitary- or special unitary transformation in $U(2^N)$ is achieved. This is equivalent to, every quantum logic gate being generable. From this follows:

Operator controllability is equivalent to universal quantum computing. A qubit array that is operator controllable, is a qubit array that allows universal quantum computing and vice versa.

From now on operator controllability will be referred to as controllability, if not stated otherwise.

2.3.2 Lie Algebras and Lie Groups

The study of Lie algebras and Lie groups is part of the mathematical Lie theory. Roughly speaking, the Lie theory shows a fundamental correspondence between different algebraic structures. The significant result, for analyzing controllability in quantum systems is that Lie algebras correspond to Lie groups via the exponential mapping. In the following one came across a few mathematical terms, that in other contexts are explained in rigorous mathematical details. It is not the goal of this thesis to cover everything about the mathematical background, but we focus on the main concepts that are important for this thesis.

Definition 2.3.4. (Lie Algebra) A **Lie algebra** \mathcal{L} over a field \mathbb{K} is a vector space V over the field \mathbb{K} , with a binary operation, that is called **Lie bracket** $[\cdot, \cdot]$, that satisfies the following conditions: Let $x, y, z \in \mathcal{L}$ and $\alpha \in \mathbb{K}$

1. **Bilinearity**

$$[x + y, z] = [x, z] + [y, z].$$

$$[x, y + z] = [x, y] + [x, z].$$

$$\alpha[x, y] = [\alpha x, y] = [x, \alpha y].$$

2. **Skew-Symmetry**

If $\mathbb{K} = \mathbb{R}$ or \mathbb{C}

$$[x, y] = -[y, x].$$

3. **Jacobi-Identity**

$$[x, [y, z]] + [y, [z, x]] + [z, [x, y]] = 0.$$

To indicate that a certain Lie bracket is defined on a specific Lie Algebra \mathcal{L} , we write $[\cdot, \cdot]_{\mathcal{L}}$.

Definition 2.3.5. (Lie Subalgebra) Let \mathcal{L} be a Lie algebra. Then a vector space \mathcal{A} is a Lie subalgebra of \mathcal{L} , if \mathcal{A} is a subspace of \mathcal{L} and if \mathcal{A} forms a Lie algebra with the Lie bracket $[\cdot, \cdot]_{\mathcal{L}}$.

A familiar example of a Lie algebra is the vector space \mathbb{R}^3 equipped with the cross-product \times of two vectors since cross-product \times is a Lie bracket. In this thesis, we are concerned with matrix Lie algebras. Consider the vector space of square matrices $\mathbb{K}^{N \times N}$, with $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$. Let $A, B \in \mathbb{K}^{N \times N}$. A **commutator** is a binary function, that is defined via $[A, B] = AB - BA$. Note that, the commutator is Lie bracket¹⁸. The vector space $\mathbb{K}^{N \times N}$ equipped with the commutator is a Lie algebra. One can prove, that every subspace V of $\mathbb{K}^{N \times N}$ equipped with the commutator generates a Lie subalgebra of $\mathbb{K}^{N \times N}$ [16]. Consider a matrix $X \in \mathbb{C}^{N \times N}$, that fulfills $X = -X^\dagger$. The matrix X is said to be a **skew-Hermitian matrix**. The set of all skew-Hermitian matrices forms an \mathbb{R} -vector space. The following are important examples of Lie algebras for this thesis:

The \mathbb{R} -vector space of **skew-Hermitian matrices** equipped with the commutator is a Lie algebra. It is written as:

$$u(N) := \{X \in \mathbb{C}^{N \times N} | X = -X^\dagger\} \quad (2.27)$$

The \mathbb{R} -vector space of **traceless skew-Hermitian matrices** equipped with the commutator is a Lie algebra. It is written as:

$$su(N) := \{Y \in u(N) | \text{tr}(Y) = 0\} \quad (2.28)$$

The Lie algebra $u(N)$ is important since skew-Hermitian matrices appear in all relevant equations of motion. For instance, consider the Schrödinger operator equation (2.7). For every time t is $iH(t)$ a skew-Hermitian matrix.

The Lie groups that are going to be considered are always matrix groups and Lie subgroups of the Lie group $Gl_N(\mathbb{C})$: That is the general linear group over the complex field and only contains square matrices with determinant different from zero. Before introducing Lie groups, we will shortly discuss another mathematical term, that is fundamental for it. Here, a **manifold** M is a subset of $\mathbb{K}^{N \times N}$, $N \in \mathbb{N}$, $\mathbb{K} = \mathbb{R}$ or \mathbb{C} , that can be homeomorphically mapped into the N -dimensional Euclidean space \mathbb{R}^N ¹⁹.

Definition 2.3.6. (Lie Group) A **Lie group** is an analytical differentiable manifold G , that has the structure of a group. The group operations inversion and multiplication are analytic functions²⁰.

If H is a subgroup and an analytical submanifold of the Lie group G , then H is said to be a **Lie subgroup** of G ²¹. Consider the following Lie subgroups of $Gl_N(\mathbb{C})$, that play a fundamental role in quantum mechanics. The **unitary group** $U(N)$ contains all quantum gates. Moreover, its elements are important for unitary evolution of quantum systems.

$$U(N) := \{U \in Gl_N(\mathbb{C}) | UU^\dagger = \mathbf{1}_N\}. \quad (2.29)$$

The **special linear group** Sl_N contains all matrices with determinant equal to one. The special matrices describe all linear transformations that leave the volume and the orientation of the

¹⁸In physics, this function goes often under the name commutator, while in mathematics, it goes under the name **standard matrix commutator**.

¹⁹A Homeomorphism is a function f between two topological spaces X and Y , that is bijective, continuous and has a continuous inverse function [17],[16].

²⁰Here, an **analytic function** is a function $f(x_1, x_2, \dots, x_n)$ that can be approximated by a Taylor-expansion in every variable, for every point of its range and every neighbourhood.

²¹Formally one would have to prove all Lie subgroup properties to show that H is a Lie subgroup of G . One can prove, that the subgroups of the general linear group are analytical submanifolds by defining a homeomorphism mapping to the euclidean space \mathbb{R}^{N^2} [17].

coordinate space invariant ²². The special linear group is defined as:

$$Sl_N := \{S \in Gl_N(\mathbb{C}) \mid \det(S) = 1\}. \quad (2.30)$$

Since $U(N)$ and Sl_N are subgroups of $Gl_N(\mathbb{C})$, their intersection is as well a subgroup of $Gl_N(\mathbb{C})$ [11].

$$SU(N) := U(N) \cap Sl_N := \{V \in Gl_N(\mathbb{C}) \mid VV^\dagger = \mathbb{1}_N, \det(V) = 1\}. \quad (2.31)$$

Since $SU(N) \subset U(N)$ it is relevant universal quantum computing. Moreover, it is important for controllability as we have seen in the definition 2.3.3. The correspondence between Lie algebras and Lie groups is given by the exponential function. The exponential function maps Lie algebras to Lie groups [17].

Definition 2.3.7. (Matrix Exponential) Let $A \in \mathbb{K}^{n,n}$. The exponential of the matrix A is defined by the following power series:

$$\mathbf{e}^A = \sum_{k=0}^{\infty} \frac{A^k}{k!} = \mathbb{1} + A + \frac{A^2}{2} + \dots$$

For every $A \in \mathbb{K}^{n,n}$, the power series converges.

Moreover, the matrix exponential has several interesting mathematical properties. Here, the following two properties are needed. Firstly it holds that $(e^A)^\dagger = e^{A^\dagger}$. Secondly, $\det(e^A) = (e^{\text{tr}(A)})$ ²³. The significance of the matrix exponential 2.3.7, becomes clear when inserting elements from an Lie algebra. By inserting in definition 2.3.7, we can conclude the following:

Corollary 2.3.8. *The matrix exponential maps the Lie algebra of skew-Hermitian matrices $u(N)$ to the Lie group of unitary matrices $U(N)$ ²⁴. Furthermore, the matrix exponential maps the Lie algebra of traceless skew-Hermitian matrices $su(N)$ to the Lie group of special unitary matrices $SU(N)$.*

$$\mathbf{e}^{u(N)} = U(N) \quad (2.32)$$

$$\mathbf{e}^{su(N)} = SU(N) \quad (2.33)$$

Proof. Consider $X \in u(N)$, therefore it fulfills the property $X = -X^\dagger$.

$$\begin{aligned} \mathbf{e}^X &= \mathbf{e}^{-X^\dagger} \\ \mathbf{e}^{X+X^\dagger} &= \mathbb{1}_N \\ \mathbf{e}^X \mathbf{e}^{X^\dagger} &= \mathbb{1}_N \\ \mathbf{e}^X (\mathbf{e}^X)^\dagger &= \mathbb{1}_N. \end{aligned}$$

Hence the image of any skew-Hermitian matrix is a unitary matrix. Likewise consider $Y \in su(N)$.

$$\det(\mathbf{e}^Y) = e^{\text{tr}(Y)} = e^{0_N} = \mathbb{1}_N.$$

It follows, that the image of any $Y \in su(N)$ is a special unitary matrix. □

²²The volume and the orientation stays the same, since the determinant describes the change of volume after a linear transformation [11].

²³Here, $\text{tr}(A)$ means the trace of the matrix A . That is the sum of its diagonal entries.

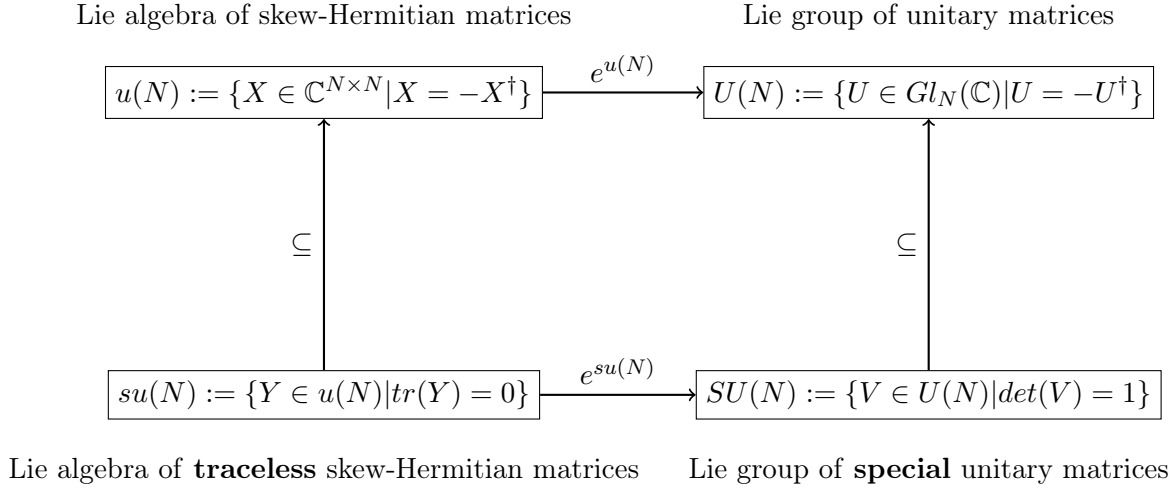


Figure 2.6: The upper diagram shows the association between Lie algebras and Lie groups via the matrix exponential and also the inclusion from $su(N)$ to $u(N)$, as well as the inclusion from $SU(N)$ to $U(N)$.

To indicate the relation to the Lie group $U(N)$, the notation of the Lie algebra $u(N)$ is used. Likewise, for the Lie group $SU(N)$ and the Lie algebra $su(N)$.

2.3.3 Determining Controllability in Quantum Systems

The goal of this section is to give the necessary framework for upcoming methods, such that one can determine if a quantum control system is controllable. The method 3.1 requires the calculation of so-called nested commutators.

Definition 2.3.9. (Nested commutators and Depth) Let $\{H_0, H_1, \dots, H_k\}$ be a set of elements in a Lie subalgebra \mathcal{S} . Then a commutator L of the form $L = [K_1, [K_2, \dots [K_p, K_{p+1}] \dots]]$ is a **nested commutator** with **depth** p and $K_i \in \{H_0, H_1, \dots, H_k\}$. The depth of a nested commutator L is the number of commutators that is necessary to generate L .

Roughly, calculating nested commutators increases the given Lie subalgebra \mathcal{S} . Each nested commutator of depth p , that is not linearly dependent, can be interpreted as a new direction that \mathcal{S} gains. If the aim is to increase the Lie subalgebra, then it is a logical step to calculate several nested commutators.

Let $\{H_0, H_1, \dots, H_k\}$ be a set of elements lying in a Lie algebra \mathcal{L} . The set of all nested commutators spans a Lie subalgebra \mathcal{S} of \mathcal{L} . \mathcal{S} is the smallest Lie subalgebra that contains $\{H_0, H_1, \dots, H_k\}$

To indicate, that we are going to calculate all nested commutators of depth p , of a given set $\{H_0, H_1, \dots, H_k\}$. We write $Lie\{H_0, H_1, \dots, H_k\}$. As a matter of fact, if we want to show that the Lie subalgebra generated by $\{H_0, H_1, \dots, H_k\}$, noted by $Lie\{H_0, H_1, \dots, H_k\}$, is equal to another Lie

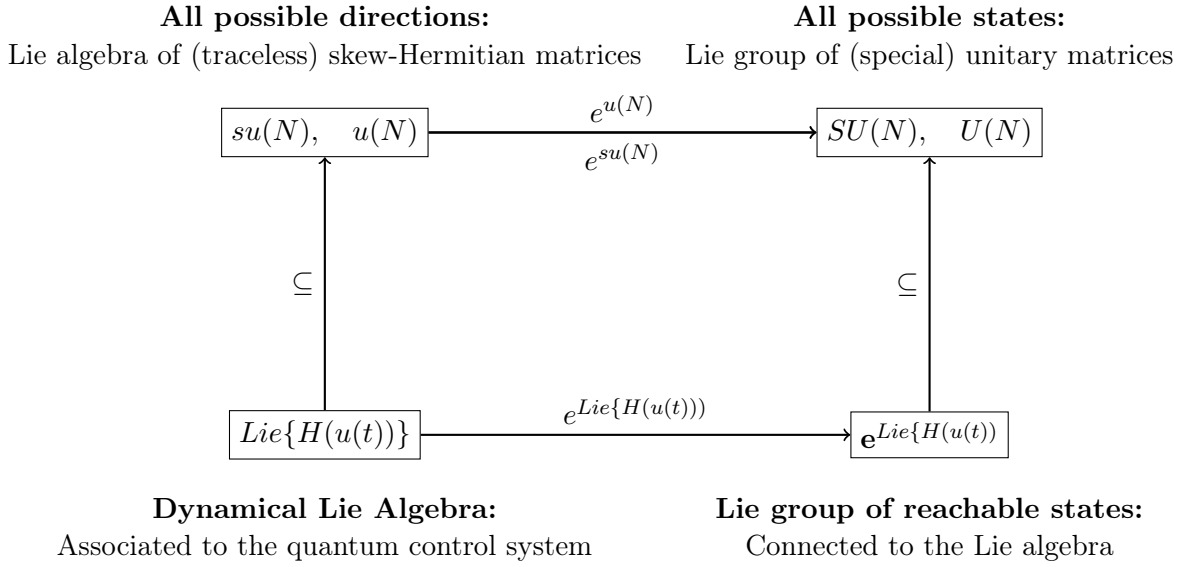


Figure 2.7: The Dynamical Lie algebra is associated with the quantum control system and encodes information in the directions that are obtainable in $u(N)$. It is always a Lie subalgebra of the Lie algebra of skew-Hermitian matrices $u(N)$. Moreover, the dynamical Lie algebra is connected to the Lie group $\mathbf{e}^{Lie\{H(u(t))\}}$, that contains all reachable states of the quantum control system. Note that, the Lie group $\mathbf{e}^{Lie\{H(u(t))\}}$ is always a Lie subgroup of $U(N)$, which contains all possible unitary states.

algebra \mathcal{T} . We have to show, that the nested commutators form a basis of \mathcal{T} . If by calculating nested commutators, one finds more elements as in the basis of \mathcal{T} , then \mathcal{T} is a Lie subalgebra of $Lie\{H_0, H_1, \dots, H_k\}$. Consider $\{\sigma_x, \sigma_y\}$ which is a subset of $su(2)$. We want to increase the set of elements and afterwards take the span of it, therefore we are going to calculate nested commutators. The nested commutator obtained at depth 1 is:

$$[\sigma_x, \sigma_y] = \sigma_x \sigma_y - \sigma_y \sigma_x = 2i\sigma_z.$$

Now, we obtained σ_z as a new direction. Calculating more nested commutators does not bring new elements. Hence, $Lie\{\sigma_x, \sigma_y\}$ is equal to $su(2)$.

Definition 2.3.10. (Dynamical Lie Algebra)

An N-dimensional quantum control system that is evolving according to the bilinear equation of motion (2.20) has an **dynamical Lie algebra** that is associated with the quantum control system.

$$Lie\{H(u(t))\} = Lie\{H_0, H_1, \dots, H_M\} \quad (2.34)$$

$M \leq N$ displays the number of terms in the control-Hamiltonian. The dynamical Lie algebra $Lie\{H(u(t))\}$ is a Lie subalgebra of $u(N)$.

Example 2.3.11. (Two-qubit system manipulated by a periodic Field) Consider example 2.2.1,

with Hamiltonian

$$H(u(t)) = \sum_{\alpha=1}^2 \frac{\omega_{\alpha}}{2} \sigma_z^{\alpha} + \sigma_x^1 \sigma_x^2 + A \cos(t) \sigma_y^2.$$

The notation $Lie\{H(u(t))\}$ means, that we interpret the terms that appear in $H(u(t))$ as a basis, therefore we write

$$Lie\{H(u(t))\} = Lie\left\{\sum_{\alpha=1}^2 \frac{\omega_{\alpha}}{2} \sigma_z^{\alpha} + \sigma_x^1 \sigma_x^2, \quad \sigma_y^2\right\}.$$

Since the control-function $u(t) = A \cos(t)$ affects the second qubit temporary via the operator σ_y^2 , we interpret σ_y^2 as another direction and do not understand $H(u(t))$ as a single direction. The dynamical Lie algebra $Lie\{H(u(t))\}$ of this particular two-qubit system is then the span of all nested commutators that can be obtained by $\{H(u(t))\}$.

The physical significance of the dynamical Lie algebra gets clearer, in terms of achievable states of the associated quantum system. If a skew-Hermitian matrix $X \in Lie\{H(u(t))\}$, then there exists a unitary matrix $U = e^X$, that is a reachable state for the quantum system. The correspondence between skew-Hermitian matrices and unitary states is given by the matrix exponential (2.32). Note that $e^{Lie\{H(u(t))\}}$ is a Lie subgroup of $U(N)$. Consider the figure 2.7 for the exact relation between Lie algebras and Lie groups, that are involved. This correspondence gives rise to the definition of the Lie group connected to associated with the dynamical Lie algebra.

Theorem 2.3.12. (*Reachable States form a Lie Group*) Let \mathcal{L} be the dynamical Lie algebra, associated with a finite-dimensional quantum system. The set of all reachable unitary states of equation (2.20), form a Lie group $e^{\mathcal{L}}$. It is the Lie group connected to the dynamical Lie algebra \mathcal{L} .

It is notable, that the Lie group connected to the dynamical Lie algebra $e^{\mathcal{L}}$ is a Lie subgroup of $U(N)$, while the dynamical Lie algebra \mathcal{L} itself is a Lie subalgebra of $u(N)$.

Theorem 2.3.13. (*Lie Algebra Rank Condition*)

Let equation (2.20) be state-equation associated to a quantum control system. Let \mathcal{L} be the dynamical Lie algebra associated with the system and $e^{\mathcal{L}}$ its connected Lie group. The quantum control system is **controllable** if one of the following two conditions can be satisfied.

