CZECH TECHNICAL UNIVERSITY IN PRAGUE
Faculty of Nuclear Sciences and Physical Engineering
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BACHELOR'S THESIS

Věrný přenos kvantových stavů na uvězněných iontech

Perfect state transfer for trapped ions

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Abstrakt: Tato práce se věnuje možnosti úplného přenosu kvantové informace na uvězněných iontech. Na začátku jsou uvedeny některé fundamentální poznatky z kvantové teorie, které jsou nutné k pochopení dalších dvou kapitol o věrném přenosu kvantové informace v obecném kontextu a o uvězněných iontech. Iontové pasti jsou prezentovány jak v základním přístupu, tak v modifikaci s externím magnetickým polem, což je experimentálně pestrý, novější přístup. Cílem prezentování modifikovaných iontových pastí tímto způsobem je budoucí nalezení Hamiltoniánů a iontových konfigurací, které umožní věrný přenos stavu. V práci je odvozena celá třída Hamiltoniánů, které vedou k úplnému přenosu informace na obecném systému, čímž je nastíněna cesta k nalezení žádaných iontových konfigurací umožňujících úplný přenos kvantové informace po pasivním kvantovém drátu z uvězněných iontů.

Klíčová slova: kvantový popis, teorie informace, kvantové počítače, uvězněné ionty, věrný přenos stavu.

Title: **Perfect state transfer for trapped ions**

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Abstract: This work focuses on possibilities of the perfect state transfer on trapped ions. In the first part some fundamental principles from quantum theory are presented that are necessary for correct understanding of next two chapters devoted to faithful transfer of quantum information in a rather general context, and to ion traps, respectively. The ion traps are presented both in elementary approach and the approach with external magnetic field, which is experimentally more diverse, more recent approach. The aim in presenting the ion traps in this way is future finding of Hamiltonians and ion configurations that allow for perfect state transfer to happen. In this work whole class of Hamiltonians is derived, that lead to perfect state transfer in general context, which shows the path to finding the demanded configurations that allow the perfect state transfer over a passive quantum wire consisting of trapped ions.

Key words: quantum description, theory of information, quantum computers, trapped ions, perfect state transfer.

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Introduction

The faithful transfer of a state is a very important part of designing a fully working quantum computer. For practical use of quantum computers for actual calculations or simulations, it is necessary to develop a reliable way of transferring the state from one component of the computer to another in analogy to classical computers. The state of the component is what carries the data, thus we could compare the transfer of the state to, for example, reading or writing the data from the hard drive of a classical computer.

There are many approaches to building a quantum computer (based on superconductors, quantum dots, nuclear magnetic resonance (NMR) - both on liquid and solid state substances, electromagnetic cavities, trapped ions or optical lattices...) and thus, not surprisingly, there is more than one possible approach to transferring the state of the components. An example of an experimental success in the Perfect State Transfer (PST) are recent experiments with rays of trapped ions communicating by transferring their states over photons and optical fibers. Currently, the two most successful (experimentally) designs of the quantum computer are the ones using trapped ions and the ones using spin resonance (the NMR methods), the reason being a long development that the NMR technology has been subjected to over the past decades and its massive commercial success. Even some of the quantum algorithms have been successfully presented on the NMR based computers. The reason for the success of the trapped ions lies in their relatively simple obtainability resulting from well-developed methods of cooling ions (e.g. sideband cooling) and the simple idea behind trapping them with rapidly varying electromagnetic fields. It was prof. Theodor W. Hänsch and his team who have demonstrated the principle of trapping them on trapping macroscopic charged lycopodium seeds with many traps of different shapes, prof. Hänsch even trapped them with a conventional paper clip and made an amusing video where the seeds dance to a ballet music in the traps. Furthermore, above the other designs, the trapped ions do not suffer from limited scalability, in principle, which is important for experiments with larger numbers of qubits.

The one method of transferring the state we shall be focusing on throughout this thesis is using the components of the quantum computer itself to transfer the information. This approach is called *passive quantum wires* and it should bring new possibilities to experiments, since, for example, photons are excellent carriers over long distances, for short distances, however, they are not very economical because the imprinting of the state onto the photon and back is a rather complicated procedure. The idea behind passive quantum wires is to use the interaction (e.g. spin interaction) between the components in a way that allows for the information to travel through the computer without a necessity of any external driving.

Even though the framework for PST that has been developed and is presented in this thesis is very general and no specialization is needed, the first step to successful experimental implementation is finding a suitable physical system that would be capable of a passive perfect state transfer. Of course it is desirable to find this system amongst the systems that are being pursued for building the quantum computers. For that we would like to explore the possibility of PST on trapped ions, because the recent development in this area suggests that the most significant advantage of the NMR methods, the well-developed technology, could be used for driving the ions in the traps and thus eliminating the major experimental obstacle of the trapped ions being used as quantum computer: the fact that expensive and rare lasers had to be used for driving the ions. The driving electromagnetic radiation that could be used for driving the ions has to be stable against variations in frequency, phase and amplitude in order to achieve long decoherence times for the quantum computer and that is difficult to achieve experimentally with lasers, however, the NMR technology is capable of producing suitable rf or mw radiation.

The theoretical research behind the quantum computers suggests that even a few tens of qubits could solve tasks that are beyond the potential of classical computers. Examples of the tasks are popular Shor's algorithm for integral factorization, or many simulations of quantum systems that could serve for finding the eigenvalues and the eigenvectors of the Hamiltonians of the quantum systems. It is the parallelism of quantum computers that allows for solving problems whose time of completion grows exponentially with the seriousness of the task. Furthermore, the simulations could help us understand the elusive world of quantum mechanics.

In order to understand the tools of quantum physics used and the PST and the approaches to trapping ions, some basic principles and experiments from quantum mechanics are described and

explained in Part I of this thesis. Part II is devoted to introducing the perfect state transfer and passive quantum wires. And finally Part III describes the trapping of the ions and shows the latest approach to driving them.

Part I
Fundamentals of Quantum Physics behind Quantum Computing

Throughout this work notation common in quantum mechanics is being used together with common mathematical conventions, such as the Dirac's bras and kets. Unless said otherwise we will identify our physical system with a separable complex Hilbert space $\mathscr{H}$, vectors of which will be denoted by kets $|k\rangle$ with dual bras $\langle b|$. As is common in quantum mechanics the scalar product with respect to incident Hilbert space will be denoted by the braket: $\langle k \,|\, b\rangle$. If we later on would like to talk about two or more systems, then the general state space of them combined will be a tensor product of the states of individual systems.

We will also be using the Pauli notation for Pauli matrices:

$$\sigma_1 = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{0.1}$$

1 Information Unit in Quantum Information Processing

1.1 Qubit

Any information is usually broken down to ones and zeros in information processing. For example the sequence of characters "eye" which is forming a word could be encoded into a sequence of ones and zeros just by assigning "e" to one and "y" to zero. The result of this would then be 101. This would be a rather simple way of encoding the information and indeed would not be using the full potential of the sequence of zeros and ones. One can easily see that 3 bits (from now on we will be calling one variable holding value of one or zero a bit) can hold $2^3 = 8$ different values and therefore 8 different numbers/values.

QIP (Quantum Information Processing) like any other information processing therefore needs a bit container, something to hold the value of the bit, from which the value could be read at any time and changed at any time. And preferably used for calculation purposes at any time. Although this work focuses on the trapped ions as carriers of the quantum bit unit – the qubit – there is no need to restrain our thoughts on the trapped ions and the simplest qubit can be any two-level quantum system. That is a system with state space spanned by two basis vectors $\{|0\rangle, |1\rangle\}$. In this work we follow the general convention and assume the basis vectors to be orthogonal and normalized with respect to the scalar product in the space:

$$\langle k \,|\, l\rangle = \delta_{kl}. \tag{1.1}$$

We will see that a qubit has many different properties from a classical bit caused by the fact that we work with qubits with tools provided by quantum physics. One of the most peculiar ones results from the fact that we called a two level system a qubit - the possibility of superposition of basic states. Because we identified qubit with two-level system, the qubit can be in any state

$$|\psi\rangle = a\,|0\rangle + b\,|1\rangle\,, \tag{1.2}$$

not only in the two that form the basis. The qubit really is a subspace/ray in the general state space.