1. $\dim(\mathcal{L}) = \dim(u(N)) = N^2$
2. $\dim(\mathcal{L}) = \dim(su(N)) = N^2 - 1$

Although both conditions state whether a system is controllable, they are not equal. The first condition in theorem 2.3.13 implies, that it is possible to manipulate all local phases and the global phase of the system. The second condition implies that only the local phases are controllable. Eventually, controlling all local phases is sufficient, since the global phase of a quantum system is not measurable. The first condition is equivalent to $\mathcal{L} = u(N)$ and $e^{\mathcal{L}} = U(N)$. Likewise the second condition is equivalent to $\mathcal{L} = su(N)$ and $e^{\mathcal{L}} = SU(N)$. Consider figure 2.7. If a quantum control system is controllable it reaches all possible directions in the Lie algebra and all possible states in the (special) unitary group. To conclude, to prove controllability we test if the dynamical Lie algebra of a quantum control system reaches $su(N)$ or $u(N)$ ²⁵.

²⁵The name **Lie algebra Rank condition** is derived from the Rank condition, which is a method that determines if a linear system is controllable. The Rank condition is described in [12].

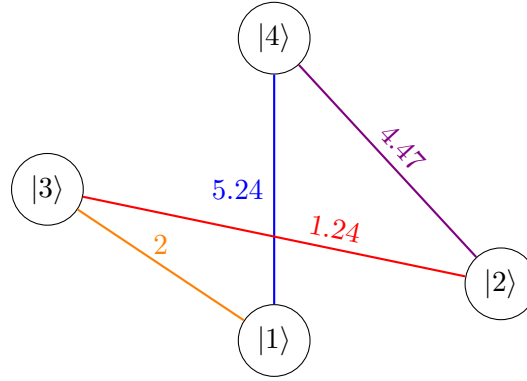


Figure 2.8: This graph corresponds to a controllable two-qubit system and shows the connection of its energy-levels. The **nodes** $\{|1\rangle, |2\rangle, |3\rangle, |4\rangle\}$ represent **energy-levels** of a two-qubit array. The nodes are sorted from lowest- to highest energy, which is indicated by the number within the ket. An **edge** between two nodes, represents that there is a difference in energy, while its **weight** represents the absolute value of the **energy-gap**. The different colors do not follow from any mathematical definition, but serve to distinguish the energy gaps. The selected colors are based on the visible spectrum, therefore **Violet** > **Blue** > **Red** > **Orange** holds. Since this graph is **connected**, it is **pure state controllable**.

2.4 Graph Theory

Graph theory is a subject of pure mathematics, that investigates the properties of networks. In Graph theory, networks are represented abstractly, since objects and their relations are displayed as nodes and edges. The question that comes along naturally while studying graphs concerns the connection of nodes or the number of edges between two nodes²⁶. Graphs are useful tools to visualize objects and their connections, as we have seen in this thesis before. Consider figure 2.2. Each node represented a qubit and each edge represented a two-qubit interaction. Furthermore, basic concepts of graph theory will become important to get insights into a quantum control system's energy levels. If all energy levels are connected by an edge, then the quantum control system is pure state controllable [14]. The graph-theoretic controllability test will be explained in more detail, in the methods chapter.

Definition 2.4.1. (Graph) A **graph** $G = (V, E)$ is a set of nodes V and edges E , where each edge (u, v) is a connection between nodes $u, v \in V$.

Definition 2.4.2. (Weighted Graph) Let $G = (V, E)$ be a graph. G is called **weighted graph**, if there exists a function $d : E \rightarrow \mathbb{R}, (u, v) \rightarrow x$, that maps every edge to a weight.

Definition 2.4.3. (Path) Let $G = (V, E)$ be a Graph. A sequence of nodes $\{v_1, v_2, \dots, v_n | v_i \in V, 1 \leq i \leq n\}$, in which 2 successive nodes are connected by an edge, is called a **path**.

Definition 2.4.4. (Connected Graph) A graph $G = (V, E)$ is a **connected** graph, if every pair of nodes $u, v \in V$ is connected by a path in G .

²⁶Furthermore, classical problems of graph theory, concern the shortest path between two arbitrary nodes within a graph [18].

Paths between nodes, allow a graph to be connected. As an example consider the figure 2.2. The 3-qubit chain and the 3-qubit loop are visualized by connected graphs. For each qubit exists a path to another qubit. The difference between both graphs is that for the 3-qubit chain, the first and the third node are not connected by a single edge. Since graphs can be connected, they also can be **disconnected**. Simply, a graph G is called disconnected, if it is not connected. For instance, consider a 3-qubit system with two coupled qubits and a decoupled qubit as in figure 2.3. Note that there is a pair of interacting qubits within the 3-qubit system, a so-called **connected component** of the graph, that is itself a connected graph [18]. Consider the connected - and weighted graph illustrated in the figure 2.8. We will find this graph again in the chapter about methods in figure 3.4. At first, it is not important how exactly this graph was obtained. It is more important to introduce the concepts of graph theory on an example that has a physical meaning.

Chapter 3

Methods

Two different methods of determining the controllability of an N -dimensional quantum system are going to be considered. The next subsection deals with how to generate a basis for the dynamical Lie algebra 2.3.10 that is associated with the N -dimensional quantum system. Therefore, nested commutators as defined in definition 2.3.9 are going to be calculated until N^2 or $N^2 - 1$ linearly independent elements are obtained. Only then one of the conditions in theorem 2.3.13 is verified. The chapter after deals with how to determine controllability in certain finite-dimensional quantum systems using concepts of graph theory.

3.1 Generating a Basis of an dynamical Lie Algebra

Given is an N -dimensional quantum system, then the following algorithm generates a basis of the dynamical Lie algebra associated with the quantum system [7].

Algorithm to generate a basis of an dynamical Lie algebra.

Let $H(u(t))$ be the Hamiltonian of a N -dimensional quantum system, that obeys to the equation (2.20). Step 0:

Consider all linear independent vectors in $H(u(t))$ to create the following set $\{H_0, H_1, \dots, H_k\}$, that we will refer as commutators of depth 0.

Step n:

1. Obtain nested commutators of depth n, by calculating the commutator with input matrices from nested commutators of depth $n - 1$ and depth 0 (obtained at step $n - 1$ and step 0).
2. Consider the commutators up to depth n and remove all linearly dependent nested commutators.
3. If N^2 or $N^2 - 1$ linear independent nested commutators, where obtained, then the procedure shall be stopped.

If N^2 linear independent nested commutators have already been generated, continuing the algorithm cannot lead to new linear independent elements. There are some mathematical tools, that can be added to the algorithm, that possibly leads to a faster calculation of linearly independent elements.

Simplifications to the Algorithm

Let $M_X := \{X_0, X_1, \dots, X_k\}$, be the set of all nested commutators gained up to depth n .

Let $L = L_d + L_i$ be a repeated Lie bracket obtained at step $n+1$, with L_i being linearly independent to any element in M_X . Instead of using L in step $n+2$, it is sufficient to use L_i .

Numerically, one could implement an algorithm similar to the Gram-Schmidt orthogonalization, that orthogonalizes an element obtained at depth n against the set of all previously obtained elements [11]. There are certain qubit systems, where one can tell for sure, that they are not controllable¹. Consider the 3-qubit system in the upper example on disconnected graphs, where two qubits couple via nearest-neighbour interaction and the third qubit is decoupled. If we set only one arbitrary local control, then this system is impossible to be controllable, since there is always one decoupled qubit.

Example 3.1.1. (Generating a Basis for a 3-Qubit Chain with Symmetries) Consider a 3-qubit chain with an σ_x -control on the first qubit. The 3-qubit chain shall have degenerate energy-levels, i.e., $\omega_1 = \omega_2 = \omega_3 = \omega, \omega \in \mathbb{R}/\{0\}$ and it shall have equal strenght coefficients $\kappa_{1,2} = \kappa_{2,3} = \kappa, \kappa \in \mathbb{R}/\{0\}$ ². The Hamiltonian of this certain 3-qubit chain is given by:

$$H(u(t)) = \frac{\omega}{2}(\sigma_z^1 + \sigma_z^2 + \sigma_z^3) + \kappa(\sigma_x^1 \sigma_x^2 + \sigma_x^2 \sigma_x^3) + u(t)\sigma_x^1$$

Note that the associated Hilbert space is the tensor product of 3 Hilbert spaces, where each Hilbert space is associated with a single qubit. Therefore, $\dim(\mathcal{H}) = 2^3 = 8$. according to 2.1.6. According to theorem 2.3.13, this 3-qubit chain is operator controllable, if $\text{Lie}\{H(u(t))\} = \mathfrak{su}(8)$. Note that $\dim(\mathfrak{su}(8)) = 8^2 - 1 = 63$. Hence, we need to calculate 63 linearly independent nested commutators, that are basis vectors of $\mathfrak{su}(8)$. Before doing the calculation, we can make another simplification by multiplying $\frac{2}{\omega}$ to $H(u(t))$ and setting $\eta = \frac{2}{\omega} \cdot \kappa$. Then the Hamiltonian:

$$H(u(t))' = \underbrace{\sum_{\alpha=1}^3 \sigma_z^\alpha + \eta(\sigma_x^1 \sigma_x^2 + \sigma_x^2 \sigma_x^3)}_{=H_0} + \underbrace{u(t)'}_{\frac{2}{\omega} u(t)} \sigma_x^1 = H_0 + u(t)' \sigma_x^1,$$

¹There are also systems, where one can tell, that they are for sure controllable. For instance, take an N-qubit system with local control on each qubit (No σ_z -control).

²Symmetries make the calculation of the nested commutator easier, which is a reason why they can be understood as simplifications to the 3-qubit system.

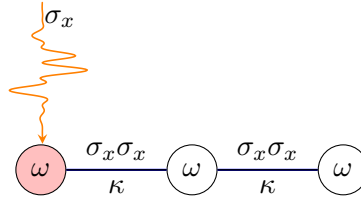


Figure 3.1: A 3-qubit chain with an σ_x -control on the first qubit can be seen. The energy degeneracy is made visible by equal ω within the nodes. Furthermore, the equal coefficients κ are made visible by the blue edges.

represents equivalent physical information as $H(u(t))$. First of all, observing the commutators of depth 0.

Depth 0: $\{H_0, \sigma_x^1\}$

$$[H_0, \sigma_x^1] = \left[\sum_{\alpha=1}^3 \sigma_x^\alpha, \sigma_x^1 \right] + \underbrace{\kappa[\sigma_x^1 \sigma_x^2 + \sigma_x^2 \sigma_x^3, \sigma_x^1]}_{=0} = 2i\sigma_y^1$$

Depth 1: $\{\sigma_y^1\}$

$$[H_0, \sigma_y^1] = \left[\sum_{\alpha=1}^3 \sigma_z^\alpha, \sigma_y^1 \right] + \kappa[\sigma_x^1 \sigma_x^2 + \sigma_x^2 \sigma_x^3, \sigma_y^1] = 2i(-\sigma_x^1 + \sigma_z^1 \sigma_x^2)$$

Note that σ_x^1 already exists in the set of elements of depth 0. Because of the simplification to the algorithm in 3.1, we can simply ignore σ_x^1 , since only $\sigma_z^1 \sigma_x^2$ contributes a new vector.

$$[\sigma_x^1, \sigma_y^1] = 2i\sigma_z^1$$

Depth 2: Consequently the set of nested commutators of depth 2 is: $\{\sigma_z^1 \sigma_x^2, \sigma_z^1\}$

This procedure will be continued n times until only linearly dependent commutators are generated and then it stops. Doing this calculation until the algorithm does not generate new elements leads us to 21 basis vectors. Hence, $\text{Lie}\{H(u(t))\}$ is a Lie subalgebra of $su(n)$. But there are 42 linear independent vectors of $su(8)$ that are not admissible. Consequently the 3-qubit chain with symmetries and a σ_x -control on the first qubit, is **not controllable**³.

³The number of generated dimensions also does not change, if we implement the σ_x -control on the third qubit, instead of the first qubit. However, implementing a σ_x -control on the second qubit generates 24 dimensions, therefore σ_x^2 is called a **preferred local control**. Physically, that could rely on the fact the σ_x -control affects the center-qubit

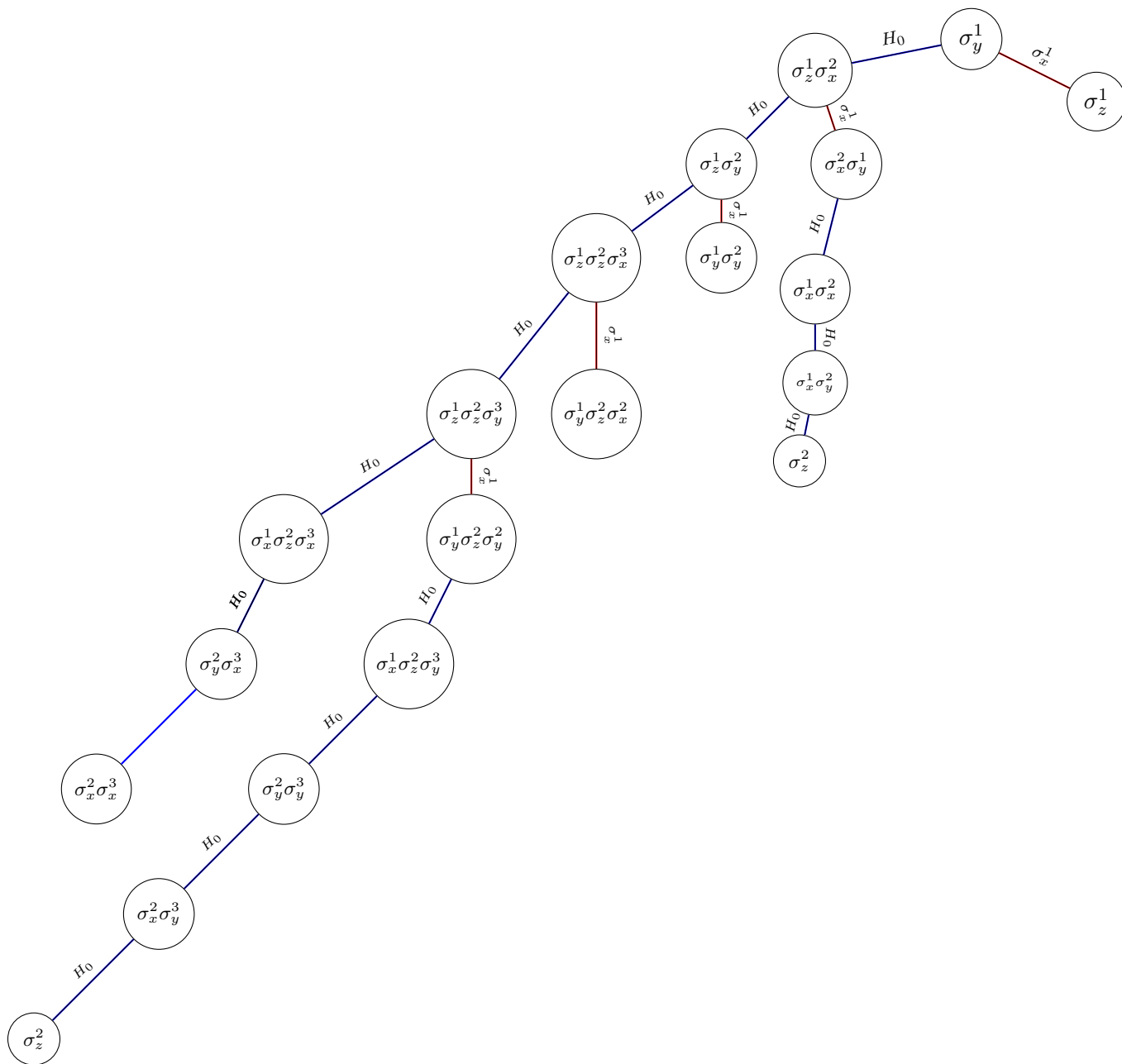


Figure 3.2: A way of visualizing the generated nested commutators includes drawing a graph. Starting from the top with depth-1 elements. Now each edge that is directed downwards represents calculating the commutator with a vector from depth 0. The edge to the left describes calculating the commutator with H_0 , $[H_0, -]$ and the edge to right describes calculating the commutator with σ_x^1 , $[\sigma_x^1, -]$. When there is no edge coming from a node, as in depth 2, consider σ_z^1 , then calculating commutators does not generate linearly independent elements. If one wonders, how a certain element was generated, one can easily go the graph up and reach the element's ancestors.

3.2 Graphic Controllability Test

Although the previous algorithm gives a basis of a dynamical Lie algebra, the direct calculation involving nested commutators can be very elaborate in high dimensions. In the following, a controllability test for bilinear control systems will be discussed, that uses notions of graph theory. One can directly apply the procedure to quantum control systems since they are modeled by bilinear control systems. Implemented in computer code, the **graphic controllability test** works more efficiently, than the direct computation of the dynamical Lie algebra basis. However, some conditions are necessary to be fulfilled, such that the graphic controllability test works properly. Let $H(u(t))$ be a Hamiltonian associated with a quantum control system:

$$H(u(t)) = A + Bu(t) = -i(H_0 + H_1u(t)). \quad (3.1)$$

As every considered quantum control system, this system has a time-independent Hamiltonian H_0 and a control-Hamiltonian $H_1u(t)$. Note that $A, B \in u(n)$ and therefore skew-Hermitian matrices [15]. Consequently, H_0, H_1 are Hermitian matrices. As seen before, $u = u(t)$ a (time-dependent) control function. We have to assume the following:

- A must be a **diagonal matrix** or equivalently H_0 is a **diagonal matrix**
- B must be a **skew-Hermitian square matrix** or equivalently H_1 is a **Hermitian square matrix** ⁴.

If there exists a control function $u(t)$ and a time T , such that one can steer the quantum control system's eigenvalue λ_i to reach the desired eigenvalue λ_j of the system, then we can transfer the state $|i\rangle$ to the target state $|j\rangle$. Hence, the arbitrary manipulation of the quantum control systems eigenvalues to reach desired eigenvalues is equivalent to **state-to-state controllability**, which is equivalent to **pure state controllability** for quantum systems.

Visualize the system's eigenvalues geometrically, as vertices of a graph, and imagine edges between the vertices describing permitted paths. Those paths are allowed state transfers of the quantum system. The following theorem states, that for any quantum control system, there exists a graph that connects the quantum control systems eigenvalues. This particular graph is said to be the **system graph** and connects the system's eigenvalues.

Theorem 3.2.1. (*Existence of the System Graph*) Let \sum_1 be a quantum control system, with state equation,

$$\frac{d}{dt}|\psi(t)\rangle = -i(H_0 + H_1u(t))|\psi(t)\rangle.$$

If H_0 is a diagonal matrix, B a skew-Hermitian square matrix and $u = u(t)$ a piecewise continuous control-function, then there exists a weighted Graph $G = (V, E)$ with the following properties,

1. $\lambda_i \in V \Leftrightarrow \lambda_i$ is an eigenvalue of H_0 .
2. $\{\lambda_i, \lambda_j\} \in E \Leftrightarrow H_{1i,j} \neq 0$.
3. The edge $\{\lambda_i, \lambda_j\}$ has the weight $\text{abs}(\lambda_i, \lambda_j) = |\lambda_i - \lambda_j|$

The weighted graph G is said to be the **system-graph** ⁵.

By measuring the quantum control systems energy, one measures an eigenvalue of $H(u(t))$, while the wave-function of the system collapses and the system reaches the eigenstate associated to the

⁴In some articles, B is restricted to be real and therefore symmetric [14].

eigenvalue. A connected path between eigenvalues describes a possible state transfer, between the associated eigenstates. But it does not provide the information, that any level-spacing is measurable and equivalently the system to reach any desired target state. Therefore, we have to modify the system Graph G of a quantum control system, to have an answer regarding pure state controllability.

Theorem 3.2.2. (*Controllability of quantum control systems*) Let \sum_1 be a quantum control system and $G = (V, E)$ its system graph. By removing all edges of G with equal weights, one obtains the **resulting system graph** G_{con} . The system \sum_1 is said to be **pure state controllable**, if the graph G_{con} is **connected**. The procedure of determining the system graph G , removing the edges with equal weights, and checking if the resulting system graph G_{con} is still connected, is called **graphic controllability test**⁶.

The matrix H_1 provides necessary information in drawing the system-graph G_{con} , since it specifies the kinematic couplings amongst the eigenstates of the system⁷. Ultimately, performing a graphic controllability test just one time does not always give a direct answer concerning controllability. For instance, if the resulting system-graph G_{con} is disconnected, it does not imply that the quantum control system is not controllable. Having such a case, one would have to calculate the commutator $[H_0, H_1] = H_{01}$ and do the graphic controllability test again, but this time starting with state-equation $\frac{d}{dt}|\psi\rangle = -i(H_{01} + H_1)|\psi\rangle$. Given is a bilinear system \sum'_1 , that unitary evolution is described by $\dot{\psi} = (A + Bu)\psi$. If the state-equation describes a quantum control system, then A, B are skew-Hermitian, but generally A is not diagonal-form. Since A is a skew-Hermitian matrix, it is always diagonalizable [11]. Let T be the transformation matrix, obtained by calculating the normed eigenvectors of A and writing them as columns, then T^\dagger is the inverse of T . Transforming the system into the eigenbasis of A goes as by transforming the matrices A and B .

$$TAT^{-1} = TAT^\dagger = D$$

$Consequently, we obtained a state-equation equivalent to the first one:$

$$\dot{|\psi\rangle} = (D + B'u(t))|\psi\rangle. \quad (3.2)$$

Note that the transformation in the eigenbasis of A , conserves the skew-Hermitian property:

$$TBT^\dagger = -TB^\dagger T^\dagger = -T(TB)^\dagger = -T^{\dagger\dagger}(TB)^\dagger = -(TBT^\dagger)^\dagger.$$

⁷As a matter of fact, assuming that H_1 is symmetric or Hermitian implies that the system Graph G_{con} is non-orientated, meaning it has no direct edges. [14]

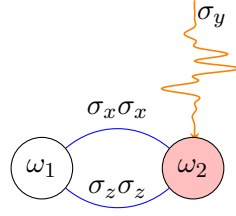


Figure 3.3: Non-degenerate two-qubit system, with σ_y -control on the second qubit and nearest-neighbour interactions $\sigma_x^1\sigma_x^2$ and $\sigma_y^1\sigma_y^2$.

Example 3.2.3. (Two-qubit system affected by periodic electromagnetic-field) Consider a two-qubit system affected by a periodic electromagnetic field, similar to the example 2.2.1 but with an additional $\sigma_z\sigma_z$ -interaction and a σ_y -control on the second qubit. The Hamiltonian of this two-qubit

system is $H(u(t)) = \underbrace{\sum_{\alpha=1}^2 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \sigma_x^1 \sigma_x^2 + \sigma_z^1 \sigma_z^2}_{=H_0} + u(t) \sigma_y^2$. In order to do the graphic controllability

test, one has to diagonalize H_0 and transform H_1 in the eigenbasis of H_0 . H_0 has eigenvalues $\{\underbrace{-2}_1, \underbrace{1-\sqrt{5}}_2, \underbrace{0}_3, \underbrace{1+\sqrt{5}}_4\}$ (Calculated with assuming $\omega_\alpha = 2$).

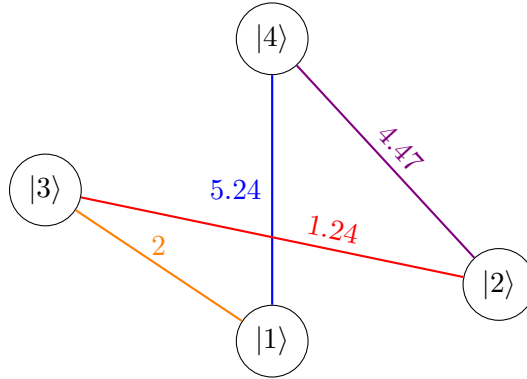


Figure 3.4: System graph associated to the 2-qubit system with σ_y -control on the second qubit. We find a connected system graph G , according to the procedure, we have now to remove the edges with equal weight. Since the graph does not have edges with equal weights, there are no edges to remove. Therefore, we have proven the pure state controllability of the system. Moreover, we gained a deeper insight into the system, since connected nodes represent allowed state transitions.

Chapter 4

Results

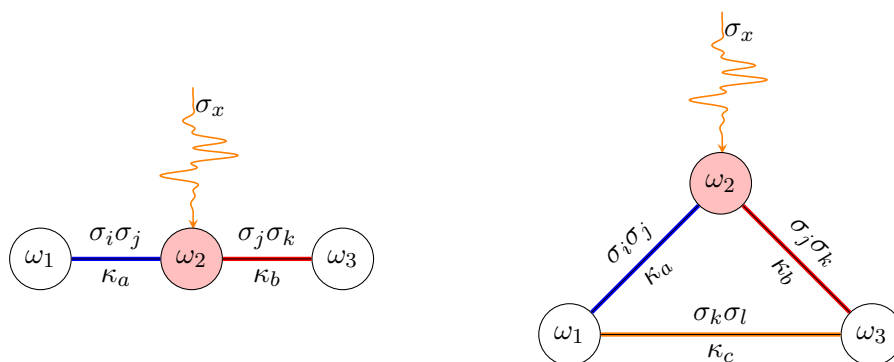


Figure 4.1: The 3-qubit arrays analyzed were the 3-qubit chain (left) and the 3-qubit loop (right). Both systems were always equipped with an σ_x -control on the middle qubit, which is shown by the arrow pointing to the middle qubit. First, cases were analyzed in which these 3-qubit arrays are controllable, in the sense of operator controllability (2.3.3). Second, after careful analysis of the controllable 3-qubit arrays, important common features that controllable 3-qubit arrays always have, were identified. The knowledge gained from the analysis could then be used to work out strategies for building controllable 3-qubit arrays with an σ_x -control on the middle qubit.

In this bachelor thesis, we aimed to indicate how one could construct a complete controllable qubit array consisting of N qubits with minimal local controls. For this purpose, we firstly investigated systems that are easier to solve, than the N -qubit array. The goal was to find criteria for controllability. Once those criteria could be found, the next step is to build a controllable N -qubit array with minimal local controls.

First, 3-qubit systems like the 3-qubit chain and the 3-qubit loop with an σ_x -control on the second qubit were studied. Then, it was carefully worked out which conditions must be satisfied for the aforementioned 3-qubit arrays to be controllable. Second, strategies could be found out, according to which one can create controllable 3-qubit systems with an σ_x -control on the second qubit. After the strategies for the creation of controllable 3-qubit arrays were worked out, there were still several open questions. For example, consider a controllable 3-qubit chain. How these systems behave

under maximized symmetries, i.e., energy degeneracy and equal coupling strength between qubits were studied. It could be verified that there are systems that are controllable despite maximized symmetry. Another interesting question deals with the possibility, that an additional two-qubit interaction could destroy the controllability.

The result chapter is divided into 4 sections. Each section will now be briefly described. The main result, i.e., the construction of controllable 3-qubit systems, can be found in section 4.1 and section 4.2. In section 4.1 we will elaborate on two strategies by which one can build controllable 3-qubit arrays when an σ_x -control has been previously attached to the second qubit. In both cases, we will see that the controllability of the 3-qubit chain depends on the quantity of nearest-neighbour interactions and on the kind of nearest-neighbour interactions. Furthermore, in section 4.1 the preservation of controllability for chains under symmetries, i.e., energy degeneracy or equal coupling strength between qubits, was studied. We will see that cases occur where an additional nearest-neighbour interaction can destroy the controllability of the system. Then, it will be explained in more detail what criteria must be fulfilled for additional two-qubit interactions to destroy the controllability of a system. Formal strategies that deal with the question, how to create controllable 3-qubit loops? will be worked out in section 4.2. In section 4.3, the system graphs for certain controllable 3-qubit chains and certain controllable 3-qubit loops were studied. Studying the graphs was necessary since it verified the current results and gives deeper insight into controllable systems. Furthermore, this will graphically illustrate what distinguishes a non-controllable system (3-qubit chains and 3-qubit loops) from a controllable system. Roughly speaking, in controllable 3-qubit arrays there exist transitions which are degenerate when a certain two-qubit interaction is taken away. Finally, we reformulate the question from the beginning and deal with how to create controllable 3-qubit arrays when the number of nearest-neighbour interactions is minimal. We study the construction of controllable 3-qubit chains with minimal nearest-neighbour interactions in section 4.4.

4.1 Controllable 3-Qubit Chains with σ_x -control

This section contains all relevant information on constructing controllable 3-qubit chains. We start with a general 3-qubit chain and local σ_x -control on the second qubit. This system is described by the Hamiltonian:

$$H(u(t)) = \sum_{\alpha=1}^3 \frac{\omega_{\alpha}}{2} \sigma_z^{\alpha} + \kappa_a \sigma_i^1 \sigma_j^2 + \kappa_b \sigma_k^2 \sigma_l^3 + u(t) \sigma_x^2. \quad (4.1)$$

This system is not controllable, because for the dynamical Lie algebra $Lie\{H(u(t))\}$ holds:

$$\dim(Lie\{H(u(t))\}) < 63,$$

for every possible nearest-neighbour interaction $\sigma_i^1 \sigma_j^2, \sigma_k^2 \sigma_l^3$ and every $\kappa_{a,b} \in \mathbb{R}$. The goal is to transform the uncontrollable system with Hamiltonian (4.1) to a controllable 3-qubit chain. Therefore, we are going to add nearest-neighbour interactions to the Hamiltonian. The goal was reached, when the dynamical Lie algebra associated with the 3-qubit chain is equal to the Lie algebra $su(8)$ or in

other words when the dimension of the dynamical Lie algebra is equal to 63¹.

In the investigation presented in this section, an σ_x -control on the second qubit is always required. However, we do not require that the nearest-neighbour interactions are fixed. The nearest-neighbour interactions can arbitrarily be chosen, before being added to the Hamiltonian (4.1). Therefore, it was important to clarify which nearest-neighbour interactions can appear in a 3-qubit chain. The nearest-neighbour interaction between qubits was defined in equation (2.15), hence a nearest-neighbour interaction is here defined as a Kronecker product of Pauli matrices and the identity matrix. It follows that all possible interactions can be determined. Ultimately, the only relevant nearest-neighbour interactions have the form, $\sigma_i^1 \sigma_j^2$ and $\sigma_k^2 \sigma_l^3$. Since there are 3 Pauli matrices $\sigma_x, \sigma_y, \sigma_z$, it follows that there are 18 possible nearest-neighbour interactions for a 3-qubit chain. Finally, to make clear which interactions are possible, the set of all nearest-neighbour interactions for a 3-qubit chain was defined:

Definition 4.1.1. (Set of nearest-neighbour interactions) The set of all possible nearest-neighbour interactions for a 3 qubit chain:

$$N_3 := \{\sigma_i^1 \sigma_j^2, \sigma_k^2 \sigma_l^3 | \sigma_{i,j,k,l} \in \{\sigma_x, \sigma_y, \sigma_z\}\}$$

Knowing the set N_3 will be important for upcoming presented concepts. Consider equation (4.1). Adding an arbitrary nearest-neighbour interaction η to $H(u(t))$, $\eta \in N_3$, that is different from the nearest-neighbour interactions that occur in $H(u(t))$, is interpreted as strengthening a coupling between a pair of qubits, in the 3-qubit chain. In the beginning, the intuition was that a high amount of different nearest-neighbour interactions correlates with a controllable system. Then, we could expect that the dimension of the dynamical Lie algebra associated with the system becomes higher, if we add η to the considered 3-qubit chain.

$$\dim(\text{Lie}\{H(u(t)) + \eta\}) \geq \dim(\text{Lie}\{H(u(t))\}).$$

Now, if we want this system to become controllable, the approach is to create a new Hamiltonian. One way that could lead to the desired result, is to repetitively add different nearest-neighbour interactions $\kappa_i \eta_i$ to $H(u(t))$, $\kappa_i \in \mathbb{R} \setminus \{0\}$, $\eta_i \in N_3$ until the dynamical Lie algebra spanned by $H(u(t))_i = H(u(t))_{i-1} + \kappa_i \eta_i$ is equal to $\text{su}(8)$. However, it is tedious to repeatedly add nearest-neighbour interactions to the 3-qubit chain and then check the dimension of its dynamical Lie algebra. Moreover, it could be the case that more interactions are included, than necessary for controllability. The procedure of repetitively adding interactions to the system was optimized. Therefore, we solved a simpler problem, that was slightly related to the original problem. Subsequently, the gained knowledge helped in constructing controllable 3-qubit chains. Consider a system of 3 uncoupled qubits and local σ_x -control on the second qubit. This system is described by the Hamiltonian:

$$H(u(t)) = \sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + u(t) \sigma_x^2. \quad (4.2)$$

The system is not controllable, because for the dynamical Lie algebra associated to the system holds:

$$\dim(\text{Lie}\{H(u(t))\}) = 4 < 63.$$

¹Formally, a 3-qubit chain is also controllable if the dynamic Lie algebra is equal to $\text{su}(8)$ or, in other words, if the dimension of the dynamic Lie algebra is equal to 64. However, such cases did not occur in the investigation.

Now, the idea is to insert a single $\eta \in N_3$ in equation (4.2) and subsequently determine the dynamical Lie algebra of the newly emerged system. Since for every element in N_3 exists a dynamical Lie algebra, it made sense to define a function that maps an arbitrary η to its dynamical Lie algebra. After this, the emerged Lie algebras were compared.

Definition 4.1.2. (Generated Subalgebra)

Let $\sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha$ be a fixed non-degenerate drift-Hamiltonian with local control $u(t)\sigma_x^2$. For $\eta \in N_3$, exists an dynamical Lie algebra, that is called **generated subalgebra** of η .

$$gs : N_3 \rightarrow su(8), \quad \eta \mapsto Lie\left\{\sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \kappa\eta + u(t)\sigma_x^2\right\}, \quad \kappa \neq 0 \quad (4.3)$$

Physically, a nearest-neighbour interaction η is mapped to a 3-qubit system with two qubits that couple via η and one qubit being decoupled from the others. Since its physical interpretation has not had a strong meaning, this definition should be understood as a mathematical tool. By determining the generated subalgebra by η , we can associate a Lie subalgebra of $su(8)$, for every $\eta \in N_3$. This definition becomes more meaningful when we start to compare generated subalgebras that are **not equal** and **do not contain each other**. Consider a pair of nearest-neighbour interactions η_1, η_2 that have generated subalgebras, that fulfill:

$$gs(\eta_1) \not\subseteq gs(\eta_2). \quad (4.4)$$

$$gs(\eta_2) \not\subseteq gs(\eta_1). \quad (4.5)$$

Note that $gs(\eta_1)$ and $gs(\eta_2)$ are Lie subalgebras of $su(8)$ that have non-empty intersections, since $\sigma_x^2 \in gs(\eta_1), gs(\eta_2)$. But roughly spoken, they mostly reach different subsets of $su(8)$. The idea is to add both interactions η_1, η_2 to the system (4.2), to get the contributions from $gs(\eta_1)$ and $gs(\eta_2)$, when we determine its dynamical Lie algebra. One obtains,

$$H(u(t)) + \kappa_1\eta_1 + \kappa_2\eta_2.$$

Now one observes that,

$$\dim(Lie\{H(u(t)) + \kappa_1\eta_1 + \kappa_2\eta_2\}) > \dim(gs(\eta_1)).$$

$$\dim(Lie\{H(u(t)) + \kappa_1\eta_1 + \kappa_2\eta_2\}) > \dim(gs(\eta_2)).$$

Since the dynamical Lie algebra is larger, then both generated subalgebras, we assume:

In order to generate a large dynamical Lie algebra, we have to add nearest-neighbour interactions $\eta_1, \eta_2, \dots, \eta_i$ that fulfill the properties (4.4) and (4.5), to the considered system (4.2).

In any case, this method will lead to a controllable 3-qubit chain, as the next example verifies.

Example 4.1.3. (Creating Controllable 3-Qubit Chain) Consider $\eta_1 = \sigma_x^1 \sigma_x^2$ and $\eta_2 = \sigma_z^2 \sigma_z^3$. In a 3-qubit chain, η_1 couples the first two qubits and η_2 couples the second and third qubit. They fulfill the properties (4.4) and (4.5), i.e., their generated subalgebras do not contain each other. Note, that this is expectable since they have a different structure as a Kronecker product.

$$\eta_1 = \sigma_x^1 \sigma_x^2 = \sigma_x \otimes \sigma_x \otimes \mathbb{1}_2.$$

$$\eta_2 = \sigma_z^2 \sigma_z^3 = \mathbb{1}_2 \otimes \sigma_z \otimes \sigma_z.$$

Assume $\kappa, \lambda \neq 0$. Consider the commutators of the generated subalgebras $gs(\eta_1), gs(\eta_2)$, obtained at depth 1:

$$\text{For } gs(\eta_1) : \left[\sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \kappa \eta_1, \sigma_x^2 \right] = \left[\sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \kappa \sigma_x^1 \sigma_x^2, \sigma_x^2 \right] = \underbrace{i\omega_2 \sigma_z^2}_{\text{local operator}}$$

$$\text{For } gs(\eta_2) : \left[\sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \lambda \eta_2, \sigma_x^2 \right] = \left[\sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \lambda \sigma_z^2 \sigma_z^3, \sigma_x^2 \right] = \underbrace{i\omega_2 \sigma_z^2}_{\text{local operator}} + \underbrace{2i\lambda \sigma_z^2 \sigma_z^3}_{\text{global operator}}$$

The commutator at depth 1 of $gs(\eta_2)$ contains a global operator, that cannot be generated in $gs(\eta_1)$. When the nested commutators of depth 2, 3, ..., n that appeared in $gs(\eta_1)$ and $gs(\eta_2)$ were compared, it was seen that they have a different structure as Kronecker product, which is why $gs(\eta_1)$ and $gs(\eta_2)$ reach different Lie subalgebras of $su(8)$, that do not contain each other.

Therefore, it makes sense to add both nearest-neighbour interactions $\sigma_x^1 \sigma_x^2$ and $\sigma_z^2 \sigma_z^3$ to our system, that is described by equation (4.2). The Hamiltonian is then given by:

$$H(u(t)) := \sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \kappa \sigma_x^1 \sigma_x^2 + \lambda \sigma_z^2 \sigma_z^3 + u(t) \sigma_x^2. \quad (4.6)$$

We find that,

$$\dim(\text{Lie}\{H(u(t))\}) > \underbrace{\dim(gs(\eta_1))}_{=11}.$$

$$\dim(\text{Lie}\{H(u(t))\}) > \underbrace{\dim(gs(\eta_2))}_{=7}.$$

But, $\dim(\text{Lie}\{H(u(t))\}) < 63$ still holds. Therefore, choose an $\eta_3 \in N_3$, such that the pair η_3, η_1 and the pair η_3, η_2 fulfills the properties (4.4) and (4.5). Consider $\eta_3 = \sigma_x^2 \sigma_x^3$ and let $\mu \neq 0$. We add $\mu \sigma_x^2 \sigma_x^3$ to the Hamiltonian (4.6) and obtain the overall Hamiltonian:

$$H(u(t)) = \sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \kappa \sigma_x^1 \sigma_x^2 + \mu \sigma_x^2 \sigma_x^3 + \lambda \sigma_z^2 \sigma_z^3 + u(t) \sigma_x^2, \quad \text{with } \dim(\text{Lie}\{H(u(t))\}) = 63. \quad (4.7)$$

Hence, a controllable 3-qubit chain with σ_x -control on the second qubit was founded, that has 3 nearest-neighbour interactions.