1.2 Representations of Qubit

A general state of any two-level system can be written as:

$$|\psi\rangle = c_1\,|0\rangle + c_2\,|1\rangle\,, \tag{1.3}$$

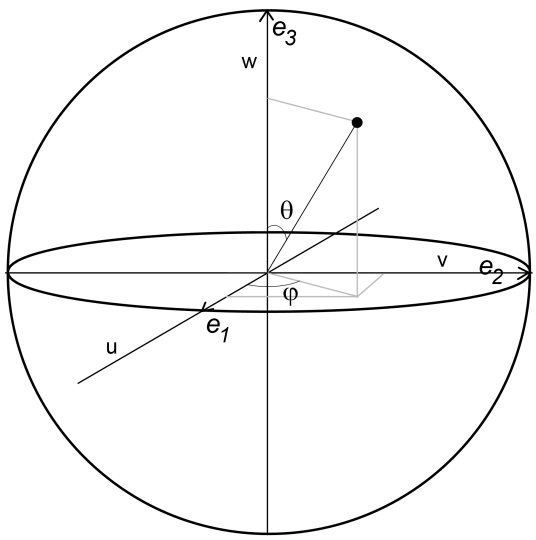

Figure 1.1: The Bloch Sphere

and $c_1, c_2 \in \mathbb{C}$. We require the general state to be normalized:

$$||\left|\psi\right\rangle||^2 = 1 = |c_1|^2 + |c_2|^2 . \tag{1.4}$$

As c_1 and c_2 are complex numbers, they are determined by four real numbers, however normalization fixes one of them and we can write general state as:

$$\left|\psi\right\rangle = e^{i\eta}\left(\cos\left(\frac{\theta}{2}\right)\left|0\right\rangle + e^{i\varphi}\sin\left(\frac{\theta}{2}\right)\left|1\right\rangle\right) \tag{1.5}$$

As the state in quantum physics is denoted by $\left|\psi\right\rangle$ up to arbitrary phase, the parameter η does not influence the state, however if we were considering multiple two-level systems, we would have to take into account relative phases [1, 2]. If we now choose to encode any information into our two level system using the numbers c_1, c_2; the basis $\{\left|0\right\rangle, \left|1\right\rangle\}$ will be called *computational basis*.

1.2.1 Bloch Sphere

A geometrical representation of a qubit is possible by defining the coordinates as follows:

$$\begin{aligned}
u := \left\langle\psi\right|\sigma_1\left|\psi\right\rangle &= \overline{c_1}c_2 + c_1\overline{c_2} && (1.6)\\
&= e^{-i\eta}\cos\left(\frac{\theta}{2}\right)e^{+i\eta}e^{i\varphi}\sin\left(\frac{\theta}{2}\right) + e^{+i\eta}\cos\left(\frac{\theta}{2}\right)e^{-i\eta}e^{-i\varphi}\sin\left(\frac{\theta}{2}\right) && (1.7)\\
&= (\cos\varphi + i\sin\varphi)\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right) + (\cos\varphi - i\sin\varphi)\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right) && (1.8)\\
&= \cos\varphi\sin\theta, && (1.9)\\
v := \left\langle\psi\right|\sigma_2\left|\psi\right\rangle &= i\left(c_1\overline{c_2} - \overline{c_1}c_2\right) = \ldots = \sin\varphi\sin\theta, && (1.10)\\
w := \left\langle\psi\right|\sigma_3\left|\psi\right\rangle &= c_1\overline{c_1} - \overline{c_2}c_2 = \ldots = \cos\theta, && (1.11)
\end{aligned}$$

where we have used (1.5) and (0.1). We will denote the u, v, w as components of a *Bloch vector*

$$\vec{R} := \begin{pmatrix} u \\ v \\ w \end{pmatrix}. \tag{1.12}$$

If we lay the coordinates on three axes we get Figure 1.1. As we can see, the general state of two-level system can be uniquely represented by a point on the Bloch sphere. This could come in

handy when talking for example about spins, as the spin operator is operator with two eigenvalues relevantly acting on vectors from $\mathbb{C}^2$ and therefore spin can be displayed on the Bloch sphere and one can associate the purely abstract idea with visual. However, it is important to note that the 3D space and the sphere is only a projection.

The representation on the Bloch sphere has several interesting properties and points. For example the state $|\psi\rangle = |0\rangle$ will be projected to the "north pole" ($w = 1, u = 0, v = 0$) and the state $|1\rangle$ to the "south pole". And we can see that two orthogonal states will be displayed as two opposite points on the sphere, because the angle α between the Bloch vectors of two different states is given by:

$$\cos\frac{\alpha}{2} = \langle\psi\,|\,\omega\rangle\,. \tag{1.13}$$

And if the states are orthogonal:

$$\cos\frac{\alpha}{2} = 0 \Rightarrow \alpha = \pi. \tag{1.14}$$

Let us now skip a little bit forward in the text and define an operator called density matrix for the two-level system using the Pauli vector from 0.1

$$\vec{\sigma} = \begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \end{pmatrix}, \tag{1.15}$$

as

$$\rho = \begin{pmatrix} c_1\overline{c_1} & c_1\overline{c_2} \\ c_2\overline{c_1} & c_2\overline{c_2} \end{pmatrix} = \frac{1}{2}\left(I + \vec{R}\cdot\vec{\sigma}\right), \tag{1.16}$$

we will be talking more about this object in the following section 2.1. It is very simple to show that if the density matrix is defined as in 2.1, for the two level system it has to take the form (1.16) and the definitions are therefore in conformity.

1.2.2 Poincaré Sphere

There is one more way of representing the general state of the two-level system on a sphere, which is called the *Poincaré sphere*. To introduce the sphere correctly, we will rewrite the general state (1.3) as follows

$$|\psi\rangle = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = c_1 \begin{pmatrix} 1 \\ z \end{pmatrix}, \tag{1.17}$$

where $z \in \mathbb{C}$ and

$$z = \frac{c_2}{c_1} = e^{i\varphi}\tan\frac{\theta}{2}. \tag{1.18}$$

We now take z and represent it by a point in the complex plane as is common and denote the real axis as axis u and the imaginary axis v, we will introduce the axis w as axis orthogonal to the two and passing through the origin of the complex plane. Next step is to perform a stereo graphical projection of the point z from the complex plane to the south pole of the sphere (See Figure 1.2) and assign the point where it penetrates the sphere to the state of the two-level system. It is very easy to see that this is a one-to-one mapping of the complex plane and therefore the point similarly to the case of Bloch sphere uniquely represents quantum state.

The Poincaré has as well several interesting properties, such as that the state $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ is represented by the north pole because $||z|| = 0$ in this case and the stereo graphical projection is rather simple in this case. Using similar path we would arrive to representation of the state $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ as the south pole. This corresponds with the Bloch sphere and its properties. In mathematics this sphere is usually called the *Riemann sphere*. If we tried to compare the two spheres, using only basic geometry we could arrive to the fact that both the spheres represent the state identically, the only difference with the Poincaré sphere is that it has additional representation of a state in z and the complex plane.

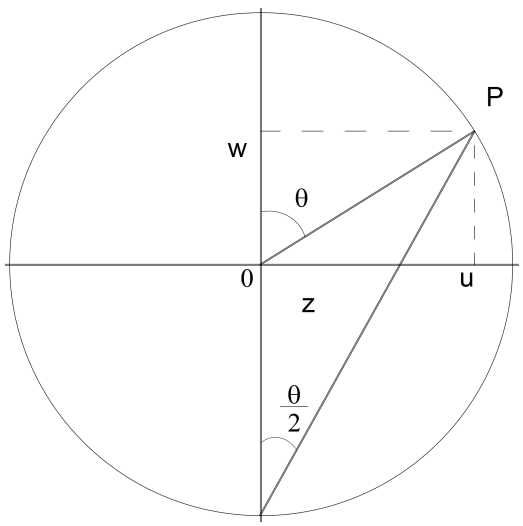

Figure 1.2: The Poincaré Sphere

Polarization of Photons and Poincaré Sphere We know that we can describe the polarization of any photon by a linear combination of the two basic linear polarizations - in the horizontal and vertical directions - $\longleftrightarrow, \updownarrow$ [1, 2]. In quantum mechanics the photon is one quantum of an electromagnetic field and to describe its polarization state the basis $\{|\leftrightarrow\rangle, |\updownarrow\rangle\}$ denoting the two basic polarizations mentioned before can be chosen [1, 2]. As such, the description of photon polarization is a beautiful example of a two-level system that can be represented by a point on the Poincaré sphere. Also it is one of the most common systems to be represented on the P-sphere.