The procedure in example 4.1.3 has a strong physical interpretation. Generally, for each η_i exists a generated subalgebra $gs(\eta_i)$ and this corresponds to a 3-qubit system with Hamiltonian $H(u(t)) = \sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \kappa_i \eta_i + u(t) \sigma_x^2$. Now, connected to the system is a Lie group $\mathbf{e}^{gs(\eta_i)}$, that is obtained through the image of the matrix exponential of $gs(\eta_i)$. The Lie group $\mathbf{e}^{gs(\eta_i)}$ is a Lie subgroup of $SU(8)$ and contains every realizable quantum logic gate for the system.

The considered interactions $\sigma_x^1 \sigma_x^2, \sigma_x^2 \sigma_x^3, \sigma_z^2 \sigma_z^3$ fulfill the properties (4.4) and (4.5), therefore their connected Lie groups do not contain each other as well ². This means, that $\mathbf{e}^{gs(\sigma_x^1 \sigma_x^2)}, \mathbf{e}^{gs(\sigma_x^2 \sigma_x^3)}, \mathbf{e}^{gs(\sigma_z^2 \sigma_z^3)}$ differ in realizable quantum logic gates, since they reach different subgroups of $SU(8)$.

A system that contains all considered interactions as in equation (4.7) has a dynamical Lie algebra $Lie\{H(u(t))\} = su(8)$. Hence, all quantum logic gates are realizable, since $\mathbf{e}^{su(8)} = SU(8)$. That means universal quantum computing is possible.

There are cases, where a pair of different nearest-neighbour interactions η_1, η_2 has the same generated subalgebra or where one is a subalgebra of the other. Then, it is of no use to implement both interactions into the system, because one cannot generate new elements. Interestingly, the definition of generated subalgebras by nearest-neighbour interactions leads naturally to an equivalence relation on the set N_3 , which divides the set into disjoint subsets ³.

Definition 4.1.4. (Subalgebra equivalence: \sim) A pair of nearest-neighbour interactions $\eta_1, \eta_2 \in N_3$ is subalgebraically equivalent, if $gs(\eta_1) = gs(\eta_2)$.

$$\eta_1 \sim \eta_2 :\Leftrightarrow gs(\eta_1) = gs(\eta_2). \quad (4.8)$$

Note that subalgebra equivalence is an equivalence relation because equality is an equivalence relation. Therefore, one can apply subalgebra equivalence \sim on the set N_3 , where one divides the elements of N_3 into 6 disjoint subsets. Each disjoint subset is an element of the **quotient set** N_3/\sim . The elements of N_3/\sim are called **classes** and they are written in tuples:

$$(11, A), (11, B), (7, A), (7, B), (4, A), (4, B).$$

The first number indicates the dimension of the generated subalgebra. For instance, if $\eta \in (11, A)$, then $\dim(gs(\eta)) = 11$. The letters A, B describe the different order of operators in the Kronecker product. For example, for $\sigma_x^1 \sigma_x^2 \in (11, A)$ with

$$\sigma_x^1 \sigma_x^2 = \sigma_x \otimes \sigma_x \otimes \mathbb{1}_2,$$

exists $\sigma_x^2 \sigma_x^3 \in (11, B)$ with

$$\sigma_x^2 \sigma_x^3 = \mathbb{1}_2 \otimes \sigma_x \otimes \sigma_x.$$

Physically, elements from A -classes connect the first two qubits, while elements from B -classes connect the second- and the third qubit.

$$(11, A) := \{\sigma_x^1 \sigma_x^2, \sigma_y^1 \sigma_y^2, \sigma_x^1 \sigma_y^2, \sigma_y^1 \sigma_x^2, \sigma_x^1 \sigma_z^2, \sigma_y^1 \sigma_z^2\}, \quad (11, B) := \{\sigma_x^2 \sigma_x^3, \sigma_y^2 \sigma_y^3, \sigma_x^2 \sigma_y^3, \sigma_y^2 \sigma_x^3, \sigma_z^2 \sigma_x^3, \sigma_z^2 \sigma_y^3\} \quad (4.9)$$

²In general, different subalgebras of $su(n)$ can also have the same image in $SU(N)$. But those cases are not relevant for our investigations.

³Disjoint = non-intercepting

Dimension of generated subalgebra	A	B
11	$\sigma_x^1 \sigma_x^2$	$\sigma_x^2 \sigma_x^3$
7	$\sigma_z^1 \sigma_z^2$	$\sigma_z^2 \sigma_z^3$
4	$\sigma_z^1 \sigma_y^2$	$\sigma_z^3 \sigma_y^2$

Figure 4.2: The diagram illustrates the 6-element quotient set N_3/\sim obtained by applying **subalgebra equivalence** to the set N_3 . The elements of N_3/\sim are disjoint classes, where each block illustrates a class of N_3/\sim . Every single block illustrates a representative of its class. In a 3-qubit chain, elements of A-classes are interactions between the first two qubits, whereas elements of B-classes are interactions between the second and the third qubit. A-classes and B-classes with equal dimensions are very similar. Mathematically, for each element in an A-class, exists a corresponding element in a B-classes, that differs from the other in its order of Pauli matrices as a Kronecker product.

$$(7, A) := \{\sigma_z^1 \sigma_z^2, \sigma_z^1 \sigma_x^2\}, \quad (7, B) := \{\sigma_z^2 \sigma_z^3, \sigma_x^2 \sigma_z^3\} \quad (4.10)$$

$$(4, A) := \{\sigma_z^1 \sigma_y^2\}, \quad (4, B) := \{\sigma_z^3 \sigma_y^2\} \quad (4.11)$$

The quotient set is given by:

$$N_3/\sim := \{(11, A), (11, B), (7, A), (7, B), (4, A), (4, B)\} \quad (4.12)$$

At first glance, the introduction of the equivalence relation and the quotient set may seem an unnecessary complication. However, we will see in the following that many simplifications will be realized with this.

Consider a 3-qubit chain with two nearest-neighbour interactions, with Hamiltonian:

$$H(u(t)) = \sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \kappa_1 \eta_1 + \kappa_2 \eta_2 + u(t) \sigma_x^2, \quad \text{with } \kappa_{1,2} \neq 0 \quad (4.13)$$

If η_1, η_2 are in the same class $\Rightarrow gs(\eta_1) = gs(\eta_2) = Lie\{H(u(t))\} \Rightarrow e^{gs(\eta_1)} = e^{gs(\eta_2)} = e^{Lie\{H(u(t))\}}$.

Implementing nearest-neighbour interactions from the same class to the system does not contribute to anything new. The dynamical Lie algebra stays the same as well as the Lie group. There are no

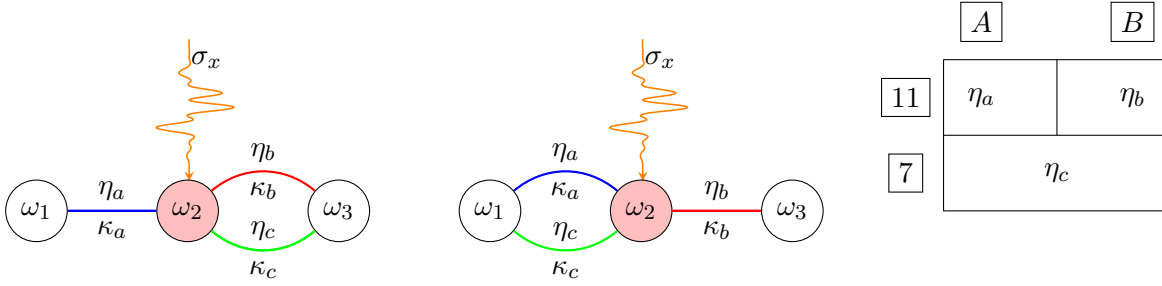


Figure 4.3: 3-qubit chains with σ_x -control on the second qubit are controllable if one chooses their nearest-neighbour interactions appropriately. The left side shows a 3-qubit chain with nearest-neighbour interactions $\eta_a \in (11, A)$, $\eta_b \in (11, B)$, $\eta_c \in (7, B)$, while on the center the 3-qubit chain has $\eta_c \in (7, A)$. The right side shows a diagram, that states how to choose $\eta_{a,b,c}$, such that the corresponding 3-qubit chain becomes controllable.

new quantum gates, that the system achieves. Now, consider the more interesting case, when η_1, η_2 are from different classes. Then, it could hold that the one is a **strict** Lie subalgebra from the other, i.e.,

$$\text{If } gs(\eta_1) \subsetneq gs(\eta_2) \Rightarrow gs(\eta_2) = \text{Lie}\{H(u(t))\}.$$

Hence, if we already have a nearest-neighbour interaction η_2 implemented in the system, then implementing η_1 does not contribute anything new. Now consider the most interesting case, η_1 and η_2 are from different classes and fulfill property (4.4) and property (4.5). Without loss of generality we assume $\dim(gs(\eta_1)) \leq \dim(gs(\eta_2))$. Then it follows,

$$\dim(gs(\eta_1)) \leq \dim(gs(\eta_2)) < \dim(\text{Lie}\{H(u(t))\}). \quad (4.14)$$

For the Lie group connected to the system holds,

1. $e^{\text{Lie}\{H(u(t))\}}$ is larger then $e^{gs(\eta_1)}$ or $e^{gs(\eta_2)}$.
2. $e^{gs(\eta_1)} \subseteq e^{\text{Lie}\{H(u(t))\}}, \quad e^{gs(\eta_2)} \subseteq e^{\text{Lie}\{H(u(t))\}}$

Physically, this means that most quantum gates are generable with η_1 and η_2 , instead of having only η_1 or η_2 . The previous algebraic procedure was necessary, to introduce the upcoming strategy for building controllable 3-qubit chains. In the following, we assume the most general case, namely that the system does not have any symmetries or coefficients equal to zero. Mathematically, this means that $\omega_i \neq \omega_j \neq 0$ for any $i, j \in \{1, 2, 3\}$ and $\kappa_a \neq \kappa_b \neq \kappa_c \neq 0$.

Result 1: Controllable 3-Qubit Chain with σ_x -control.

A 3-qubit chain, that has a non-degenerate Hamiltonian with $\eta_a, \eta_b, \eta_c \in N_3$ and σ_x^2 -control,

$$H(u(t)) = \sum_{\alpha}^3 \frac{\omega_{\alpha}}{2} \sigma_z^{\alpha} + \kappa_a \eta_a + \kappa_b \eta_b + \kappa_c \eta_c + u(t) \sigma_x^2, \quad \kappa_a, \kappa_b, \kappa_c \in \mathbb{R} \quad (4.15)$$

is **controllable**, if one of the following condition holds:

1. $\eta_a \in (11, A), \eta_b \in (11, B), \eta_c \in (7, A)$.
2. $\eta_a \in (11, A), \eta_b \in (11, B), \eta_c \in (7, B)$.

Both conditions can be summarized in a single equation.

A 3-qubit chain is controllable, if the nearest-neighbour interactions in $H(u(t))$, fulfill

$$\eta_a \in (11, A), \eta_b \in (11, B), \eta_c \in (7, A) \cup (7, B). \quad (4.16)$$

A 3-qubit chain with Hamiltonian, that fulfills equation (4.16), has a dynamical Lie algebra $Lie\{H(u(t))\}$ with,

$$Lie\{H(u(t))\} = su(8).$$

Consequently, the Lie group connected to $Lie\{H(u(t))\}$ is $e^{su(8)} = SU(8)$. Hence, any special unitary transformation is generable, in other words, any quantum gate is realizable. Therefore, universal quantum computing is possible. From result 1, we can deduce another interesting insight, that states the minimum number of different nearest-neighbour interactions for a 3-qubit chain:

A controllable 3-qubit chain, with one local control σ_x^2 , has at least 3 different nearest-neighbour interaction terms η_a, η_b, η_c .

This observation could be important since it could lead to a rule that is about the number of interactions constructing controllable systems. But what if generally, any 3-qubit system needs at least 3 two-qubit interactions to be controllable? Therefore, we keep this fact in mind, since it could be interesting for the construction of controllable 3-qubit loops. Formally, a way was presented how controllable 3-qubit chains with a single local control can be constructed. We have not commented on the practical effort of implementing certain nearest-neighbour interactions. However, if for some practical reason nearest-neighbour interactions $\eta \in (7, A) \cup (7, B)$ are difficult to realize, another way how to construct controllable 3-qubit chains, that does not involve the classes $(7, A)$ or $(7, B)$, will be presented in the following. From an academic point of view, it illustrates that there is not a unique way of constructing controllable 3-qubit chains with an σ_x -control and exactly three nearest-neighbour interactions. For the following section, the goal will be to create a controllable 3-qubit chain without the classes $(7, A)$ and $(7, B)$. Therefore, the classes $(11, A), (11, B), (4, A), (4, B)$ where considered. It was observed, that we cannot simply swap $(4, A)$ with $(7, A)$ and $(4, B)$ with $(7, B)$ in equation (4.3). A 3-qubit chain with σ_x -control on the second qubit and 3 nearest-neighbour interactions is generally not controllable, if $\eta_a \in (11, A), \eta_b \in (11, B), \eta_c \in (4, A) \cup (4, B)$. However, there are special cases, where the 3-qubit chain becomes controllable. In those cases, there are only certain elements from $(11, A)$ and $(11, B)$, that form controllable 3-qubit chains with elements from $(4, A)$ or $(4, B)$. Interestingly, those elements are founded to be in specified equivalence classes within $(11, A)$ and $(11, B)$. Each nearest-neighbour interaction $\eta \in (11, A)$ is a Kronecker product of the form $\eta = \sigma_i^1 \sigma_j^2$. In corollary 2.1.9 was seen, that Kronecker products can be understood

as mappings. Hence, the nearest-neighbour interactions for a 3-qubit chain can be understood as mappings with three arguments:

$$(\sigma_i, \sigma_j, \mathbb{1}_2) \mapsto \sigma_i \otimes \sigma_j \otimes \mathbb{1}_2 = \sigma_i^1 \sigma_j^2.$$

Nearest-neighbour interactions, that have an equal second argument play an important role for controllable 3-qubit chains, if we consider the classes $(4, A)$ and $(4, B)$. Therefore, we will once again, define an equivalence relation.

Definition 4.1.5. (2 argument equivalence: \sim_2) A pair of Kronecker products $A = A_1 \otimes A_2 \otimes A_3$ and $B = B_1 \otimes B_2 \otimes B_3$ is **2 argument equivalent**, if $A_2 = B_2$.

Formally, \sim_2 is an equivalence relation because equality is a equivalence relation. The second argument equivalence \sim_2 applied on $(11, A)$, divides this six-element set into 3 classes:

$$(11, A)_{X^2} := \{\sigma_x^1 \sigma_x^2, \sigma_y^1 \sigma_x^2\}. \quad (4.17)$$

$$(11, A)_{Y^2} := \{\sigma_x^1 \sigma_y^2, \sigma_y^1 \sigma_y^2\}. \quad (4.18)$$

$$(11, A)_{Z^2} := \{\sigma_x^1 \sigma_z^2, \sigma_y^1 \sigma_z^2\}. \quad (4.19)$$

The quotient set is defined as:

$$(11, A)/\sim_2 := \{(11, A)_{X^2}, (11, A)_{Y^2}, (11, A)_{Z^2}\}. \quad (4.20)$$

The index, for instance, X^2 means here, that all elements in this class have σ_x as a second argument. Similarly, \sim_2 divides $(11, B)$ into classes with equal second argument. As we will see in the upcoming result, the classes $(11, A)_{Y^2}$ and $(11, B)_{Y^2}$ are important in the context of controllability for 3-qubit chains. The next result reads very similar to result 1, the difference is that $(11, A)_{Y^2}, (11, B)_{Y^2}, (4, A), (4, B)$ are the classes, from which the interactions η_a, η_b, η_c have to be chosen.

Result 2: Controllable 3-Qubit Chain with σ_x -control.

A 3-qubit chain, that has a non-degenerate Hamiltonian,

$$H(u(t)) = \sum_{\alpha}^3 \frac{\omega_{\alpha}}{2} \sigma_z^{\alpha} + \kappa_a \eta_a + \kappa_b \eta_b + \kappa_c \eta_c + u(t) \sigma_x^2, \kappa_a, \kappa_b, \kappa_c \in \mathbb{R} \quad (4.21)$$

is **controllable**, if one of the following condition holds:

1. $\eta_a \in (11, A)_{Y^2}, \eta_b \in (11, B)_{Y^2}, \eta_c \in (4, A)$
2. $\eta_a \in (11, A)_{Y^2}, \eta_b \in (11, B)_{Y^2}, \eta_c \in (4, B)$

A 3-qubit chain is controllable if it has 3 nearest-neighbour interactions, that fulfill

$$\eta_a \in (11, A)_{Y^2}, \eta_b \in (11, B)_{Y^2}, \eta_c \in (4, A) \cup (4, B). \quad (4.22)$$

Classes with elements that have σ_y as a second argument are important for controllability. One possible explanation could rely on the fact, that the local control on the second qubit, creates the second argument equivalence. The fact that it is an σ_x -control, creates the preference of σ_y as a

second argument. Calculating commutators of Kronecker products and the local control σ_x^2 implies that there can not be a preference of σ_x as a second argument, since $[\sigma_j^\alpha \sigma_x^2, \sigma_x^2] = 0$. In contrast $[\sigma_j^\alpha \sigma_z^2, \sigma_x^2] = 2i\sigma_j^\alpha \sigma_y^2$, $[\sigma_j^\alpha \sigma_y^2, \sigma_j^\alpha \sigma_x^2] = -2i\sigma_j^\alpha \sigma_z^2$ generate new two-qubit interactions. Consequently, there has to be another reason, that excludes σ_z from being preferred as second argument. One reason for that could be related to the fact, that σ_z is a generally a bad choice for a local control, since it commutes with the drift-Hamiltonian. To conclude the first two results, there are 2 strategies to build controllable 3-qubit chains with local control. A 3-qubit chain with a single local control $u(t)\sigma_x^2$ on the second qubit is controllable, if the qubit-chain has at least 3 nearest-neighbour interactions, that are chosen according to equation (4.16) or equation (4.22). Generally, symmetries are harmful to the controllability of any qubit array. This is why, non-degeneracy $\omega_i \neq \omega_j$ and $\kappa_i \neq \kappa_j$ for $i, j \in \{1, 2, 3\}$ was assumed in result 1 and result 2. A qubit array that contains symmetries, leads to non-controllability of the system since its dynamical Lie algebra is a strict subalgebra of $su(8)$. Therefore the Lie group connected to the system is always a strict Lie subgroup of $SU(8)$. This implies, that not every unitary matrix can be generated. Consequently, universal quantum computing is not possible. However, there might be cases where symmetries are unavoidable. For instance, certain experimental set-ups could require equal strength coefficients or strong external perturbations could create degeneracies. Also, symmetries could appear, which might be unexpected. This is the reason that motivates the next question:

Does a 3-qubit chain with minimal local controls exists, such that the system's controllability remains under symmetries ?

To find an answer to the above question, we considered result 1 and checked if controllable 3-qubit chains remain controllable for 4 types of symmetry: Let $i, j \in \{1, 2, 3\}$.

1. degeneracy: $\omega_i = \omega_j \neq 0$.
2. equal strength coefficients: $\kappa_i = \kappa_j \neq 0$.
3. degeneracy and equal strength coefficients: $\omega_i = \omega_j \neq 0$ and $\kappa_i = \kappa_j \neq 0$.
4. maximized symmetry: $\omega_i = \omega_j = \kappa_i = \kappa_j \neq 0$.

Note that, maximized symmetry is the strongest type of symmetry that could occur in a qubit array. Given is a generic controllable 3-qubit chain, that is built according to equation 4.16. After each special case was included, it was checked if the controllability of the 3-qubit chain remains.

It was found that a generic 3-qubit chain, that is built according to equation 4.16 remains controllable, for each special case of symmetry. The dynamical Lie Algebra associated with the 3-qubit chain does not lose any dimension when setting all of the coefficients in its Hamiltonian equal.

Result 3: Preservation of Controllability for 3-Qubit Chains under Symmetry.

The controllability of a 3-qubit chain with σ_x^2 -control and nearest-neighbour interactions η_a, η_b, η_c ,

$$\eta_a \in (11, A), \eta_b \in (11, B), \eta_c \in (7, A) \cup (7, B). \quad (4.23)$$

remains, for every type of symmetry.

In the beginning, the intuition was the more interactions between a given set-up of qubits, the more

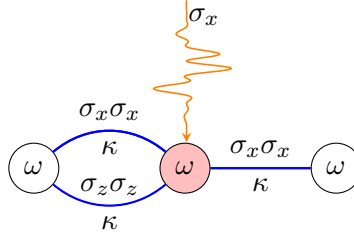


Figure 4.4: 3-qubit chain with σ_x -control on the center-qubit, degeneracy, equal strength coefficients κ and nearest-neighbour interactions $\sigma_x^1\sigma_x^2$, $\sigma_z^1\sigma_z^2$ and $\sigma_x^2\sigma_x^3$. This 3-qubit chain is controllable. Note it's asymmetric structure around the center.

likely is the system to be controllable because different nearest-neighbour interactions can contribute to a larger dynamical Lie algebra. In realizing a 3-qubit chain with local control on the second qubit, the interactions between the qubits could be resolved by external perturbations. This would lead to the decoupling of the qubits, which ultimately removes the controllability of the system. Adding nearest-neighbour interactions to the system was interpreted as strength coupling between a pair of qubits. Therefore, it is needed to protect the system from the environment. One could assume that adding certain nearest-neighbour interactions strengthens the coupling between the qubits so that, ideally, external disturbances cannot break the coupling, and ultimately the controllability remains. However, could it be that in trying to strengthen the coupling between the qubits of a controllable system, controllability gets destroyed? This would mean, that adding nearest-neighbour interactions to a controllable 3-qubit chain destroys the system's controllability.

Can an additional nearest-neighbour interaction destroy the controllability of a controllable 3-qubit chain?

To find an answer to the upper question, controllable 3-qubit chains were studied, to find an additional nearest-neighbour interaction term, that probably destroys the system's controllability. In the previous result, about controllability and symmetries, we have seen that controllability only depends on the arrangement of qubits. That means controllability depends on the number of qubits and the choice of their nearest-neighbour interactions. Adding interactions to a controllable 3-qubit chain is changing the system. Consider a nearest-neighbour interaction η that is coupling a pair of qubits. We could assume, that an additional nearest-neighbour interaction $\eta_d \in N_3$ removes the contribution to the dynamical Lie algebra, that comes from η . Therefore, it is not far-fetched to say, that controllability probably could get lost. Consider a 3-qubit chain, with Hamiltonian

$$H_1(u(t)) = \sum_{\alpha=1}^3 \frac{\omega}{2} \sigma_z^\alpha + \kappa(\sigma_x^1\sigma_x^2 + \sigma_x^2\sigma_x^3 + \sigma_z^1\sigma_z^2) + u(t)\sigma_x^2. \quad (4.24)$$

Note that this system has degeneracies and equal strength coefficients, but since the nearest-neighbour interactions are chosen according to equation 4.16, this 3-qubit system is **controllable**, according to result 3. Geometrically, it is **not symmetric** around it's center qubit, because an nearest-neighbour interaction of the form $\kappa\sigma_z^2\sigma_z^3$ is missing. What would happen, if the fourth term that is added creates a symmetry around the center qubit? The Hamiltonian of the emerging 3-qubit

chain is then given by,

$$H_2(u(t)) = H_1(u(t)) + \kappa \sigma_z^2 \sigma_z^3. \quad (4.25)$$

This system is **not controllable**. To answer the upper question, there are indeed additional nearest-neighbour interactions that destroy controllability. The term that destroys the controllability, depends on the nearest-neighbour interactions of the 3-qubit chain and requires degeneracy as well as equal strength coefficients. Furthermore, this example indicates, that there is a connection between geometric symmetries and non-controllability.

As we will see in the upcoming result, this example is not a special case of a controllability-losing system, because we can systematically tell, when a 3-qubit chain will lose its controllability, when a fourth interaction is added. The following rules have been identified that are indeed harmful to the controllability of 3-qubit chains.

Result 4: An additional interaction can destroy controllability.

A controllable 3-qubit chain, with Hamiltonian

$$H(u(t)) = \sum_{\alpha=1}^3 \frac{\omega_{\alpha}}{2} \sigma_z^{\alpha} + \kappa_a \eta_a + \kappa_b \eta_b + \kappa_c \eta_c + u(t) \sigma_x^2$$

and $\eta_a \in (11, A), \eta_b \in (11, B), \eta_c \in (7, A)$, **loses controllability**, if a fourth nearest-neighbour interaction $\kappa_d \eta_d$, with $\eta_d \in (7, B), \kappa_d \neq 0$ is added to the Hamiltonian, when the following 4 statements are **simultaneously** true:

1. $\eta_a = \sigma_i^1 \sigma_j^2, \quad \eta_b = \sigma_i^2 \sigma_j^3.$
2. $\eta_c = \sigma_k^1 \sigma_l^2, \quad \eta_d = \sigma_k^2 \sigma_l^3.$
3. Degeneracy: $\omega_{\alpha} = \omega.$
4. Equal strenght coefficients : $\kappa_a = \kappa_b = \kappa_c = \kappa_d = \kappa, \kappa \neq 0.$

Adding certain terms can be harmful to the system's controllability. Moreover, it is the case that the controllability-destroying term depends on the system. This can occur to be a counter-intuitive result, but adding a certain nearest-neighbour interaction to the system may remove the contribution from a nearest-neighbour interaction in the dynamical Lie algebra. The third and the fourth rule in result 4 are said to be symmetries. They are in particular geometric symmetries. Additionally,

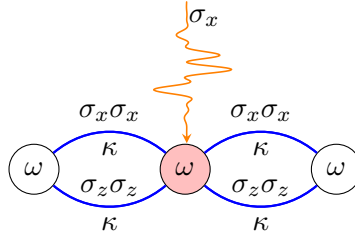


Figure 4.5: In comparison to the 3-qubit chain presented in figure 4.4, this 3-qubit chain contains an additional $\kappa \sigma_z^2 \sigma_z^3$ -interaction. This 3-qubit chain is not controllable. Note that it is symmetric around the center.

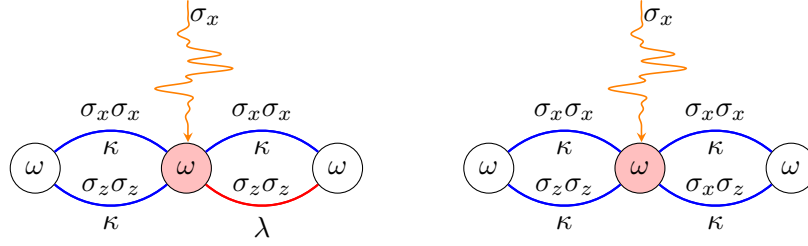


Figure 4.6: Two 3-qubit chains with an σ_x -control on the second qubit and 4 nearest-neighbour interactions. Note that in both cases, the symmetry around the center qubit is destroyed. On the left side, the coefficient λ destroys the geometric symmetry. On the right side the symmetry is destroyed by a Kronecker product $\sigma_x^2 \sigma_z^3 \neq \sigma_z^2 \sigma_z^3$. Both 3-qubit chains are controllable, probably because of the asymmetry.

if the appearing nearest-neighbour interactions contain the same Pauli matrices, the system gains geometric symmetry. Therefore, each statement in result 4, is understandable as a geometric symmetry. If every statement is fulfilled, then the system is not controllable. But one has geometric symmetry around the center qubit. Also, the considered controllable 3-qubit chains in result 1, were always asymmetric around the center qubit. This leads to the following conjecture:

Geometric asymmetries causing controllability. Geometric symmetries causing non-controllability.

Every controllable 3-qubit chain that is built according to result 1, has its controllability-destroying term. Consider a two different controllable 3-qubit chains with Hamiltonian $H_1(u(t))$ and $H_2(u(t))$. Adding a fourth interaction η_4 to $H_1(u(t))$ might destroy this systems controllability, but adding η_4 to a different Hamiltonian $H_2(u(t))$ could remain the controllability. To strengthen a coupling between a pair of qubits, through adding interactions, may preserve the system's controllability. Knowing the examined criteria in result 4 is therefore helpful since it is now known, which term should not be added.

Result 5: Adding interactions that preserve Controllability

A controllable 3-qubit chain, with Hamiltonian

$$H(u(t)) = \sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \kappa_a \eta_a + \kappa_b \eta_b + \kappa_c \eta_c + u(t) \sigma_x^2$$

and $\eta_a \in (11, A)$, $\eta_b \in (11, B)$, $\eta_c \in (7, A)$, **remains controllable** when a fourth nearest-neighbour interaction $\eta_4 \in (7, B)$ is added, if one conditions in statements in result 4 is false.

Consider the controllable 3-qubit chain, with the Hamiltonian $H_1(u(t))$ (4.24). According to result 5, the system's controllability remains by adding $\lambda \sigma_z^2 \sigma_z^3$, $\lambda \neq \kappa$ or adding $\kappa \sigma_x^2 \sigma_z^3$ to the systems Hamiltonian $H_1(u(t))$. To conclude the last 3 results, certain properties of controllable 3-qubit chains, that were built according to result 1 were studied. Result 3 states that controllable 3-qubit chains remain controllable, for every symmetry caused by degeneracy and equal strength coefficients. In result 4, it was found out, that a controllable 3-qubit chain with degeneracy and equal strength

coefficients can lose its controllability when a certain nearest-neighbour interaction is added to the system. This particular nearest-neighbour interaction is system-dependent and a strategy was provided on how to identify it (To possibly avoid it). The statements that are formulated in result 4, allow a geometric interpretation, that matches with physical expectation. It was assumed, that geometric symmetries are related to non-controllability and geometric asymmetries to controllability. In all considered examples in this section, symmetries around the center qubit were always harmful to the controllability of the system, and asymmetries around the center qubit indicated controllability. So far the geometric interpretation, allows us roughly to determine if a system remains controllable after one includes a certain symmetry. Result 4 leads to result 5. Result 5 states that nearest-neighbour interactions can be added and the system remains controllable if one of the 4 statements in result 4 is false. This result could be helpful, to strengthen a coupling between qubits, such it resists external disturbances. It is a natural question to ask if we can find strategies for a different setup of 3 qubits. Therefore, in the upcoming analysis, it is the goal to find strategies to build controllable 3-qubit loops.

4.2 Controllable 3-Qubit Loops with σ_x -control

According to equation (2.24), a 3-qubit loop is a 3-qubit chain with an additional loop interaction. Considering the example 2.1.12, with an additional local control σ_x^2 , such that the obtained Hamiltonian is:

$$H(u(t))_{Loop} = \underbrace{\kappa_a \sigma_x^1 \sigma_x^2 + \kappa_b \sigma_x^2 \sigma_x^3}_{H_{0,chain}} + \underbrace{\kappa_c \sigma_x^1 \sigma_x^3}_{Loop} + u(t) \sigma_x^2.$$

A 3-qubit loop consists of a 3-qubit chain with an additional loop interaction that allows the first and third qubits to interact. In contrast to the 3-qubit chain, a 3-qubit loop does not have a center-qubit. Only the choice of the local control creates a center. The goal was to create controllable 3-qubit loops with an σ_x -control on the second qubit, analogous to the previous section. It was aimed to give a strategy, how a controllable 3-qubit loop can be constructed.

The starting point is almost identical to the starting point of the previous section. We start from a general 3-qubit chain with σ_x -control on the second qubit, that has 2 nearest-neighbour interactions $\eta_a, \eta_b \in N_3$. This system is described by the Hamiltonian:

$$H(u(t)) = \sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \kappa_a \eta_a + \kappa_b \eta_b + u(t) \sigma_x^2. \quad (4.26)$$

In the previous section, it was found out that every controllable 3-qubit chain has at least 3 nearest-neighbour interactions. The system described by equation (4.26) cannot be controllable, since it only consists of two nearest-neighbour interactions. The goal is to transform the uncontrollable chain with Hamiltonian (4.26) to a controllable 3-qubit loop. Therefore, we want to find the loop interaction ζ , such that the emerging 3-qubit loop becomes controllable:

$$Lie\{H(u(t)) + \kappa_c \zeta\} = su(8). \quad (4.27)$$

To achieve the goal, it is first necessary to think about how to choose the two nearest-neighbour interactions η_a, η_b in the 3-qubit chain (4.26). We have avoided to choose η_a and η_b randomly, and

formulated a systematic approach. We used the result given in equation 4.12, and created 3 cases, to choose the nearest-neighbour interactions. We consider three cases:

$$\eta_a \in (11, A), \quad \eta_b \in (11, B). \quad (4.28)$$

$$\eta_a \in (11, A), \quad \eta_b \in (7, B). \quad (4.29)$$

$$\eta_a \in (11, A), \quad \eta_b \in (4, B). \quad (4.30)$$

Secondly, to determine equation (4.27), it is needed to know which loop interactions are possible. We consider loop interactions, that couple the first- and the third qubit. There are 9 different loop interactions since there are 3 Pauli matrices and a loop interaction is a Kronecker product of 2 Pauli matrices and the identity matrix.

Definition 4.2.1. (Set of all Loop-interactions) The set of all loop-interactions for a 3-qubit system is defined as:

$$L_3 := \{\sigma_i^1 \sigma_j^3 | \sigma_i, \sigma_j \in \{\sigma_x, \sigma_y, \sigma_z\}\}$$

The aim of the upper definition is ultimately to calculate the dynamical Lie algebra of the emerging the 3-qubit loop, while the parameters of the 3-qubit chain are fixed, as the loop-interaction varies in L_3 . Consider a 3-qubit chain with Hamiltonian $H(u(t)) = H_{drift} + H_{chain} + \kappa_c \zeta + u(t) \sigma_x^2$. The drift-Hamiltonian $H_{drift} = \sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha$ is assumed to be general, that is why $\omega_i \neq \omega_j \neq 0$ was required. Furthermore, $H_{chain} = \kappa_a \eta_1 + \kappa_b \eta_2$ with $\eta_1, \eta_2 \in N_3$ be fixed but arbitrary. The previous analysis of 3-qubit chains, where the generated subalgebra depended on a nearest-neighbour interaction, motivates the next procedure. In analogy, a function was built that calculated the dynamical Lie algebra $Lie\{H(u(t)) + \kappa_c \zeta\}$ of the 3-qubit loop and only depends on the loop-term $\zeta \in L_3$.

Definition 4.2.2. (Generated Subalgebra of η_a, η_b, ζ)

A 3-qubit chain, with non-degeneracies and an σ_x -control on the second qubit has the Hamiltonian

$$H(u(t)) = \sum_{\alpha}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \kappa_a \eta_a + \kappa_b \eta_b + u(t) \sigma_x^2.$$

For $\zeta \in L_3$ and $\eta_1, \eta_2 \in N_3$, exists a dynamical Lie algebra that is called generated subalgebra of ζ, η_a, η_b .

$$gs : N_3 \times N_3 \times L_3 \rightarrow su(8), \quad (\eta_a, \eta_b, \zeta) \rightarrow Lie\{H(u(t)) + \kappa_c \zeta\}.$$

We were able to identify a strategy, to build controllable 3-qubit loops with an σ_x -control on the second qubit. Consider the generated subalgebra for the first case (4.28), i.e.,

$$gs : (11, A) \times (11, B) \times L_3 \rightarrow su(8). \quad (4.31)$$

We find that, $gs(\eta_a, \eta_b, \zeta) = su(8)$ for $\zeta \in M \subset L_3$. The set M is defined through:

$$M := \{\sigma_x^1 \sigma_x^3, \sigma_y^1 \sigma_y^3, \sigma_z^1 \sigma_z^3, \sigma_x^1 \sigma_y^3, \sigma_y^1 \sigma_x^3\}. \quad (4.32)$$

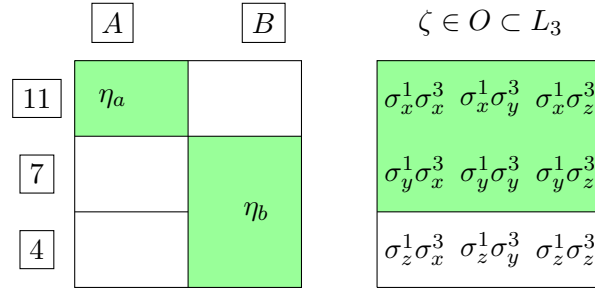


Figure 4.7: The green colored areas show how the interactions η_a, η_b, ζ have to be chosen, for a controllable 3-qubit loop with local control $u(t)\sigma_x^2$ emerges. It is a visualization of the second-and the third statement of **result 6**.

For the second case (4.29) and the third case (4.30) holds, that $gs(\eta_a, \eta_b, \zeta) = su(8)$ for $\zeta \in O \subset L_3$, where O is defined through:

$$O := \{\sigma_x^1 \sigma_x^3, \sigma_y^1 \sigma_y^3, \sigma_x^1 \sigma_y^3, \sigma_y^1 \sigma_x^3, \sigma_x^1 \sigma_z^3, \sigma_y^1 \sigma_z^3\}. \quad (4.33)$$

We summarize the observations in our next result.

Result 6: Controllable 3-Qubit Loops with σ_x -control.

A 3-qubit loop with non-degeneracies and σ_x^2 -control on the second qubit with Hamiltonian

$$H(u(t)) = \sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \kappa_a \eta_a + \kappa_b \eta_b + \kappa_c \zeta + u(t) \sigma_x^2 \quad (4.34)$$

is **controllable**, if one of the following 3 conditions is true.

1. $\eta_a \in (11, A)$, $\eta_b \in (11, B)$ and $\zeta \in M$
2. $\eta_a \in (11, A)$, $\eta_b \in (7, B)$ and $\zeta \in O$
3. $\eta_a \in (11, A)$, $\eta_b \in (4, B)$ and $\zeta \in O$

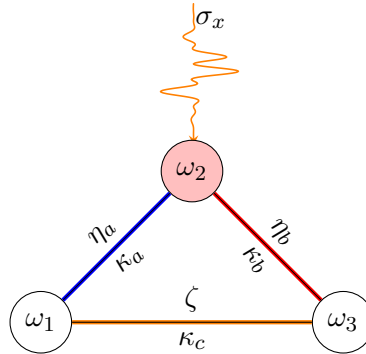


Figure 4.8: A 3-qubit loop with σ_x -control on the second qubit is recognizable. If the interactions η_a, η_b, ζ are chosen according to result 6, then the 3-qubit loop is controllable.

Note that the loop-interactions in the second and the third statement are the same. This could be expected, since $gs(\eta_1) \subset gs(\eta_2)$, for $\eta_1 \in (4, B)$ and $\eta_2 \in (7, B)$. We find that, within the set of all loop interactions L_3 , there are certain subsets M, O that are important for the controllability of 3-qubit loops. Interestingly, they have interceptions. From this follows directly, that a 3-qubit loop is controllable if the interactions are chosen in the following way:

$$\eta_a \in (11, A), \quad \eta_b \in (11, B) \cup (7, B) \cup (4, B), \quad \zeta \in M \cap O. \quad (4.35)$$

Moreover, a statement about the minimum number of interactions for a controllable 3-qubit loop follows from result 6.