To see how it can be represented and what tools we are provided we will now denote the two states by

$$|\updownarrow\rangle =: \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |\longleftrightarrow\rangle =: \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{1.19}$$

so that we are able to use the theory from previous subsections. Another basis that could be equivalently used is a basis that is achieved by rotating the previous basis vectors by $\frac{\pi}{4}$ in the real plane, which can be written in the previous basis as:

$$|\nearrow\rangle = \frac{1}{\sqrt{2}} \left(|1\rangle + |0\rangle\right), \tag{1.20}$$

$$|\nwarrow\rangle = \frac{1}{\sqrt{2}} \left(|1\rangle - |0\rangle\right). \tag{1.21}$$

We know [2] that the angle α between two Bloch vectors which represent two different states is given by

$$\cos\frac{\alpha}{2} = \frac{\langle\varphi\,|\,\psi\rangle}{||\varphi||\,||\psi||}, \tag{1.22}$$

which specially for two vectors from the two bases gives

$$\cos\frac{\alpha}{2} = \langle\updownarrow|\nearrow\rangle = \frac{1}{\sqrt{2}} \tag{1.23}$$

from which we can see that the angle between these two vectors must be $\frac{\pi}{2}$. In direct analogy to previous subsections and as a consequence to how we chose the basis vectors it is easy to see which states are represented by north and south poles.

The circularly polarized photons can be described by linear combination of the vectors we chose as basis by [2]:

$$|\circlearrowright\rangle = \frac{1}{\sqrt{2}} \left(|1\rangle + i\,|0\rangle\right), \tag{1.24}$$

$$|\circlearrowleft\rangle = \frac{1}{\sqrt{2}} \left(|1\rangle - i\,|0\rangle\right). \tag{1.25}$$

Polarization of Electromagnetic Fields and Poincaré Sphere, Stokes Vector Alternatively we can use the Poincaré sphere to describe a polarization state of an electromagnetic field, which can be viewed as very similar to previous paragraph as we will be essentially treating photons as well. Without limiting the generality of experiment, we will consider a transverse wave in the z-direction. With that said we know we can write the components of the electric field as [1, 2]:

$$E_x = A_1 \cos \omega t, \tag{1.26}$$

$$E_y = A_2 \cos (\omega t + \delta) . \tag{1.27}$$

We can now switch to a phasor representation, which is more illustrative for the terms from previous paragraph as circular or linear polarization:

$$\begin{pmatrix} E_x \\ E_y \end{pmatrix} = Re\left(e^{i\omega t}\begin{pmatrix} \mathcal{E}_x \\ \mathcal{E}_y \end{pmatrix}\right) = Re\left(e^{i\omega t}\begin{pmatrix} A_1 \\ A_2 e^{i\delta} \end{pmatrix}\right). \tag{1.28}$$

This gives

$$\frac{\mathcal{E}_y}{\mathcal{E}_x} = \frac{A_2}{A_1} e^{i\delta}, \tag{1.29}$$

which shows that δ is a relative phase of the phasors $\mathcal{E}_x, \mathcal{E}_y$ in the complex plane. If we now have $\delta = m\pi, m \in \mathbb{N}$, the phasors are in opposite directions and the polarization is linear. For $\delta = \pm\frac{\pi}{2}$ and $A_1 = A_2$ we can see that the phasors are of the same size and the polarization is circular. For $\delta > 0$ is the polarization called *right-handed* and for $\delta < 0$ *left-handed*. Using simple derivations from the formulas above it is possible to show that in general the polarization is elliptic (the E_x and E_y with δ as parameter satisfy the equation for ellipse), however the process is not important and if reader wanted to see the process, it can be found in [2].

Alternative and for experimental measurements very important way of describing the polarization of electromagnetic waves are the *Stokes parameters/Stokes vector*. The parameters are defined by:

$$s_1 = \begin{pmatrix} \mathcal{E}_x, & \mathcal{E}_y e^{-i\delta} \end{pmatrix} \sigma_3 \begin{pmatrix} \mathcal{E}_x \\ \mathcal{E}_y e^{i\delta} \end{pmatrix} = A_1^2 - A_2^2, \tag{1.30}$$

$$s_2 = \begin{pmatrix} \mathcal{E}_x, & \mathcal{E}_y e^{-i\delta} \end{pmatrix} \sigma_1 \begin{pmatrix} \mathcal{E}_x \\ \mathcal{E}_y e^{i\delta} \end{pmatrix} = 2A_1 A_2 \cos\delta, \tag{1.31}$$

$$s_3 = \begin{pmatrix} \mathcal{E}_x, & \mathcal{E}_y e^{-i\delta} \end{pmatrix} \sigma_2 \begin{pmatrix} \mathcal{E}_x \\ \mathcal{E}_y e^{i\delta} \end{pmatrix} = 2A_1 A_2 \sin\delta. \tag{1.32}$$

Sometimes are these parameters considered as components of the Stokes vector of length

$$||s|| = s_1^2 + s_3^2 + s_3^2 = \left(A_1^2 + A_2^2\right)^2 . \tag{1.33}$$

And this vector can be directly represented on the Poincaré sphere introduced in the previous subsection 1.2.2, only with different orientation, that should show us relation between the two paragraphs (Polarization of Photons and Poincaré Sphere and this one), because the circular polarization with $\delta = \pm\frac{\pi}{2}, A_1 = A_2 = A$ yields

$$\vec{s} = \left(0, 0, \pm 2A^2\right), \tag{1.34}$$

which are in correspondence with previous paragraph north and south poles of the sphere. It can be shown [2] that the linear polarization is represented by equator which separates the north half of right-handed polarization from the south one of left-handed polarization. It can also be shown that the angle between two Stokes vectors is in direct relation to the phase difference δ. The experimental significance of the Stokes parameters lies in their simple measurement using polarization filters [1].

2 No State Cloning in Quantum Mechanics

One would think why is it necessary to investigate the perfect state transfer, wouldn't it be easier to clone the state of one component of the quantum computer to another similarly to how we

reproduce many copies of the same photograph? In this section we want to focus on why that is not a possibility and therefore why the PST has to be investigated. We will demonstrate in two ways why coning is not allowed and we will explore the possibility of "almost" faithful copying of the state.

2.1 Density Operator

One of the basic rules in quantum mechanics is that every system can be described by a state vector $|\psi\rangle$. However, knowing exactly in what state the system is doesn't always have to be possible. Example of that can be taken even from classical mechanics, the large ensembles of many subsystems. So how do we describe such a large quantum system? The answer is: with a set of possible states $\{|\psi_i\rangle\}$ each occurring with certain probability.

Definition. If it is possible to describe the system with a single state vector $|\psi\rangle$, we will call that a *pure state*, otherwise a *mixed state*.

Let us now investigate an ensemble of quantum systems with a set of possible states $\{|\psi_i\rangle\}$, where state $|\psi_i\rangle$ occurs with the frequency/probability p_i, $p_i \in \mathbb{R}_0^+$, obeying $\sum_i p_i = 1$. The p_i's can be easily measured for many systems starting with gases of fluids.