For 3-qubit loops with σ_x -control on the second qubit holds, the minimum number for two-qubit interaction terms is 3. Those are two nearest-neighbour interactions and one loop interaction.

Interestingly, we find that for controllable 3-qubit systems, the minimum number of two-qubit interaction terms is 3. In the case of the 3-qubit chain, it was 3 nearest-neighbour interactions. We hypothesize that the number of qubits and the number of local controls determines the number of minimal interactions.

4.3 System Graphs associated with Controllable 3-Qubit Arrays

The founded criteria on how to construct controllable 3-qubit systems with one local σ_x -control on the second qubit, does not allow deeper insight into the system. The question remains, why those systems are controllable. Analyzing the system graphs associated with controllable 3-qubit systems is important because of two major reasons. Firstly, it gives us a deeper insight into the system, because the graphic controllability test illustrates allowed state transitions. Secondly, it can be considered as proof of our previous results, since the graphic controllability test proves pure state controllability³. However, it should be added that the graphic controllability test is a weaker verification since pure state controllability does not imply operator controllability⁴. It also has to be mentioned, that due to the variety of graph structures occurring in controllable 3-qubit systems, not all occurring graphs could be considered in this work due to space and time constraints. Take $\sigma_x^1 \sigma_x^2 \in (11, A)$ and $\sigma_x^2 \sigma_x^3 \in (11, B)$. Consider the 3-qubit chain with Hamiltonian

$$H(u(t)) = \sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \kappa_{1,2} \sigma_x^1 \sigma_x^2 + \kappa_{2,3} \sigma_x^2 \sigma_x^3 + u(t) \sigma_x^2 \quad (4.36)$$

As seen in the previous section about the 3-qubit chain and the 3-qubit loop, the system's controllability largely depends on three interaction terms. Hence, the system associated with the upper Hamiltonian is not controllable, since it only has 2 interaction terms. When examining the system graph, it was found that not every state transition between eigenstates is possible. This follows from the graph being disconnected. The structure of this graph is illustrated in figure 4.9. By carefully analyzing several 3-qubit chains with exactly two nearest-neighbour interaction terms, an interesting connection became clear. Many 3-qubit chains with two nearest-neighbour interactions, share the **same graph structure**, which is illustrated in figure 4.9. Here, same graph structure means that the

⁴Since operator controllability implies pure state controllability, but not the other way around, pure state controllability is weaker.

arrangement of nodes and edges is identical, although the weight may differ ⁵. Consider Kronecker products of the form:

$$\sigma_i^1 \sigma_j^2, \quad \sigma_i^2 \sigma_j^3, \quad \text{with } \sigma_i, \sigma_j \in \{\sigma_x, \sigma_y\}. \quad (4.37)$$

We choose η_a, η_b to obey the form of equation (4.37), then

$$\eta_a \in \{\sigma_x^1 \sigma_x^2, \sigma_y^1 \sigma_y^2, \sigma_x^1 \sigma_y^2, \sigma_y^1 \sigma_x^2\} \subset (11, A) \text{ and } \eta_b \in \{\sigma_x^2 \sigma_x^3, \sigma_y^2 \sigma_y^3, \sigma_x^2 \sigma_y^3, \sigma_y^2 \sigma_x^3\} \subset (11, B). \quad (4.38)$$

When η_a, η_b are simultaneously chosen in this way, the system that corresponds to the Hamiltonian,

$$H(u(t)) = \sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \kappa_a \eta_a + \kappa_b \eta_b + u(t) \sigma_x^2 \quad (4.39)$$

has a system graph that always has the structure illustrated in figure 4.9.

The fact that the system graphs have the same structure can be explained as follows. Although the eigenstates and eigenvalues of the Hamiltonian vary for different interaction terms, the number of different eigenvalues and the number of eigenstates in the cases considered remains the same.

⁵One cannot conclude that these systems have the same eigenvalues or eigenvectors just because their graphs have the same structure. Two systems with the same graph structure, generally have different eigenvalues and different eigenvectors.

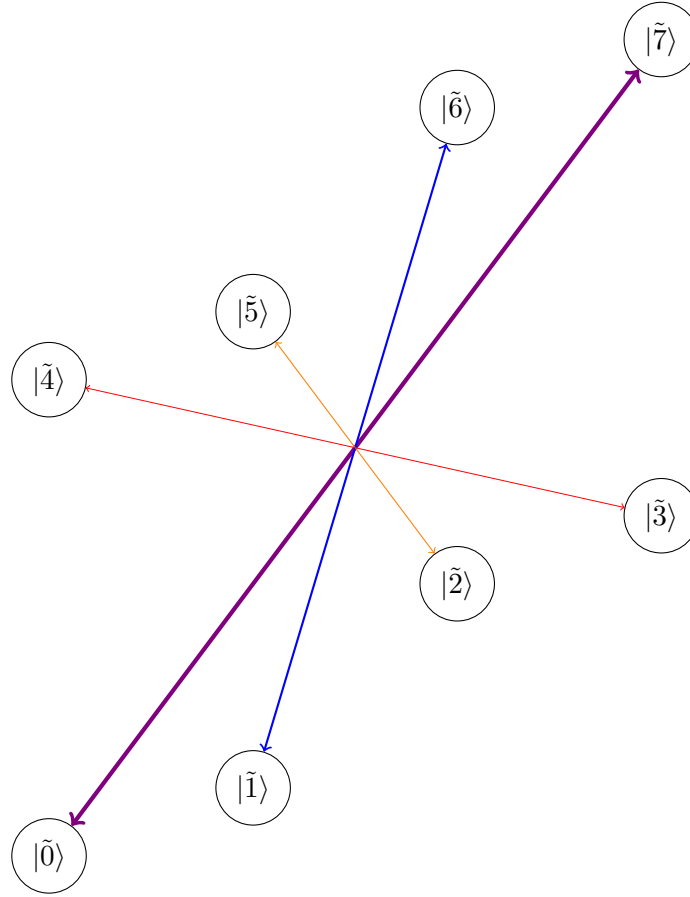


Figure 4.9: The system graph shows, the allowed state transitions for a 3-qubit chain with exactly two nearest-neighbour interactions that are chosen according to (4.38). Each node is associated to an eigenvalue that is indicated by $0, 1, 2, \dots, 7$. The eigenstates $|0\rangle, |1\rangle, |2\rangle, \dots, |7\rangle$, that correspond to the eigenvalue is written inside the node. The states are sorted from the lowest (indicated by 0) to the highest, which is indicated by 7. The **different colours** are meant to represent **different energy-gaps** in the following way: **Violet** $>$ **Blue** $>$ **Red** $>$ **Orange**. The **thickness** of an edge also corresponds to the magnitude of **energy-gap**. The thicker the edge, then the higher the energy-gap. Since the graph is **disconnected**, there are state transitions that are not allowed for this system. For instance, since there is not an edge then connects the node $|1\rangle$ and $|2\rangle$, this state transition is not allowed. Consequently, steering the system from an arbitrary initial state to an arbitrary final state is impossible. That is why any system with a system graph that corresponds to this graph structure is **not controllable**. Comparing two different 3-qubit chains with exactly two nearest-neighbour interactions, with nearest-neighbour interactions chosen as explained above, then both system's associated system graphs would have the same structure. Generally, the eigenvalues, the eigenstates, and the weights differ, but the arrangement of nodes and edges stays the same.

The resulting system graph is a disconnected graph. It is to interpret that not every state transition is admissible or in other words, only certain state transitions are allowed. Consider the states $|2\rangle$ and $|5\rangle$. Since they are connected, we can use the local control $u(t)\sigma_x^2$ to steer the system's state from $|2\rangle$

to $|5\rangle$ (If the system was in the state $|2\rangle$ before). Because only certain and not every state transition is possible, any system that has a system graph that obeys this structure is not controllable.

Consider an nearest-neighbour interaction term $\kappa_c \eta_c$, $\kappa_c \neq 0$ with $\eta_c \in \{\sigma_z^1 \sigma_z^2, \sigma_z^2 \sigma_z^3\}$. When $\kappa_c \eta_c$ is added to the system (4.39), then the system becomes controllable, according to result 1. The fact, that the resulting system graph is connected is a weak verification of result 1. Physically, adding a third nearest-neighbour term provides splitting of energy or in other words, removes the energy degeneration.

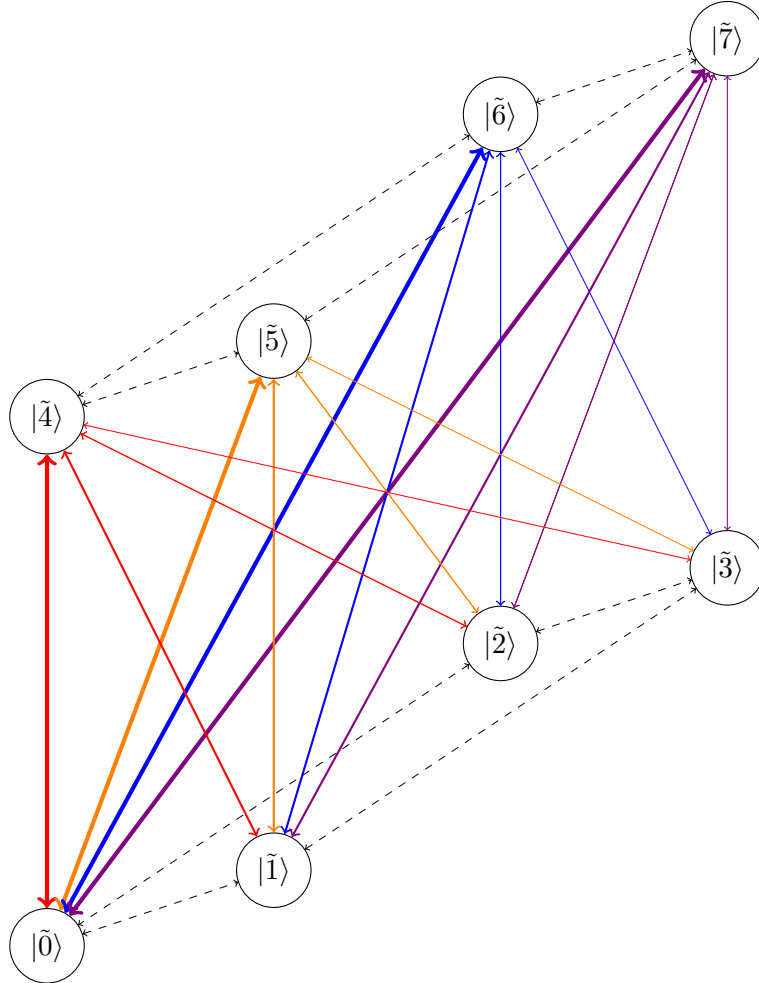


Figure 4.10: The resulting graph corresponds to a 3-qubit chain (4.39) with an additional term $\sigma_z^i \sigma_z^{i+1}, i \in \{1, 2\}$. The graph is **connected**, hence any 3-qubit system with this graph structure, is a controllable system. Also here, the different colours are meant to represent different energy-gaps: **Violet** > **Blue** > **Red** > **Orange**. The thickness of an edge is proportional to the magnitude of the energy gap. A grey dashed line between two nodes represents a path between those nodes, that is greater than a single edge. Physically, a dashed line means the system has to be steered from an initial state to another state before it can reach the target state.

Every state $|0\rangle, |1\rangle, |2\rangle, |3\rangle$ gained 3 more transitions, compared to figure 4.9, we assume that the additional third term has removed existing energy-degenerations. Furthermore, it is noticeable that the nodes $|0\rangle, |1\rangle, |2\rangle, |3\rangle$ are connected to the nodes $|4\rangle, |5\rangle, |6\rangle, |7\rangle$ by a single edge. We will refer to the upper graph structure, as **graph-1 structure**. Any 3-qubit chain that has an associated system graph with graph-1 structure has to be (pure state) controllable since the graph is connected. It is worth noting that many controllable 3-qubit chains have a system graph with a graph-1 structure. How to generate 3-qubit chains with graph-1 structure is summarized in Result 7.

Result 7: System graphs of 3-qubit chains with graph-1 structure.

The resulting system graph G_{con} of a controllable 3-qubit chain with Hamiltonian

$$H(u(t)) = \sum_{\alpha=1}^3 \frac{\omega_{\alpha}}{2} \sigma_z^{\alpha} + \kappa_a \eta_a + \kappa_b \eta_b + \kappa_c \eta_c + u(t) \sigma_x^2,$$

has **graph-1 structure**, if one of the following three conditions hold:

1. $\eta_a \in \{\sigma_i^1 \sigma_j^2 | \sigma_i, \sigma_j \in \{\sigma_x, \sigma_y\}\}, \quad \eta_b \in \{\sigma_i^2 \sigma_j^3 | \sigma_i, \sigma_j \in \{\sigma_x, \sigma_y\}\}$ and $\eta_c \in \{\sigma_z^1 \sigma_z^2, \sigma_z^2 \sigma_z^3\}$.
2. $\eta_a \in \{\sigma_i^1 \sigma_j^2 | \sigma_i, \sigma_j \in \{\sigma_x, \sigma_y\}\}, \quad \eta_b \in \{\sigma_z^2 \sigma_x^3, \sigma_z^2 \sigma_y^3\}$ and $\eta_c = \sigma_z^2 \sigma_z^3$.
3. $\eta_a \in \{\sigma_x^1 \sigma_z^2, \sigma_y^1 \sigma_z^2\}, \quad \eta_b \in \{\sigma_i^2 \sigma_j^3 | \sigma_i, \sigma_j \in \{\sigma_x, \sigma_y\}\}$ and $\eta_c = \sigma_z^1 \sigma_z^2$.

Result 6, instructs how to create controllable 3-qubit loops with an σ_x -control on the second qubit. Interestingly, certain controllable 3-qubit loops also have a graph-1 structure.

Result 8: System graphs of 3-qubit loops with graph-1 structure.

The resulting system graph G_{con} of a controllable 3-qubit loop with

$$H(u(t)) = \sum_{\alpha=1}^3 \frac{\omega_{\alpha}}{2} \sigma_z^{\alpha} + \kappa_a \sigma_i^1 \sigma_j^2 + \kappa_b \sigma_i^2 \sigma_j^3 + \kappa_c \zeta + u(t) \sigma_x^2,$$

with $\sigma_i, \sigma_j \in \{\sigma_x, \sigma_y\}$ and $i \neq j$ has **graph-1 structure**, if $\zeta \in \{\sigma_x^1 \sigma_x^3, \sigma_y^1 \sigma_y^3, \sigma_z^1 \sigma_z^3\}$.

Interestingly, there are 3-qubit chains and 3-qubit loops that have the same graph structure. This could be the case, because without the loop interaction ζ , the Hamiltonian $H(u(t))$ describes a chain with two nearest-neighbour interactions as in equation (4.39). Hence, the system without the loop interaction corresponds to the graph structure shown in the figure 4.9. Therefore, the loop interaction ζ lifts the degeneracy, just as the third nearest-neighbour interaction η_c in result 7.

4.4 Controllable 3-Qubit Chains with minimal interactions

Consider a non-degenerate 3-qubit chain with exactly two nearest-neighbour interactions $\eta_a, \eta_b \in N_3$.

$$H_0 = \sum_{\alpha=1}^3 \frac{\omega_{\alpha}}{2} \sigma_z^{\alpha} + \kappa_a \eta_a + \kappa_b \eta_b. \quad (4.40)$$

If the second qubit would be equipped with an σ_x -control, then the system does not become controllable, because this system only has two interactions. In results 1 and 2, controllable 3-qubit chains were created by specifically choosing 3 nearest-neighbour interactions. However, in the previous study of the 3-qubit system, we did not address the challenges one faces when implementing multiple interactions between two qubits. It might be practically difficult to implement more than one interaction between two qubits. Therefore, we deal with how to create controllable 3-qubit chains when a minimum number of interactions is assumed. The trivial solution would be to control each qubit individually, however, this does not solve the lack of space problem, that was addressed in the introduction. Therefore, we cannot just control each qubit individually, since we are interested in the minimum number of local controls. The question, that is going to be answered is stated as follows:

What is the minimum number of local controls, for which a 3-qubit chain with minimal nearest-neighbour interactions becomes controllable?

Now consider H_0 from equation (4.40). We added a local control $u(t)\sigma_i$ to equation (4.40) and determined the dynamical Lie algebra $Lie\{H_0 + u(t)\sigma_i^\alpha\}$. It was observed, that the dimension of the dynamical Lie algebra varies for $\sigma_i \in \{\sigma_x, \sigma_y, \sigma_z\}$ and $\alpha \in \{1, 2, 3\}$. This has been interpreted that different local controls are of different quality. How good a local control is, is measured by the dimension of the dynamical Lie algebra it generates. Here, the larger the dynamic Lie algebra generated, the better the local control.

Definition 4.4.1. (Preferred Local Control)

Consider a 3-qubit chain described by

$$H_0 = \sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \kappa_a \eta_a + \kappa_b \eta_b.$$

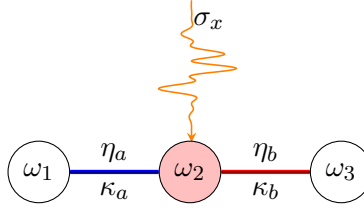
A local control $u(t)\sigma_i^\alpha$, $1 \leq \alpha \leq 3$ is said to be a **preferred local control**, if the following equation holds:

$$\dim(Lie\{H_0 + u(t)\sigma_i^\alpha\}) \geq \dim(Lie\{H_0 + u(t)\sigma_j^{\alpha'}\}), \quad \forall \sigma_j \in \{\sigma_x, \sigma_y, \sigma_z\}, 1 \leq \alpha' \leq 3. \quad (4.41)$$

A preferred local control always generates the largest dynamical Lie algebra possible. It is not unique, there can be two different Pauli matrices σ_i, σ_j , that could generate a dynamical Lie algebra of equal dimension. Also, it depends on the system. If $u(t)\sigma_i$ is a preferred local control for a 3-qubit chain with minimal interactions H_{01} , it is generally not a preferred local control for another 3-qubit chain with minimal interactions H_{02} . Consider a 3-qubit chain with Hamiltonian:

$$H(u(t)) = \sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \kappa_a \eta_a + \kappa_b \eta_b + u(t)\sigma_i^\alpha, \quad 1 \leq \alpha \leq 3. \quad (4.42)$$

A property that generally differs good local controls from bad local controls, is that it ideally does not commute with H_0 . Choosing $\sigma_i = \sigma_z$, then $u(t)\sigma_z^\alpha$ is a bad choice for a local control. Since σ_z^α



commutes with the drift-Hamiltonian:

$$\left[\sum_{\alpha=1}^3 \frac{\omega_{\alpha}}{2} \sigma_z^{\alpha}, \sigma_z^{\alpha'} \right] = \sum_{\alpha=1}^3 \frac{\omega_{\alpha}}{2} [\sigma_z^{\alpha}, \sigma_z^{\alpha'}] \delta_{\alpha', \alpha} = [\sigma_z^{\alpha'}, \sigma_z^{\alpha'}] = 0. \quad (4.43)$$

The less a local operator σ_i^{α} commutes with terms in H_0 , the more likely $u(t)\sigma_i^{\alpha}$ is a good choice for a local control.