The average value of any observable A is then given by following relation:

$$\langle A\rangle = \sum_i p_i \langle\psi_i| A |\psi_i\rangle = Tr(\rho A). \tag{2.1}$$

Where we have defined the density operator as follows from (2.1) as:

$$\rho = \sum_i p_i |\psi_i\rangle \langle\psi_i| . \tag{2.2}$$

Now, we could ask if the definition of density operator is dependent of the basis in which we express the vectors $|\psi_i\rangle$. Let us write the average value of A using arbitrary basis $\{\varphi_\mu\}$:

$$\langle A\rangle = \sum_{\mu\upsilon} \langle\varphi_\mu| A |\varphi_\upsilon\rangle \langle\varphi_\upsilon| \rho |\varphi_\mu\rangle . \tag{2.3}$$

And we see that (2.1) can be evaluated in any basis using (2.3).

Note. It is important to note that there is no requirement on the vectors $|\psi_i\rangle$, they don't have to form a basis (i.e. they do not have to be orthogonal nor complete). In case they are orthogonal, we call (2.2) the spectral decomposition of ρ.

The kind of systems where the density operator comes into the picture are systems where we do not have complete control of all the parameters and we cannot be sure in which of the states we prepare our systems; we only know probabilities for each state and we treat the system as a quantum ensemble; example of that could be a beam of photons, where we are not sure of the polarization of photons.

Interesting thing to mention about the density operator is that even knowing the matrix elements for the density operator $\langle\varphi_\mu| \rho |\varphi_\upsilon\rangle$ is not equal to knowing what state the ensemble is in, because there are many states that produce the same statistics. Example of that can be a system of four two-level systems, e.g. photons. If we label the photons 1..4 and compare following cases, we will come to the searched conclusion. First case is when the first photon is in polarization state $|\longleftrightarrow\rangle$ and the other photons are in state $|\updownarrow\rangle$, then the probability of $|\longleftrightarrow\rangle$ is $\frac{1}{4}$ and of the $|\updownarrow\rangle$ state $\frac{3}{4}$. It is easy to see that the same statistics would be valid for the state of the system where it would be the second, the third... photon in the state $|\longleftrightarrow\rangle$, however, the state of the system of four photons would be different each time. This property of the density operator is not surprising as we started using it when we were not certain of the state the system is in.

Another way we can view the quantum ensemble under investigation is as a set of subsets of systems in states $|\psi^{(k)}\rangle$. If we denote the number of systems in the subset k by N_k, we can rewrite (2.2) as follows:

$$\rho = \sum_i \frac{N_i}{N} |\psi_i\rangle \langle\psi_i| , \tag{2.4}$$

with $\sum_i N_i = N =$ total number of systems present in the ensemble. If we now change the index i which runs through all the states present to index k that will go through all the subsets in states $|\psi^{(k)}\rangle$, we can rewrite the density operator to form:

$$\rho = \frac{1}{N} \sum_k |\psi^{(k)}\rangle \langle\psi^{(k)}| . \tag{2.5}$$

For $p_i = \delta_{i0}$ equation (2.2) gives a very simple result for an ensemble where only one state $|\psi_0\rangle$ is present. In this case the density operator becomes a projector, thus:

$$\rho^2 = \rho, \tag{2.6}$$

holds. We have called such a state a pure state. For any state obeying (2.6) we have $\mathrm{Tr}\left(\rho^2 - \rho\right) = 1$ and $Tr\,\rho^2 = 1$, we will use that later to test if the state is pure or if more then one state is present in the system. Consider a system with more then two $p_i > 0$. Then we get for the trace:

$$\begin{aligned} \mathrm{Tr}\rho^2 &= \sum_{i,j} p_i p_j \mathrm{Tr}(|\psi_i\rangle \langle\psi_i | \psi_j\rangle \langle\psi_j|) \\ &= \sum_{ij} p_i p_j \, |\langle\psi_i | \psi_j\rangle|^2 \leq \sum_i p_i \sum_j p_j = 1. \end{aligned} \tag{2.7}$$

Now, we can see that when the states $|\psi_i\rangle$ are linearly independent, the sum must be:

$$\sum_i p_i^2 < 1. \tag{2.8}$$

And so for a given density matrix, we can decide if the state is pure or mixed.

2.2 Correlated States and Schmidt Decomposition

Let us consider two systems S_1 and S_2 determined by their bases $\{|\varphi_i\rangle_1\}$ and $\left\{|\varphi_j\rangle_2\right\}$, respectively. Then, as mentioned before, the basis in the combined space is given by states of the form:

$$\left\{|\varphi_i\rangle_1 \otimes |\varphi_j\rangle_2\right\}, \, i, j \in \mathbb{N}. \tag{2.9}$$

The scalar product in the combined space is given as a product of scalar products in involved systems.

The general pure state can be written as:

$$|\psi\rangle_{12} = \sum_{i,j} C_{i,j} \, |\varphi_i\rangle_1 \, |\varphi_j\rangle_2 . \tag{2.10}$$

If the coefficients can be written as $C_{i,j} = a_i \cdot b_j$, then the state can be factorized and is called separable:

$$|\psi\rangle_{12} = |\alpha\rangle_1 \, |\beta\rangle_2 , \tag{2.11}$$

with

$$|\alpha\rangle_1 = \sum_i a_i \, |\varphi_i\rangle_1 , \; |\beta\rangle_2 = \sum_j b_j \, |\varphi_j\rangle_2 , \tag{2.12}$$

and every probability statement about the combination of the systems becomes product of probability statements about each system separately. We, nevertheless, have to take into consideration even states which can not be factorized - the non-separable states. These states are called *correlated* and in QIP are of significant importance.

If we had a system in a special state (linear combination of tensor products of the same state vectors from the basis):

$$|\psi\rangle_{12} = \sum_i C_i \, |\varphi_i\rangle_1 \, |\varphi_i\rangle_2 , \tag{2.13}$$

we could easily show how measurement on one of the systems affects the other one by calculating the probability of occurrence of a state $|\varphi_\alpha\rangle_1 |\varphi_\beta\rangle_2$ in the system (2.13):

$$_{12}\langle\psi\,|\,\varphi_\alpha\rangle_1 |\varphi_\beta\rangle_2\,{}_2\langle\varphi_\beta|_1 \langle\varphi_\alpha\,|\,\psi\rangle_{12} = |C_\alpha|^2 \delta_{\alpha\beta}. \tag{2.14}$$

From that we can see that the systems S_1 and S_2 cannot be found in states with different α's, and any measurement on one of the systems determines outcomes of all later investigations of the other system. And we haven't been mentioning any spatial distance between the two systems. This property is sometimes referred to as to *Non-locality of quantum theory* [2] and is caused by strong correlation between the two systems.

We will now come back to the non-separable state of the two systems (2.10). To achieve this kind of combination of the two systems, one has to let them interact, no action carried out on them separately could cause this state; even if the systems are not interacting in the present, to posses entanglement they must have interacted in the past. Another possibility, of course, is interaction with common third system.

We would now like to find the mapping ω of the states $\{|\varphi_j\rangle_2\}$ so that the basis states $\{|\omega\,[\varphi_j]\rangle_1\}$ are the states entangled/conditioned by the observations of states $\{|\varphi_j\rangle_2\}$ similarly to (2.13).

Next we write the state (2.10) as:

$$|\psi\rangle_{12} = \sum_\alpha N_\alpha\, |\omega\,[\varphi_\alpha]\rangle_1 |\varphi_\alpha\rangle_2\,, \tag{2.15}$$

defining the states:

$$|\omega\,[\varphi_\alpha]\rangle_1 := N_\alpha^{-1} \sum_i C_{i\alpha}\, |\varphi_i\rangle_1\,, \tag{2.16}$$
$$N_\alpha^2 := \sum_i |C_{i\alpha}|^2\,.$$

If we now choose to perform measurement on the system S_2 and we measure that it is in the basis state $|\varphi_\alpha\rangle_2$, we will know that all the measurements on the system S_1 must be carried out knowing that it is in the associated state $|\omega\,[\varphi_j]\rangle_1$. It is easy to see from (2.15) that probability of that happening is:

$$P_\alpha = N_\alpha^2\,, \tag{2.17}$$

which using (2.16) is seen to be normalized:

$$\sum_\alpha P_\alpha = \sum_{\alpha,i} |C_{i\alpha}|^2 = 1. \tag{2.18}$$

What we can do now is execute large number of measurements on the system S_2, which would give us frequencies of states $|\varphi_\alpha\rangle_2$ appearing in our measurements, in other words, we would measure the N_α^2's. Note again that any prediction made for system S_1 after measuring $|\varphi_\alpha\rangle_2$ must be based on the presumption that S_1 is in $|\omega\,[\varphi_\alpha]\rangle_1$. Following that and using (2.17) and the definition of density operator we can now see the density operator of the system S_1 must be:

$$\rho_{S_1} := \sum_\alpha N_\alpha^2\, |\omega\,[\varphi_\alpha]\rangle_{1\,1} \langle\omega\,[\varphi_\alpha]|\,. \tag{2.19}$$

Different way of deducing (2.19) would be (as suggested by Paul Dirac in 1930) forming a reduced density matrix by partially tracing the general density matrix over the states of S_2 (by "tracing out" the system S_2):

$$\rho_{S_1} = Tr_{\,S_2}\rho = \sum_\alpha {}_2\langle\varphi_\alpha|\,|\psi\rangle_{12\,12}\langle\psi|\,|\varphi_\alpha\rangle_2\,. \tag{2.20}$$

From which we can derive (2.19) by inserting (2.15).

If we wanted to calculate the expectation value of some observable A_{S_1} in the system S_1, we would use the reduced density operator:

$$\langle A_{S_1}\rangle = Tr\,(A_{S_1}\rho) = Tr_{\,S_1}\,Tr_{\,S_2}\,(A_{S_1}\rho) = Tr_{\,S_1}\,(A_{S_1}\rho_{S_1})\,. \tag{2.21}$$

In the general case, the states $\{|\omega\,[\varphi_\alpha]\rangle_1\}$ are neither orthogonal nor complete. We could ask when they would form a basis... Let $\alpha \neq \beta$ determine two different states $|\omega\,[\varphi_\alpha]\rangle_1$, $|\omega\,[\varphi_\beta]\rangle_1$ and to see when these two are orthogonal we have to ask for:

$$N_\alpha N_{\beta\,1}\langle\omega\,[\varphi_\alpha]\,|\,\omega\,[\varphi_\beta]\rangle_1 = {}_{12}\langle\psi\,|\,\varphi_\alpha\rangle_2 \left(\sum_i |v_i\rangle_{1\,1}\langle v_i|\right) {}_2\langle\varphi_\beta\,|\,\psi\rangle_{12} = N_\alpha^2\delta_{\alpha\beta}, \tag{2.22}$$

with $\{|v_i\rangle_1\}$ being arbitrary orthonormal basis. If we now multiply previous equation by $|\varphi_\beta\rangle_2$ from the left and sum it over β, we obtain:

$$\sum_i {}_1\langle v_i\,|\,\psi\rangle_{12\,12}\langle\psi\,|\,v_i\rangle_1\,|\varphi_\alpha\rangle_2 = Tr_{\,S_1}\,(|\psi\rangle_{12\,12}\langle\psi|)\,|\varphi_\alpha\rangle_2 = N_\alpha^2\,|\varphi_\alpha\rangle_2\,. \tag{2.23}$$

And from that we can see that the condition required for the states $\{|\omega\,[\varphi_\alpha]\rangle_1\}$ to form a basis is equivalent to asking the states $\{|\varphi_\alpha\rangle_2\}$ to be the eigenstates of reduced density operator

$$\rho_{S_2} = Tr_{\,S_1}\,(|\psi\rangle_{12\,12}\langle\psi|)\,. \tag{2.24}$$

From (2.15) it can be seen that these states are as well eigenstates of ρ_{S_1}. In this situation ($\{|\omega\,[\varphi_\alpha]\rangle_1\}$ being the eigenstates of reduced density operators) the (2.15) is called a *Schmidt decomposition* and it always exists [2].

2.3 State Cloning Is Not Allowed

The quantum perspective of the world is in many ways different from the classical one. One of the differences is that from the classical point of view we could inspect a classical system at will and produce arbitrary number of identical copies of it, from the quantum point of view we can not produce any copy of a given quantum system, we will demonstrate this fact based on following thoughts.

First we need to define what exactly we mean by state cloning. Let us assume that we have two systems labeled S as <u>s</u>ource and D as <u>d</u>estination/target in arbitrary states $|\varphi\rangle_S$ and $|0\rangle_D$, respectively. And we now define cloning as a unitary transformation U_{SD} which will act on the tensor product of the two states in a specific way:

$$U_{SD}\,|\varphi\rangle_S\,|0\rangle_D = |\varphi\rangle_S\,|\varphi\rangle_D\,. \tag{2.25}$$

The first way of showing that cloning is not allowed [2] is taking two arbitrary (but different) states $|\varphi_1\rangle_S\,|0\rangle_D$ and $|\varphi_2\rangle_S\,|0\rangle_D$ and applying the transformation to both. If we then take a look at the results, we see that their scalar product is:

$$\begin{aligned} {}_S\langle\varphi_2\,|\,\varphi_1\rangle_{SD}\,\langle\varphi_2\,|\,\varphi_1\rangle_D &= {}_S\langle\varphi_2|_D\,\langle 0|\,U_{SD}^\dagger U_{SD}\,|0\rangle_D\,|\varphi_1\rangle_S \\ &= {}_S\langle\varphi_2\,|\,\varphi_1\rangle_{SD}\,\langle 0\,|\,0\rangle_D\,, \end{aligned} \tag{2.26}$$

from which one can immediately see that ${}_S\langle\varphi_2\rangle\,\varphi_{1\,S}$ has to be 1 or 0. In the former case $|\varphi_1\rangle = |\varphi_2\rangle$ which is in conflict which our presumption that the two states are different; in the latter case $|\varphi_1\rangle$ and $|\varphi_2\rangle$ are part of certain basis and therefore not arbitrary. And so we see that there is no such a unitary transformation possible.

One more of the basic principles of quantum physics forbids the state cloning, the requirement of the state space being a linear space where all the elements belong with their linear combinations. Let us consider a state:

$$|\psi\rangle_S = c_1\,|\varphi_1\rangle_S + c_2\,|\varphi_2\rangle_S\,. \tag{2.27}$$

What happens if we now apply transformation (2.25) to (2.27):

$$U_{SD}\,|\psi\rangle_S\,|0\rangle_D = c_1\,|\varphi_1\rangle_S\,|\varphi_1\rangle_D + c_2\,|\varphi_2\rangle_S\,|\varphi_2\rangle_D\,, \tag{2.28}$$

we see that the result of such a cloning operation would not be $|\psi\rangle_S\,|\psi\rangle_D$, which would be the proper result of state cloning.

Note. From (2.26) we can see that cloning of arbitrary state can not be possible; however, we also see that if we choose basis in the space $\{|\varphi_1\rangle, |\varphi_2\rangle, \ldots\}$, we can always design a cloning operation of these orthogonal states.

2.4 Possibility of Almost Faithful State Copying

After we have seen that there is no state cloning allowed in QM, one could ask how well could it be "almost" copied. Let the basis of our space be $\{|0\rangle, |1\rangle\}$ and let the source system be in state:

$$|\varphi_1\rangle_S = \alpha\,|0\rangle_S + \beta\,|1\rangle_S\,. \tag{2.29}$$

And let the state be chosen to be normalized:

$$\alpha\overline{\alpha} + \beta\overline{\beta} = 1. \tag{2.30}$$

We would like to transfer this state to the destination system as faithfully as possible while keeping the source system in its original state. To achieve this, we will need the A (as <u>a</u>ncillary) system to be used.

Notation.

$$|a\rangle_S\,|b\rangle_D\,|c\rangle_A =: |a\,b\,c\rangle\,. \tag{2.31}$$

Let us say that we would like to have the following transformation:

$$\begin{aligned} |0\,0\,0\rangle &\to \sqrt{\frac{2}{3}}\,|0\,0\,0\rangle - \frac{1}{\sqrt{6}}\left(|0\,1\,1\rangle + |1\,0\,1\rangle\right), \\ |1\,0\,0\rangle &\to -\sqrt{\frac{2}{3}}\,|1\,1\,1\rangle + \frac{1}{\sqrt{6}}\left(|0\,1\,0\rangle + |1\,0\,0\rangle\right). \end{aligned} \tag{2.32}$$

As we can see, the transformation maps orthogonal vectors onto orthogonal vectors, therefore we know that such a unitary transformation can be found (Note from 2.3 on Page 16).