Consider a 3-qubit chain, with Hamiltonian

$$H_0 = \sum_{\alpha=1}^3 \frac{\omega_{\alpha}}{2} \sigma_z^{\alpha} + \kappa_a \sigma_x^1 \sigma_x^2 + \kappa_b \sigma_x^2 \sigma_x^3.$$

A preferred local control $u(t)\sigma_i^{\alpha}$, can be found through testing all local controls that are possible for this system. We know that $|\{\sigma_x, \sigma_y, \sigma_z\}| = 3$ and $\alpha \leq 3$. Since σ_z -controls are always bad choices, we simply ignore them. Eventually, there are 6 possibilities for better local controls. Determining $\text{Lie}\{H_0 + u(t)\sigma_i^{\alpha}\}$, for the Pauli matrices that are left, leads to the preferred local controls σ_x^2, σ_y^2 as preferred local controls. Also, it is not a coincidence that $\sigma_x^1 \sigma_x^2 \in (11, A)$ and $\sigma_x^2 \sigma_x^3 \in (11, B)$, as we will see in the following:

A 3-qubit chain with Hamiltonian,

$$H_0 = \sum_{\alpha=1}^3 \frac{\omega_{\alpha}}{2} \sigma_z^{\alpha} + \kappa_a \eta_a + \kappa_b \eta_b, \quad (4.44)$$

with $\eta_a \in (11, A), \eta_b \in (11, B)$. always has preferred local controls $\{\sigma_x^2, \sigma_y^2\}$.

By exhaustive search it was obtained that $\dim(\text{Lie}\{H_0 + u(t)\sigma_x^2\}) = \dim(\text{Lie}\{H_0 + u(t)\sigma_y^2\}) = 36 \geq \dim(\text{Lie}\{H(u(t)) + u(t)\sigma_i^{\alpha}\})$ with $\sigma_i \in \{\sigma_x, \sigma_y, \sigma_z\}$ and $\alpha \in \{1, 2, 3\}$. This minor result states, that the generated Lie algebra reachest the highest dimension possible, when using $u(t)\sigma_{x,y}$ as local control. A possible explanation why in this considered case σ_x^2 and σ_y^2 are preferred local controls, could be related to the fact that they act on the center qubit. Ultimately, the action on the center-qubit creates a geometric symmetry around the center. This lead to the conjecture, that preferred local controls would always act on the center-qubit. However, there are 3-qubit chains with minimal nearest-neighbour interactions, that have a preferred local control that is not acting on the center qubit. For instance, consider the Hamiltonian H_0 with $\eta_1 = \sigma_x^1 \sigma_z^2$, $\eta_2 = \sigma_x^2 \sigma_z^3$.

$$H_0 = \sum_{\alpha=1}^3 \frac{\omega_{\alpha}}{2} \sigma_z^{\alpha} + \kappa_a \sigma_x^1 \sigma_z^2 + \kappa_b \sigma_x^2 \sigma_z^3. \quad (4.45)$$

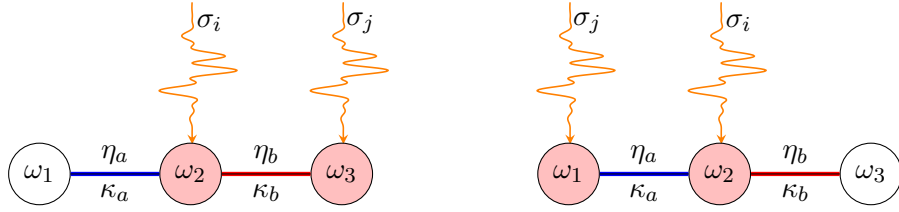


Figure 4.11: On the left and the right side, a 3-qubit chain is shown. This 3-qubit chain has minimal interactions and two local controls $\sigma_{i,j}$, each acting on a qubit. On both pictures one local control σ_i acts on the middle qubit. However, on the left side the σ_j -control acts on the third qubit, and the right side the second local control σ_j -control acts on the first qubit. Both systems describe a controllable 3-qubit chain, if one chooses $\sigma_i, \sigma_j \in \{\sigma_x, \sigma_y\}$ and $\eta_a \in (11, A), \eta_b \in (11, B)$.

Note that, the previous minor result is not holding for this system, because $\eta_1 \in (11, A)$ and $\eta_2 \in (7, B)$. The preferred local controls of the system (4.45) are $u(t)\sigma_{x,y}^3$. Hence, the conjecture about preferred local controls acting on the center-qubit does not hold generally. Eventually, we focused on 3-qubit chains with $\eta_a \in (11, A)$ and $\eta_b \in (11, B)$, for the rest of the analysis. Consider a system with Hamiltonian,

$$H(u(t)) = \underbrace{\sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \kappa_a \eta_a + \kappa_b \eta_b}_{H_0} + u_1(t) \sigma_x^2. \quad (4.46)$$

The goal is to add a second local control $u_2(t)\sigma_i^\alpha$ to $H(u(t))$, such that the emerging 3-qubit chain with two local controls becomes controllable. One could think, adding $u_2(t)\sigma_y$ to $H(u(t))$ is the right step towards the desired goal, since $u_2(t)\sigma_y$ is a preferred local control for this system.

But in this case, it holds that,

$$\text{Lie}\{H_0 + u_1(t)\sigma_x\} = \text{Lie}\{H_0 + u_2(t)\sigma_y\}.$$

Therefore adding $u_2(t)\sigma_y$ to $H(u(t))$ does not contribute new basis vectors in the dynamical Lie algebra. The next best strategy is testing for which $\sigma_i^\alpha \in \{\sigma_x^1, \sigma_x^3, \sigma_y^1, \sigma_y^3\}$ the dynamical Lie algebra of the system becomes the largest. We find that,

$$\dim(\text{Lie}\{H(u(t)) + u_2(t)\sigma_i^\alpha\}) = 63 > \dim(\text{Lie}\{H(u(t))\}), \quad \forall \sigma_i^\alpha \in \{\sigma_x^1, \sigma_x^3, \sigma_y^1, \sigma_y^3\}$$

Consequently $\text{Lie}\{H(u(t)) + u_2(t)\sigma_i^\alpha\} = \mathfrak{su}(8)$, which means that the 3-qubit chain with two local controls becomes controllable. We summarize the observations in the next Result:

Result 9: Controllable 3-qubit chains with minimal interactions

A 3-qubit chain with Hamiltonian,

$$H(u_1(t), u_2(t)) = \sum_{\alpha=1}^3 \frac{\omega_{\alpha}}{2} \sigma_z^{\alpha} + \kappa_a \eta_a + \kappa_b \eta_b + u_1(t) \sigma_i^{\alpha} + u_2(t) \sigma_j^{\alpha'}, \quad (4.47)$$

with two nearest-neighbour interactions η_1, η_2 and two local controls $u_1(t) \sigma_i^{\alpha}, u_2(t) \sigma_j^{\alpha'}$ is **controllable**, if all of the following conditions hold.

1. $\eta_1 \in (11, A), \quad \eta_2 \in (11, B)$.
2. σ_i^{α} is a preferred local control $\Leftrightarrow \sigma_i^{\alpha} \in \{\sigma_x^2, \sigma_y^2\}$.
3. $\sigma_j^{\alpha'} \in \{\sigma_x^1, \sigma_x^3, \sigma_y^1, \sigma_y^3\}$.

We find that the minimum number of local controls of a controllable 3-qubit chain with minimal interactions is 2 when the nearest-neighbour interactions and the local controls are chosen appropriately, that is according to result 9. But the question of why this system is controllable in the first place remains. Note that in the figure 4.4, the considered 3-qubit chains have asymmetries around the center. According to our conjecture about geometrical symmetries, asymmetries around the center could result in controllability. Formally, since we have two local controls, the previous conjecture on symmetries is not completely applicable to this case, but the reason why the 3-qubit chain is controllable may be related to its asymmetric geometry. Also, note that the number of interactions and local controls adds up to 4. Likewise, the number of interactions and local controls were 4 in results 1, 2, and 6. Therefore, one could conjecture that controllability could also rise from the right amount of interactions and controls. In addition, the second local control should cancel the energy degeneracy of (4.44), similar to what is shown in the figures. Formally, however, one would have to examine the system graphs with the method 3.2.2.

4.5 Summary

In the beginning, we asked if a qubit array could be controllable with fewer local controls than qubits. Especially, we were interested in the minimum number of local controls, due to the lack of space in quantum computer chips. We found that a 3-qubit array with one single σ_x -control can be controllable. Moreover, result 1, result 2, and result 6 can be considered as strategies, that will always generate controllable 3-qubit systems with a single σ_x -control on the second qubit.

Firstly, controllability depends on where the local control acts. In results 1, 2, and 6 the σ_x -control always acted on the second qubit. Secondly, the controllability of the 3-qubit chain and the 3-qubit loop depends then on the quantity and the choice of two-qubit interactions. In section 4.1 we defined, that all possible nearest-neighbour interactions $\eta = \sigma_i^{\alpha} \sigma_j^{\alpha+1}, \alpha = 1, 2$ for a 3-qubit chain are elements of a set N_3 . Then, we introduced notions to see how large the dynamical Lie algebra becomes when it only depends on a single interaction η . That was called subalgebra generated by η . It was then seen, that we can construct controllable 3-qubit chains with local control $u(t) \sigma_x^2$ if we include only certain nearest-neighbour interactions to the system. Those nearest-neighbour interactions fulfilled the property, and their associated subalgebras did not contain each other. It was found, that those certain nearest-neighbour interactions are elements of certain classes. For instance,

$$\eta_a \in (11, A), \quad \eta_b \in (11, B), \quad \eta_c \in (7, A).$$

The idea was that each nearest-neighbour interaction is added to the system, contributing a "different" subalgebra, such that the dynamical Lie algebra of the whole system becomes the Lie algebra $su(8)$, as seen in result 1.

We also saw, that there are multiple ways of creating controllable 3-qubit chains. For instance, if one chooses the nearest-neighbour interactions

$$\eta_a \in (11, A)_{Y^2}, \quad \eta_b \in (11, B)_{Y^2}, \quad \eta_c \in (4, A)$$

One can create a controllable 3-qubit chain without the use of the class $(7, A)$ or $(7, B)$ (result 2). Then, 3-qubit chains that are built according to result 1 were studied in more detail as seen in results 3, 4, and 5. Result 3 stated that, controllability remains under maximized symmetry, i.e., energy degeneracy and equal strenght coefficients $\kappa_{a,b,c} = \kappa \neq 0$. Result 4 stated that an additional fourth nearest-neighbour interaction can destroy controllability if the system has maximized symmetries and the considered nearest-neighbour interactions contain the same Pauli matrices. Finally, result 5 has stated that an additional nearest-neighbour interaction can also preserve the 3-qubit chain's controllability, in multiple cases. For instance, if we require that the system does not have maximized symmetries. In section 4.2, we observed that by adding a loop-interaction to a non-controllable 3-qubit chain with σ_x -control on the second qubit, that there are certain cases, where it transforms to a controllable 3-qubit loop. This requires that, the non-controllable 3-qubit chain has minimal nearest-neighbour interactions and that we have to choose all two-qubit interactions in a certain way. The associated two-qubit interactions, also follow the principle of being in disjoint sets. For instance, consider a loop-interaction $\zeta \in M$, where M is a subset of the set of all loop-interactions L . Then if,

$$\eta_a \in (11, A), \quad \eta_b \in (11, B), \quad \zeta \in M.$$

The associated 3-qubit loop is controllable. Therefore, result 6 states how controllable 3-qubit loops can be constructed. The strategies discussed in results 1, 2 and 6, explain how to create controllable 3-qubit arrays with an σ_x -control, but do not answer why those systems are controllable. Also, the current results, do not give deeper insight into the system. This is why certain resulting system graphs that are associated with controllable 3-qubit systems were studied in section 4.3. It was found that certain 3-qubit systems share the same graph structure. In figure 4.9 and figure 4.10 one can see, how an additional third two-qubit interaction lifts the energy-degeneration of the system, such that overall the emerging 3-qubit system is controllable. In section 4.4 the goal was to construct a controllable 3-qubit chain when the number of interactions has to be minimal. Since a 3-qubit chain with minimal interactions and a single σ_x -control is not controllable, the strategy was to include local controls in the system. But firstly, it was seen that not every local control is equally good, if the desired goal is to create a high dynamical Lie algebra. It was investigated that the dynamical Lie algebra of a 3-qubit chain that has minimal interactions $\eta_a \in (11, A), \eta_b \in (11, B)$, equipped with a single local control $u(t)\sigma_i^\alpha$, differs in dimension for $\sigma_i \in \{\sigma_x, \sigma_y, \sigma_z\}$ and $\alpha \in \{1, 2, 3\}$. This investigation lead to the notion of **preferred local controls**, which simply describes for which Pauli matrix σ_i and for which qubit α , the dynamical Lie algebra becomes the largest. Preferred local controls contribute the most in generating the Lie algebra with the highest dimension possible. We identified the preferred local controls $u(t)\sigma_{x,y}$, for 3-qubit chains with minimal nearest-neighbour interactions, that have $\eta_1 \in (11, A)$ and $\eta_2 \in (11, B)$. As a small but noteworthy side result, we saw in (4.45) that in certain systems the preferred local control does not have to act on the center-qubit. Finally in result 9, it was obtained that certain 3-qubit-chains with minimal nearest-neighbour

interactions $\eta_1 \in (11, A)$ and $\eta_2 \in (11, B)$, only need 2 local controls. Here, one local control $u(t)\sigma_{x,y}^2$ must act on the middle qubit and the other local control $u(t)\sigma_{x,y}^\alpha$ must act on the first - or the third qubit.

Chapter 5

Outlook

5.1 Continuation of the results

This section is a summary of research ideas that occur while working on this thesis. Those research ideas are directly connected to the results.

Controllable 3-qubit arrays with a local control acting on the first or the third qubit

Throughout the whole analysis of the 3-qubit system a σ_x -control, that acts on the second qubit was required. The original choice of an σ_x -control on the second qubit, was motivated by example 3.1.1. It was investigated, that an σ_x -control on the second qubit generates the largest dynamical Lie algebra possible when compared to the local control $u(t)\sigma_x^{1,3}$. Moreover, choosing $u(t)\sigma_x^2$ as a local control is the best choice if for the nearest neighbour interactions, $\eta_a \in (11, A), \eta_b \in (11, B)$ holds. This was a minor result in section 4.4. Also in section 4.4, the 3-qubit chain 4.45 was discovered. This system has nearest-neighbour interactions $\eta_a \in (11, A), \eta_c \in (7, B)$ and preferred local controls that are not acting on the center qubit. It's preferred local controls are $u(t)\sigma_{x,y}^3$. For instance, consider the Hamiltonians:

$$H(u(t))_1 = \sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \kappa_a \eta_a + \kappa_c \eta_c + u(t) \sigma_x^1. \quad (5.1)$$

$$H(u(t))_3 = \sum_{\alpha=1}^3 \frac{\omega_\alpha}{2} \sigma_z^\alpha + \kappa_a \eta_a + \kappa_c \eta_c + u(t) \sigma_x^3. \quad (5.2)$$

Now that we have set up the equations, we could proceed in the same way as in sections 4.1 and 4.2, that is adding interactions to the Hamiltonian. Therefore, one could ask the question:

Can we add two-qubit interactions, such that either one of those systems becomes controllable?

There are at least two ways to tackle this question. One way would be to simply add interactions and then check if the emerging system is controllable. The second way, would involve that we change our notion of subalgebra and substitute σ_x^2 with $\sigma_{x,y}^{1,3}$ in equation (4.3). From there, we would do

the same analysis as in the section 4.1. We would then apply the equivalence relation **subalgebra equivalence** on N_3 and obtain another quotient set N_3/\sim , that probably contains "other" classes than $\{(11, A), (11, B), (7, A), \dots\}$. The next step would then be to see, if one could detect a rule of creating controllable 3-qubit systems, that is similar to result 1. From a more theoretical point of view, it would be interesting to know, how the classes differ for different local controls. For instance, the dimension of the generated subalgebra for each class is either a prime 11, 7 or a prime power 4. It would be an interesting fact, if for different local controls $u(t)\sigma_{x,y}^{1,3}$, the dimension of the subalgebras would maintain the prime number pattern.

Deeper analysis of result 2

In result 2, we came across a different method on how controllable 3-qubit chains with an σ_x -control can be constructed. Doing deeper investigation, where one observes how the system behaves for maximized symmetries and searches if there is an additional nearest-neighbour interaction, that destroys the controllability of the system was not done but would be reasonable for completeness reasons.

Classification of system graphs for the controllable 3-qubit system

While analyzing the resulting system graphs, it was noticeable that controllable 3-qubit chains, that were built according to result 1, can have different resulting system graphs in general. From an academic perspective, it would be interesting to clarify the correspondence between controllable 3-qubit systems and their system graphs. As we have seen in the figure 4.10 some systems are likely to have the same graph structure, therefore one could ask the question: **how many and which graph structures does the controllable 3-qubit system have?**

5.2 Geometric Symmetries and Controllability

To determine if a qubit array is controllable, we have calculated the dynamical Lie algebra or performed the graphic controllability test. Calculating the basis vectors of the dynamic Lie algebra becomes more tedious with each qubit. The graphical controllability test is more efficient, but the system graph quickly becomes confusing for a system with many qubits. Therefore, developing a method that determines if a qubit array is controllable, that is fast and gives clear results, could among interest. Instead of calculating the dynamical Lie algebra or performing the graphic controllability test to determine if a qubit array is controllable, it would be great if we could directly determine if a system is controllable by simply **drawing it in the right way**. We would have to keep in mind, the following conjecture:

Conjecture 1

Geometric symmetries around the center qubit are harmful to controllability, while geometric asymmetries around the center qubit are important for controllability.

Each condition in result 4 can be visualized in a diagram like in the figure 5.1, with the following correspondence:

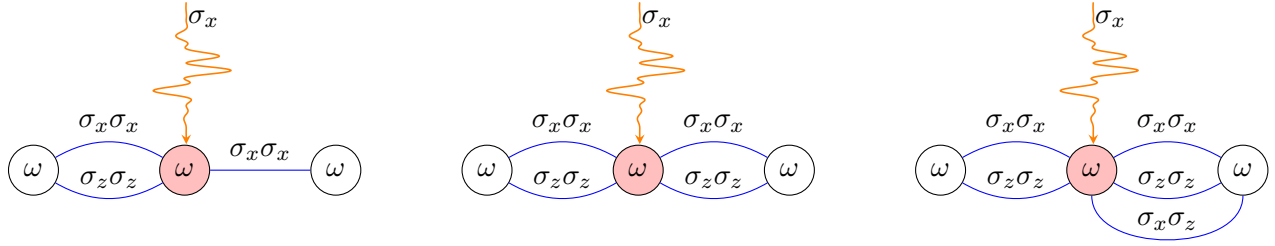


Figure 5.1: The coefficients κ_i is not written, since all strength coefficients are equal. **Left:** Asymmetric 3-qubit chain with σ_x -control on the center-qubit, that is **controllable**. **Center:** Symmetric 3-qubit chain with σ_x -control on the center-qubit, that is **not controllable**. **Right:** Asymmetric 3-qubit chain with σ_x -control. Note that the $\sigma_x \sigma_z$ -interaction destroys the symmetry and perhaps creates controllability.

- Equal Pauli matrices \leftrightarrow Equal labeling of the edges.
- Degeneracy \leftrightarrow equal ω inside the nodes.
- Equal strength coefficients \leftrightarrow equal colour of the edges.