We will now apply the transformation on the state

$$|\psi\rangle_{SDA} = |\varphi_1\,0\,0\rangle\,, \tag{2.33}$$

where $|\varphi_1\rangle_S$ is taken from (2.29). From that we get:

$$\begin{aligned} |\psi\rangle_{SDA} \to &\sqrt{\frac{2}{3}}\left(\alpha\,|0\,0\,0\rangle - \beta\,|1\,1\,1\rangle\right) - \frac{\alpha}{\sqrt{6}}\left(|0\,1\,1\rangle + |1\,0\,1\rangle\right) \\ &+ \frac{\beta}{\sqrt{6}}\left(|0\,1\,0\rangle + |1\,0\,0\rangle\right) =: \left|\tilde{\psi}\right\rangle_{SDA}. \end{aligned} \tag{2.34}$$

If we now calculate the reduced density matrices in source and destination systems by tracing out the other degrees of freedom

$$\begin{aligned} \rho_S &= \mathrm{Tr}_{DA}\,\rho, \\ \rho_D &= \mathrm{Tr}_{SA}\,\rho, \end{aligned} \tag{2.35}$$

by first calculating $\rho = |\tilde{\psi}\rangle_{SDA\,SDA}\langle\tilde{\psi}|$. And then from ρ we get ρ_S by identifying the terms that contain:

$$\begin{aligned} \{\,&|0\rangle_D\,|0\rangle_{A\,A}\langle 0|_D\,\langle 0|\,;\ |0\rangle_D\,|1\rangle_{A\,A}\langle 1|_D\,\langle 0|\,; \\ &|1\rangle_D\,|0\rangle_{A\,A}\langle 0|_D\,\langle 1|\,;\ |1\rangle_D\,|1\rangle_{A\,A}\langle 1|_D\,\langle 1|\}. \end{aligned} \tag{2.36}$$

Putting the remaining terms together we get:

$$\rho_S = \rho_{out} = \frac{1}{6}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{2}{3}\begin{pmatrix} \alpha\overline{\alpha} & \alpha\overline{\beta} \\ \overline{\alpha}\beta & \beta\overline{\beta} \end{pmatrix} = \frac{1}{6}I + \frac{2}{3}\rho_{in}, \tag{2.37}$$

where ρ_{in} corresponds to the initial state (2.29). If we now perform exactly the same operations for ρ_D, we get expression identical to (2.37). And so we see that both systems S and D contain the same level of information about the initial state (2.29) of the source system.

We can now rewrite (2.37) as follows:

$$\rho_{out} = \frac{5}{6}\left|\psi\right\rangle_{SDA\,SDA}\left\langle\psi\right| + \frac{1}{6}\left(I - \left|\psi\right\rangle_{SDA\,SDA}\left\langle\psi\right|\right). \tag{2.38}$$

And use this expression to calculate the expectation value of projector $\left|\psi\right\rangle\left\langle\psi\right|$, which will give us the probability of finding either of the systems $\{S, D\}$ in the state (2.29):

$$\left\langle\left|\psi\right\rangle_{SDA\,SDA}\left\langle\psi\right|\right\rangle = {}_{SDA}\left\langle\psi\right|\rho_{out}\left|\psi\right\rangle_{SDA} = \frac{5}{6}. \tag{2.39}$$

And so we have shown that there is an operation that will copy the original state of the source system to the destination system with probability of $\simeq 83\%$. This number is called *fidelity* and it can be shown [2] that this is the extreme value in the investigated situation. It follows from (2.37) that the Bloch vector from page 7 is transformed in the process as:

$$\overrightarrow{R}_{out} = \frac{2}{3}\overrightarrow{R}_{in}, \tag{2.40}$$

the norm of which is:

$$\left|\left|\vec{R}_{out}\right|\right| = \frac{4}{9} < 1. \tag{2.41}$$

And that indicates the loss of information, we can imagine that in previous analogy with the photos as a process where the first picture coming out of the machine is perfect, with sharp edges and the second one would come out as a blurry copy of the first one.

3 Experiments Associated with Spin Operator

Let us now move in the text to some fundamental experiments that led to introducing the spin operator, an event in physics that allowed the Paul traps and trapping ions to be developed. In this section we will explain using these experiments basic ideas behind the trapped ions and quantum computation on the trapped ions.

3.1 Stern–Gerlach Experiment, Spin

Named after Otto Stern and Walther Gerlach, the Stern-Gerlach experiment is a well-known demonstration of certain quantum properties such as the spin of the particles. Alternatively it can serve as a demonstration of how measurement in quantum mechanics affects the system itself. The experiment is based on sending a beam of particles through an inhomogeneous magnetic field and observing their deflection (See Figure 3.1). Most usually particles with no charge are used to neglect the deflection due to known laws of movement of a charged particle through a magnetic field (the Lorentz force). The deflection of the particles (e.g. electrons) observed is rather remarkable as it can not be understood using any quantum analogue of a classical property. What is observed in the experiments is a splitting of particles into two separate beams. Based on the experiments it has been necessary to introduce an analogue to angular momentum - the intrinsic angular momentum/the spin which every particle possesses and that can only take certain quantized values (Landé, Stoner, Pauli 1923-25).

In order to introduce the spin/the intrinsic angular momentum operator correctly, we now need to switch from original space $\mathscr{H}$ to space $\mathscr{H} \otimes \mathbb{C}^2$, this can be viewed as switching from a one-component Hilbert space $\mathscr{H}$ to a two-component Hilbert space $\mathscr{H} \otimes \mathbb{C}^2$, where each component of a vector is from $\mathscr{H}$; and therefore describing the state of the system by a linear combination of vectors from the original Hilbert space. Operators acting on the new Hilbert space will now

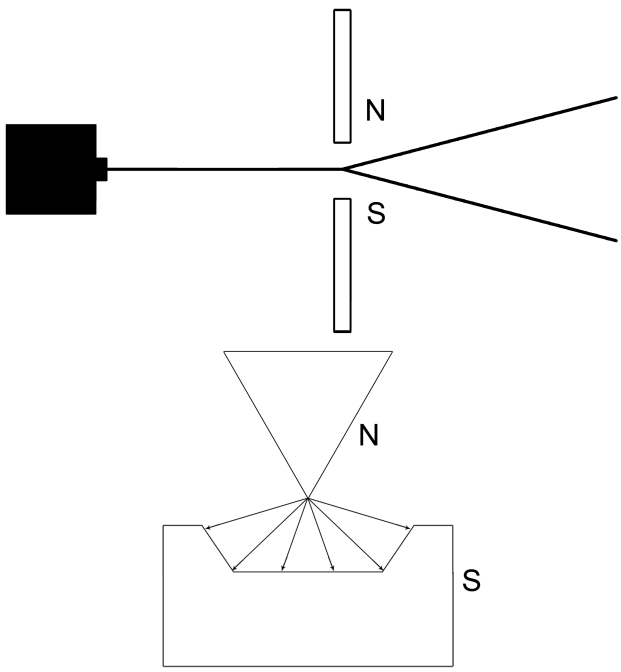

Figure 3.1: The Stern-Gerlach Experiment

be denoted by matrices of operators $A \in \mathscr{B}\left(\mathscr{H} \otimes \mathbb{C}^2\right)$, where $\mathscr{B}$ denotes a Banach space of all continuous linear maps, $A = \{A_{ij}\}_{i,j=1}^{2}, A_{ij} \in \mathscr{B}(\mathscr{H})$. It is worth noticing that the new space truly is a Hilbert space; with the scalar product of vectors defined by

$$(u, v) := \sum_{i=1}^{2}(u_i, v_i), \qquad u_i, v_i \in \mathscr{H}, u, v \in \mathscr{H} \otimes \mathbb{C}^2, \tag{3.1}$$

$$u = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}, v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}. \tag{3.2}$$