Consider a 3-qubit chain with Hamiltonian:

$$H(u(t)) = \sum_{\alpha=1}^3 \frac{\omega}{2} \sigma_z^\alpha + \kappa(\sigma_x^1 \sigma_x^2 + \sigma_x^2 \sigma_x^3 + \sigma_z^1 \sigma_z^2) + u(t) \sigma_x^2. \quad (5.3)$$

The Hamiltonian corresponds to the left picture in the figure 5.1. It corresponds to a controllable 3-qubit chain, according to result 1. Note its asymmetric structure around the center in figure 5.1. According to result 4, adding $\kappa \sigma_z^2 \sigma_z^3$ destroys the controllability:

$$H(u(t)) = \sum_{\alpha=1}^3 \frac{\omega}{2} \sigma_z^\alpha + \kappa(\sigma_x^1 \sigma_x^2 + \sigma_x^2 \sigma_x^3 + \sigma_z^1 \sigma_z^2 + \sigma_z^2 \sigma_z^3) + u(t) \sigma_x^2. \quad (5.4)$$

But it also creates a geometric symmetry around the center, which is illustrated in the middle picture of the figure 5.1. Choose an nearest-neighbour interaction $\eta \in N_3$, $\eta = \sigma_i^\alpha \sigma_j^{\alpha+1}$, $\alpha = 1, 2$, that is not included in the upper equation. It is not trivial to ask what would happen to the system's controllability, if the another term is added to the Hamiltonian? The additional term is destroying the symmetry around the center. Interestingly, it does not depend on the term, the symmetry is destroyed in any case. According to conjecture 1, the emerging system has to be controllable. The system could regain controllability if the conjecture is correct.

We could choose $\eta \in (7, B)$, $\eta = \sigma_x^2 \sigma_z^3$ and the resulting system is asymmetric as illustrated on the right side of figure 5.1 and therefore probably controllable. The question now is, could we continue exactly as we are, creating or destroying controllability with each additional nearest-neighbour interaction?

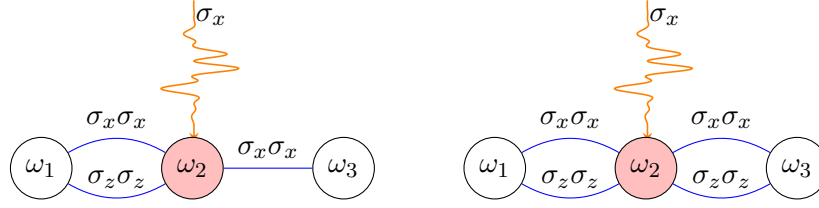


Figure 5.2: On the left side is the 3-qubit chain from the figure 4.4 and on the right side is the 3-qubit loop from the figure 4.5. To create a controllable two-dimensional array, the goal is to merge both systems. Hence, consider figure 5.3.

5.3 Controllable Two-Dimensional Qubit-Arrays

Conjecture 2

A two-dimensional qubit array, that is a composition of controllable 3-qubit chains or controllable 3-qubit loops, is **controllable** if the following two conditions hold:

1. The qubit array has local control, that acts on its center qubit.
2. The qubit array has an asymmetric structure around its center.
3. Every collection of connected qubits is a controllable array.

Consider result 1 and result 6. Consider two 3-qubit chains, that with Hamiltonian:

$$H(u(t))_1 = \sum_{\alpha=1}^3 \frac{\omega_{\alpha}}{2} \sigma_z^{\alpha} + \kappa(\sigma_x^1 \sigma_x^2 + \sigma_x^2 \sigma_x^3 + \sigma_z^1 \sigma_z^2) + u(t) \sigma_x^2. \quad (5.5)$$

$$H(u(t))_2 = H(u(t))_1 + \kappa \sigma_z^2 \sigma_z^3. \quad (5.6)$$

Note that both Hamiltonians $H(u(t))_1, H(u(t))_2$ correspond to controllable 3-qubit chains, as illustrated in 5.2. In both cases, the nearest-neighbour interactions are chosen according to result 1. Furthermore, $H(u(t))_1$ remains controllable under symmetries $\kappa_i = \kappa$, because of result 3. $H(u(t))_2$ has 4 interaction terms and equal strength coefficients. But since we choose a non-degenerate drift-Hamiltonian, the system is controllable according to result 5. Now the idea is to create a two-dimensional qubit array out of the systems $H(u(t))_1$ and $H(u(t))_2$. We cannot simply add them up, because this would result in a 3-qubit chain. Consider the 4-qubit array illustrated in the figure 5.3. Because of its structure, this system will be referred to as **T-network**. The Hamiltonian that corresponds to the T-network is,

$$H(u(t))_T = H(u(t))_1 + \kappa(\sigma_x^2 \sigma_x^4 + \sigma_z^2 \sigma_z^4). \quad (5.7)$$

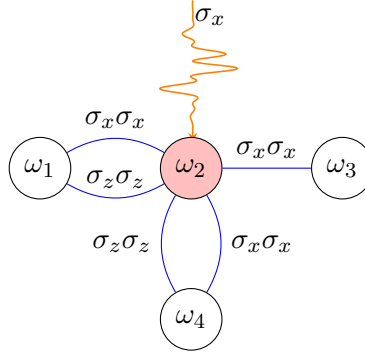


Figure 5.3: The T-network is a two-dimensional qubit array, that consists of 4 qubits. Each collection of 3 connected qubits involves the center qubit, with the local control $u(t)\sigma_x^2$. Since every collection of 3 connected qubits, is a controllable 3-qubit chain, we conjecture that the T-network is controllable.

Each collection of connected qubits within the T-network so called, contains at least 3 qubits and always the center qubit. Hence each collection contains the σ_x -control. If we just consider the collection of nodes $\{\omega_1, \omega_2, \omega_3\}$, it is a controllable 3-qubit chain, that is equivalent to $H(u(t))_2$. Moreover, the collections $\{\omega_1, \omega_2, \omega_4\}$ and $\{\omega_4, \omega_2, \omega_3\}$ are also understandable as controllable 3-qubit chains, that are equivalent to $H(u(t))_1$.

5.4 Controllable N-Qubit Chains

Conjecture 3:

Creating a controllable N-qubit chain out of controllable 3-qubit chains. An N-qubit chain is controllable if its qubit cells are controllable 3-qubit chains.

Consider the Hamiltonian,

$$H(u_1(t)) = \sum_{\alpha=1}^3 \frac{\omega}{2} \sigma_z^\alpha + \kappa(\sigma_x^1 \sigma_x^2 + \sigma_x^2 \sigma_x^3 + \sigma_z^1 \sigma_z^2) + u_1(t) \sigma_x^2. \quad (5.8)$$

Note that $\sigma_x^1 \sigma_x^2 \in (11, A)$, $\sigma_x^2 \sigma_x^3 \in (11, B)$, and $\sigma_z^1 \sigma_z^2 \in (7, A)$. We pictured this particular system in the figure 4.4. Note that it is built according to result 1 and its symmetries are according to result 5 not harmful for the system's controllability. Now, the goal is to build a controllable N-qubit chain with a minimum number of k local controls, $k < N$. The question is, how could this be effectively done? Consider system (5.8). From the conjecture, we can derive the following idea: If one would have 2 copies of system (5.8) and connect both in a line, then the emerging qubit chain is controllable because it consists of controllable 3-qubit systems. In that sense, one refers to system (5.8) as **qubit cell**, since it is used as the building block for a larger qubit chain. There are at least two ways, that deliver controllable N-qubit chains with minimal local controls. One could consider to connect two qubit cells through a nearest-neighbour interaction, such that the emerging system is a 6-qubit chain with just two local controls $u_1(t)\sigma_x^2$ and $u_2(t)\sigma_x^5$. However, this idea is not quite rigorous since currently, we do not know if a nearest-neighbour interaction exists, that connects both qubit cells

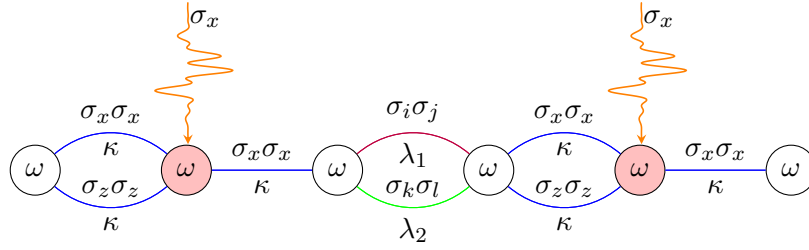


Figure 5.4: A 6-qubit chain with 2 local controls can be recognized. This system is a composition of the 3-qubit chain illustrated in figure 4.4. The coupling between the third- and the fourth qubit is described by an $\lambda_1 \sigma_i^3 \sigma_j^4$ -interaction and an $\lambda_1 \sigma_j^3 \sigma_k^4$ -interaction. If these interactions can be found so that the 6-qubit array is controllable, then a controllable qubit chain consisting of $3N$ -qubits is imaginable.

and preserves controllability. So the problem is how to choose the nearest-neighbour interaction between the third -and the fourth qubit. Therefore, one would have to test for which Pauli matrices the Kronecker product $\lambda_i \sigma_i^3 \sigma_j^4$ leads to a controllable 6-qubit chain. Possibly, one nearest-neighbour interaction term between the third and the fourth qubit is not sufficient. Hence, one would have to add a different Kronecker product of the form $\lambda_2 \sigma_k^3 \sigma_l^4$ and do the testing again.

If the system illustrated in 5.4 is controllable, then one could take N copies of system (5.8), connect each 3-qubit chain through the nearest-neighbour interactions $\lambda_1 \sigma_i^3 \sigma_j^4 + \lambda_2 \sigma_i^3 \sigma_k^4$ and the resulting system would be an controllable $3N$ -qubit chain. For this a proof by induction would be conceivable.

Another way, that could lead to the desired result: Consider again, 2 copies of system (5.8). The idea is, that the last qubit of the original 3-qubit chain is treated as the first qubit of the second 3-qubit chain. Such that we ultimately obtain a 5-qubit chain, that has a σ_x -control on the second qubit and on the fourth qubit. Mathematically, we expand the 3-qubit chain to a 5-qubit chain, by adding what is required:

$$H(u_1(t), u_2(t)) = H(u_1(t)) + H_3^5(u_2(t)), \text{ with } H_3^5(u_2(t)) = \sum_{\alpha=4}^5 \frac{\omega}{2} \sigma_z^\alpha + \sigma_x^3 \sigma_x^4 + \sigma_z^3 \sigma_z^4 + \sigma_x^4 \sigma_x^5 + u_2(t) \sigma_x^4 \quad (5.9)$$

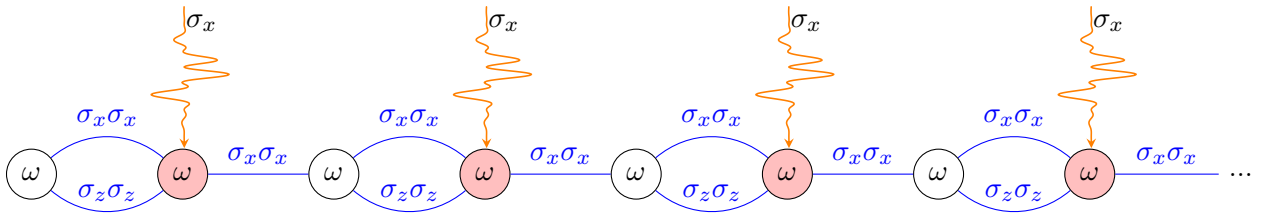


Figure 5.5: The emerging composite system is a qubit chain, that contains $2N+3$ qubits. It is noticeable, that the number of qubits is always odd.

In H_3^5 The low and the upper index, are showing how the number of qubits changes from 3 to 5. Note that by doing this expansion the dynamical Lie algebra of the system gets larger. Hence, $iH(u_1(t), u_2(t)) \in su(32)$ ¹. Formally, one could define an operator that describes the expansion of the Lie algebra:

$$T : su(8) \rightarrow su(32), \quad iH(u_1(t)) \rightarrow iH(u_1(t)) + iH_3^5(u_2(t)). \quad (5.10)$$

We have to adjust the definition of controllability for $su(32)$. Note that, $\dim(su(32)) := (32)^2 - 1 = 1023$, hence there are 1023 basis vectors that have to be calculated for controllability. Following this thought, applying the expansion operator T twice on our 3-qubit Hamiltonian, we would gain 4 new qubits, such that there are 7 qubits in total and σ_x -controls on the second, fourth and sixth qubit.

$$T^2(iH(u_1(t))) = T \circ T(iH(u_1(t))) = T \circ (iH(u_1(t)) + iH_3^5) = iH(u_1(t)) + iH_3^5 + iH_5^7 = iH(u_1(t), u_2(t), u_3(t))$$

$$T^2 : su(32) \rightarrow su(128), \quad iH(u_1(t)) \rightarrow iH(u_1(t), u_2(t), u_3(t)) \quad (5.11)$$

Since $\dim(su(128)) = (128)^2 - 1 = 16383$, this is the total number of basis vectors that have to be calculated, for controllability. Applying N times the expansion-operator T on the 3-qubit chain, then the total number of qubits becomes $2N + 3$. The system is controllable if the dynamical Lie algebra becomes $su(2^{2N+3})$, while the number of local controls is $N + 1$.

$$T^N : su(8) \rightarrow su(2^{2N+3}), iH(u_1(t)) + iH_3^{3+2N} \quad (5.12)$$

This system would have $\dim(su(2^{2N+3})) = (2^{2N+3})^2 - 1$ basis vectors that would need to be calculated. The conjecture, states that at least with the qubit cell described by $H(u_1(t))$ one could derive a qubit chain, that contains $2N + 3$ -qubits and totally $N + 1$ local controls, which is less than half of the total amount of qubits. If this conjecture would be true, it could help design new computer chips, that don't share the lack-of-space problem that current quantum computers have.

5.5 Analytic Research

Avoiding an exhaustive search and giving analytical proof requires a deep understanding of the subject's matter and can contribute to the subject by showing connections that possibly lead to a stronger framework. The methods that were introduced, were implemented in python and therefore the problems were solved numerically. However, analytical proof for the results is still missing. Calculating the dynamical Lie algebra of an N -qubit system, one has to calculate a lot of nested commutators. The main goal of this subsection is, therefore, to introduce an analytical approach to prove the results of this bachelor thesis, but avoids the direct calculation of nested commutators. The approach is to determine mathematical identities, that will simplify the calculation of the dynamical Lie algebra for a given N -qubit system. This subsection is more mathematical since every identity needs solid mathematical proof. In this subsection we use P, Q, R, S as symbols for arbitrary Pauli matrices $\sigma_x, \sigma_y, \sigma_z$, since the derived identities are better readable.

Starting with the easiest commutators that can occur, the commutator of local operators. The following two statements are the only possible outcomes.

¹Note that $H(u_1(t))$ is a Hermitian matrix for all t , hence $iH(u_1(t))$ is a skew-Hermitian matrix, with $iH(u_1(t)) \in su(8)$, for all t .

1. If two local actions P^n, Q^m act on different Hilbert spaces, ($n \neq m$) they commute to the zero action².
2. If two local actions P^n, Q^m act on the same Hilbert space, ($n = m$) they commute to a different local action or commute to zero if $P = Q$.

Both statements can be summarized in the following theorem.

Theorem 5.5.1. (*Commutator of Local Operators*) Let $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \dots \otimes \mathcal{H}_N$ be a Hilbert space associated to a N -qubit system. Let P^n and Q^m be local operators, then

$$[P^n, Q^m] = 2i\epsilon_{P,Q,R} R^n \delta_{n,m}.$$

Proof. Firstly, assume the local actions affect different Hilbert spaces and note that the notation for a two-qubit interaction is not restricted by order of the operators, then it follows

$$[P^n, Q^m] = P^n Q^m - \underbrace{Q^m P^n}_{=P^n Q^m} = 0.$$

Secondly, assume they act on the same Hilbert space, then it follows $[P^n, Q^n] = 2i\epsilon_{P,Q,R} R^n$. Note that for $P = Q$ the epsilon tensor is automatically equal to zero. \square

Now we can expand this idea and do the next more complex thing and observe how the commutator of a linear combination of local actions behaves.

Theorem 5.5.2. (*Commutator of linear combinations of local operators*) Let $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \dots \otimes \mathcal{H}_N$ be a Hilbert space associated to a N -qubit system. Let $A = \sum_{\alpha} \kappa_{\alpha} P_i^{\alpha}$ and $\sum_{\beta} \lambda_{\beta} Q_i^{\beta}$ be local operators, then

$$[A, B] = \sum_{\alpha=1}^N 2i\kappa_{\alpha} \lambda_{\alpha} \epsilon_{(P_i Q_i R_i)} R_i^{\alpha}.$$

Thanks to 5.5.1, the proof of 5.5.2 is nearly already given.

Theorem 5.5.3. Let $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \dots \otimes \mathcal{H}_N$ be a Hilbert space associated to a N -qubit system. The commutator of a local action P^n and a two-qubit interaction $Q^m R^l$ is,

1. equal to zero, for different Hilbert space actions $n \neq m \neq l$.
2. equal to zero, if $P^n = Q^m$ or $P^n = R^l$.
3. A two-qubit interaction if $n = m$ and $P = Q$, or $n = l$ and $P = R$.

Proof. Firstly, assume that the operators act on different Hilbert spaces $n \neq m \neq l$.

$$[P^n, Q^m R^l] = P^n Q^m R^l - \underbrace{Q^m R^l P^n}_{=P^n Q^m R^l} = 0.$$

²The zero action is not a number, in this case it is a Kronecker product of N zero matrices. $\otimes_{i=1}^N 0_{2 \times 2}$

Secondly, assume that $n = m$ and $m \neq l$ (Otherwise it would not be a two-qubit interaction). Then, $[P^n, Q^n R^l] = P^n Q^n R^l - Q^n R^l P^n = ([P^n, Q^n])R^l = 2i\epsilon_{P,Q,S}S^n R^l$. Note that, this conclusion is completely symmetric to the case, where $n = l$ holds. Moreover, this implicates (3). \square

In the next theorem we will not discuss every single case, how the zero-interaction can emerge, but remark that if the given conditions do not hold, the emerging commutator is zero.

Theorem 5.5.4. (*Commutator of two-qubit interactions*) Let $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \dots \otimes \mathcal{H}_N$ be a Hilbert space associated to a N -qubit system. The commutator of 2 two-qubit interactions $A = P^n Q^m$ and $B = R^l S^k$ is,

1. a three-qubit interaction if, only one operator in each two-qubit interaction act on the same Hilbert space. $P \neq R, n = l, m \neq k$.
2. a local action if both terms share exactly one operator, e.g. $P^n = R^l$ and $m = k$. In every other case the commutator is zero.

The proof of this theorem is somewhat more technical and can be inferred from the theorems above. Since the full proof would only unnecessarily lengthen this section, it is skipped completely. To sum up the theorems:

1. The commutator of two local operators is either another local operator or zero.
2. The commutator of a local operator and a two-qubit interaction is a two-qubit action or zero.
3. The commutator of 2 two-qubit interactions is a local action, a three-qubit interaction, or zero.

It is not the goal of this subsection to give a general mathematical identity for every single commutator possible for n -qubit interactions. Such an approach is firstly very elaborate and secondly not practical. The conjecture is:

Only those mathematical identities are needed, that generate local operators and two-qubit interactions.

Recall that each commutator is element of the Lie algebra $su(n)$. For each commutator, exists a unitary transformation in $SU(n)$ ³. The local operators correspond to the 1-qubit gates. The two-qubit interactions correspond to the CNOT-gate. We can use the central result of the paper [2]:

All 1-qubit gates and the CNOT-gate form a **universal set**, which means that every unitary transformation is a product of elements in this set. Consequently, all quantum logic gates are realizable, and universal quantum computing is possible.

Universal quantum computing implies the controllability of the considered qubit array. Therefore, to prove the controllability of a qubit array, generating all local operators and all two-qubit interactions is sufficient.

³The matrix exponential maps $su(n)$ to $SU(N)$

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Final Words

Not only have I learned many new things in this bachelor thesis, but I have also finally been able to see that many different concepts from physics, mathematics, and computer science merge into one big whole. Working on this bachelor thesis was an up-and-down process, which is why I am very happy to have achieved results. Many thanks to the reader!

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SELBSTSTÄNDIGKEITSERKLÄRUNG

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