All the operators we have been using so far have been acting only on $\mathscr{H}$ and we can now view them as tensor products of the original operator with unity operator, for example the Hamiltonian operator will now be:

$$H = H \otimes I_{\mathbb{C}^2}. \tag{3.3}$$

To a projection of the intrinsic angular momentum to the z-axis we will now assign operator:

$$\mu_z = \begin{pmatrix} \mu_0 & 0 \\ 0 & -\mu_0 \end{pmatrix}, \tag{3.4}$$

where $\mu_0 = \frac{e\hbar}{2M}$ is the Bohr magneton ($\mu_0 \doteq 0,9274 \cdot 10^{-23} JT^{-1}$ for electron). Notice that the operator of projection of the spin to z-axis acts only as a multiplication by a constant factor in the original Hilbert space and it is nontrivial operator only in the $\mathbb{C}^2$. In complete analogy to commutation relations of components of the angular momentum [1, 3] we will now define the spin operator as a vector operator $\vec{S}$ nontrivial only on $\mathbb{C}^2$, components of which follow the commutation relations:

$$[S_i, S_j] = i\hbar\epsilon_{ijk}S_k, \tag{3.5}$$

where $[A, B] := AB - BA$ and where the relation follows the Einstein summation convention with ϵ_{ijk} being the Levi-Civita symbol [1]. It would be straightforward to show that the components of the spin operator must be in a following relation with the Pauli matrices (0.1):

$$S_i = \frac{\hbar}{2}\sigma_i, \forall i \in \{1..3\}. \tag{3.6}$$

We will now define the intrinsic magnetic moment (analogue to magnetic moment [3]) by

$$\vec{\mu} := \frac{2\mu_0}{\hbar}\vec{S}, \tag{3.7}$$

which will allow us to write the Hamiltonian of a particle in an electromagnetic field as dependent on the spin of the particle in the following form:

$$H = \frac{1}{2M}\left[P - eA\right]^2 + e\phi - \mu_0\vec{B}\cdot\vec{\sigma}, \tag{3.8}$$

where P is the operator of the momentum, e is the charge of the particle, A and ϕ are the electromagnetic potentials:

$$\vec{E} = -\boldsymbol{\nabla}\phi - \frac{\partial\vec{A}}{\partial t}, \vec{B} = \boldsymbol{\nabla}\times\vec{A}, \tag{3.9}$$

and $\vec{E}, \vec{B}$ are the electric field and the magnetic field. The equation:

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi, \tag{3.10}$$

where H is taken from (3.9) and ψ being the two-component function is called Pauli equation, the corresponding equation

$$H\psi = E\psi, \tag{3.11}$$

is called time-independent Pauli equation.

3.2 Zeeman Shift

The Stern-Gerlach experiment is not the only experiment that led to introducing the spin operator, also putting atoms into magnetic field (similarly to Stark effect for electric field [1, 3]) was showing some properties that were not in correspondence with the theory. If we tried to solve the motion of electrons in atoms in external homogeneous magnetic field using only the correspondence principle [1] without the spin interaction, we would learn that the eigenenergy corresponding to state vector $|E, l, m\rangle$ of electron in a spherically symmetric potential of the core would with the magnetic field become $(E - \mu_0 m)$ and depend on the magnetic quantum number, we would see from this fact that the magnetic field would change the degeneracy of the spectrum of the Hamiltonian. To each state vector corresponding to azimuthal quantum number l the magnetic field would create $(2l+1)$ different possible energy levels with distance $\mu_0\left|\left|\vec{B}\right|\right|$. This prognosis has, however, not been confirmed by experiment as according to this formula, there should be no degeneracy of the ground state with magnetic field present, but the experiments have proven, that even the ground state will split into two levels with the magnetic field present.

As mentioned before, the solution to this is to introduce the spin operator and the spin interaction with magnetic field and come to the form of Hamiltonian (3.8). We will now attempt to find this solution for homogeneous time-independent magnetic field $\vec{B} \neq \vec{B}(t)$. It is possible to show that solving of the Pauli equation can be directly transformed to solving the Schrödinger equation, because it is possible to show that if $\phi_j, j = 1, 2$ are solutions of the Schrödinger equation:

$$i\hbar\frac{\partial\psi}{\partial t} = H_1\psi, \tag{3.12}$$

where H_1 is the spin-independent part of (3.8) then the solution of Pauli equation can be written as

$$\begin{pmatrix} \psi_1(\vec{x}, t) \\ \psi_2(\vec{x}, t) \end{pmatrix} = e^{\frac{i}{\hbar}\vec{\mu}\cdot\vec{B}t}\begin{pmatrix} \phi_1(\vec{x}, t) \\ \phi_2(\vec{x}, t) \end{pmatrix}, \tag{3.13}$$

with

$$e^{\frac{i}{\hbar}\vec{\mu}\cdot\vec{B}t} = \cos\left(\frac{\mu_0}{\hbar}\left|\left|\vec{B}\right|\right|t\right) + i\frac{\vec{B}\vec{\sigma}}{\left|\left|\vec{B}\right|\right|}\sin\left(\frac{\mu_0}{\hbar}\left|\left|\vec{B}\right|\right|t\right). \tag{3.14}$$

The correct splitting of energy levels we can now get from the Pauli Hamiltonian:

$$H_P = H_0 - \frac{\mu_0}{\hbar}\vec{B}\cdot\vec{L} - \frac{2\mu_0}{\hbar}\vec{B}\cdot\vec{S}, \tag{3.15}$$

where H_0 describes the part of the Hamiltonian that does not depend on the spin (e.g. the Hamiltonian of particle in a Coulombic field). We can derive the energy splitting by solving time-independent Pauli equation

$$H_P\psi = E\psi \tag{3.16}$$

with known solution to the Schrödinger equation.

For spherically symmetric Hamiltonian without limiting the generality we can choose the z-axis in the direction of magnetic field. It would now be easy to verify that if the particle had energy $E_0 = E_{nl}$ when the magnetic field was not present; therefore E_{nl} is the eigenvalue of H_0 with $\psi_{n,l,m}$ being the eigenfunction of H, L^2, L_z - of the Hamiltonian, angular momentum squared and the third component of the angular momentum - then functions

$$\psi_{n,l,m,+}(\vec{x}) = \begin{pmatrix} \psi_{n,l,m}(\vec{x}) \\ 0 \end{pmatrix}, \psi_{n,l,m,-}(\vec{x}) = \begin{pmatrix} 0 \\ \psi_{n,l,m}(\vec{x}) \end{pmatrix}, \tag{3.17}$$

are the eigenfunctions of the Pauli Hamiltonian with eigenenergies

$$E_{n,l,m,\pm} = E_{nl} - \mu_0 B_z\,(m \pm 1) \tag{3.18}$$

The number of the new energy levels in this case is $(2l+3)\,, l = 1, 2, 3, ...$ for $l = 0$ we are getting two energy levels, which corresponds with both experiments. This splitting of energy levels in magnetic field is called the *Zeeman shift*.

Part II
Perfect State Transfer

An essential part of any quantum computer is a faithful transfer of arbitrary state between two components of a quantum computer [4]. In order to achieve this, we have to attempt to engineer a quantum wire. Quantum wires should serve as a transport for a state of one component to another, meaning that the stationary state of the starting component has to be encoded onto a "flying" qubit which will then be transferred through the wire and encoded back to stationary state of the destination component. It is important to note that the state of the starting component can not be copied, only transferred (see page 11 [No State Cloning in QM]) without any losses of information.

Two approaches seem to have been developed in this area – active and passive quantum wires. Example of the former one could be a photon transmitted over large distances through optical fiber. Photons are known to be excellent carriers even over large distances, however, the most promising ideas for quantum computers are based on for example trapped ions, atoms or solid-state systems and physical realization of such a state-imprinting onto the photon and back does not always have to be an easy task. Therefore for short distances, such as transport of the information between two quantum processors, alternative path seems to be more appropriate, the passive quantum wires.

Passive quantum wire should be a system fully compatible with the quantum computer itself. Passive quantum wires tend to use the elements of the quantum computer itself to achieve the Perfect State Transfer. Usually the quantum computer is composed of several quantum mechanical objects of one kind who form a linear chain (ions, quantum dots...) with bipartite interactions, whose strength can be manipulated for desirable effect (usually to provide different kinds of interactions). The idea behind the passive wire is to imprint the state on the first element of our network and only using unperturbed time evolution let the system evolve for a well defined time to a situation, where the last site of the chain is in the initial state of the first one.

Although there is no dissipation or dephasing present in passive wires, another obstacle prevents the passive wires to be an easy task for physicists – the dispersion of the quantum information over the wire [4]. Also there is a major advantage in using the passive wires and that is minimal

necessary control of the system, there has to be no measurement or external control, which is important for practical use.

This work focuses on the passive quantum wires and their application for computers based on trapped ions. So far the existence of the perfect passive quantum wires has been shown for systems involving coupled harmonic oscillators, arrays of quantum dots, and spin chains [4, 5]. This work aims to summarize previous work in the field of designing interactions – couplings etc. – that force the information to be refocused after a well defined time at certain site of the chain [4, 5]. In the following text some of the previous results are presented: determining form of Hamiltonians suitable for PST and showing that there are infinitely many without setting any prior restrictions on topology of network or coupling interactions, from there we will see that there are no PST Hamiltonians with NN (nearest-neighbor) interactions only for onecycle permutations of the states of the sites. Based on these results the process of quantum wire engineering has been suggested and finally it will be shown that the passive wires can be used as so called logical buses where several sites communicate using the same shared media.

4 One-cycle Permutations in Perfect State Transfer

4.1 Requirements

Let the $\mathbb{S}_n = \{1, 2, 3, \ldots, n\}$ be a set of permanently coupled quantum objects labeled by $1, 2, 3, \ldots, n$ respectively, the $\mathbb{S}_n$ will be our network; we will also require the site labeled 1 to be prepared in an arbitrary input state $|1\rangle$ and the remaining sites to be prepared in their ground states $|0\rangle$. If we can achieve transfer of a single qubit state, that will be sufficient for transferring arbitrary multi qubit states. In the simplest case we can use the same quantum wire multiple times or if the total number of excitations and the transmitted state are preserved, the global Hilbert space can be decomposed into one excitation subspaces and treated separately. On a contrary to Subsection 2.4, we will not be interested in state copying from the first site as well as we will not be interested in state cloning because we know that the basic laws of QM forbid such a behavior (see Subsection 2.3). We will rather attempt to construct a whole class of Hamiltonians $\mathfrak{C}_{\mathcal{H}}$ that only by unperturbed (with no external control) time evolution leads to perfect state transfer from the first site to the n-th site after a well defined time t with unit efficiency. Instead of using t for measuring the time we will be using a dimensionless quantity $\tau = t/J$, where J is our time units. It will allow us to work with a rather general framework as the physical realization of such networks can be a wide variety of systems, where J can be characterizing energy of the system, a coupling constant or tunneling rate. The parameter τ doesn't even have to be continuous variable, in passive linear optical networks the excitation of photons is governed by practically instant unitary evolutions and τ would present a number of these transformations applied. We will also assume that the network does not disturb the transmitted state (the system Hamiltonian $\mathcal{H}$ preserves the total number of excitations) and the only source of possible dissipation is that the wave packet spreads along the network. Specifically for the networks formed by spin chains or quantum dots this would be guaranteed when the Hamiltonian commutes with total spin operator [4].

Our way of satisfying all of these conditions will be to concentrate on Hamiltonians for which the time evolution leads to a permutation matrix after "time" τ:

$$\mathcal{U}(\tau) \equiv e^{-i\mathcal{H}\tau} = \mathcal{P}, \tag{4.1}$$

where

$$\mathcal{P} = \begin{pmatrix} 0 & & & \\ \vdots & & \tilde{\mathcal{P}} & \\ 0 & & & \\ 1 & 0 & \ldots & 0 \end{pmatrix}, \tag{4.2}$$

is a permutation matrix as $\tilde{P}$ is also a permutation matrix in the computational basis. This condition will guarantee that after "time" τ the information will refocus on the last site; if we denote the state of the system where excitation is present on the α-th site by:

$$|\alpha\rangle := |0\rangle_1 \ldots |1\rangle_\alpha \ldots |0\rangle_n \,, \tag{4.3}$$

we can easily see that the time evolution leads to:

$$\mathcal{U}(\tau)\,|1\rangle = |n\rangle \,. \tag{4.4}$$

The condition 4.1 is severely restrictive for the Hamiltonians; nevertheless, we will show that infinitely many Hamiltonians fulfill it, many of which contain previously derived PST Hamiltonians [4].

In general we can find $(n-1)!$ permutations in the form (4.2) as we have $(n-1)$ positions to fill; we will attempt to find associated Hamiltonians for each of these permutations. We will, at first, distinguish between one and many cycle permutations.

4.2 Permutations

To correctly understand our approach, we need to correctly define permutations and their distinction important for our approach.

Definition. Let $\mathbb{S}$ be an ordered set of arbitrary objects. Bijection $\mathcal{P}$ from $\mathbb{S}$ to itself is called a *permutation*.

Another way of understanding permutations is to consider the permutation a map of the set $\mathbb{S}$ to itself for which every element of $\mathbb{S}$ appears exactly once as image value and we see that permutation introduces rearrangement of the set $\mathbb{S}$. This view is equivalent to our definition, but it can help a better imagination of permutations.

We can denote the permutation in two ways, first and rather simple to understand is a two-line notation. If we had a set $\{1,2,3,4\}$ and a permutation that would map this set onto $\{2,3,4,1\}$, we could denote the permutation by writing the original order on the first line of a two-line matrix and the result on the second line:

$$\mathcal{P} = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 3 & 4 & 1 \end{pmatrix}. \tag{4.5}$$

Another way of denoting the permutations is to decompose them into disjoint *cycles* corresponding to *orbits*. It works as follows: starting from first element of the set $\mathbb{S}$, we write into parenthesis subsequent images of the first element until we get the original element, at which point we close the parenthesis and start writing the same for next unincluded element:

$$\left(x, \mathcal{P}(x), \mathcal{P}(\mathcal{P}(x)), \ldots, \mathcal{P}^i(x)\right), \text{ where } \mathcal{P}^{i+1}(x) = x, (\ldots), \ldots \tag{4.6}$$

One parenthesis is an *orbit* (we would not call it orbit if it only had one element) and the corresponding permutation is called a *cycle*. In the following will not distinguish orbits and corresponding permutations.

The example from the previous can be rewritten using the next notation as:

$$(1,2,3,4)\,. \tag{4.7}$$

Example of a two-cycle permutation could be:

$$\mathcal{P} = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 4 & 3 & 2 & 1 \end{pmatrix}, \tag{4.8}$$

which is easily seen to be decomposed into two cycles of *length* 2:

$$C_1 = (1,4) \text{ and } C_2 = (2,3)\,. \tag{4.9}$$

Definition. The cycles of length 2 are called *transpositions*.

Note. One can easily see that if the cycles are disjoint, they commute and the order of their application is irrelevant for the result.

4.3 Hamiltonians Associated With One-Cycle Permutations.

For n-sites there are $(n-2)!$ possible one-cycle permutations. We can see that from the simplest permutation:

$$\mathcal{P} = \begin{pmatrix} 0 & 1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 1 \\ 1 & 0 & \cdots & 0 \end{pmatrix}. \tag{4.10}$$

The other permutations would be achieved by relabeling the sites $\{2, \ldots, n-1\}$. Next we will derive the class of Hamiltonians leading to (4.10). First we need to find the spectrum $\sigma(\mathcal{P})$ of the operator $\mathcal{P}$, characteristic equation for which is:

$$0 = \begin{vmatrix} -\lambda & 1 & \ldots & 0 \\ \vdots & \ddots & & \vdots \\ 0 & 0 & \ddots & 1 \\ 1 & 0 & \ldots & -\lambda \end{vmatrix}. \tag{4.11}$$

Next we assume $\lambda \neq 0$ and we derive the equation for λ's by adding the first line multiplied by $\frac{1}{\lambda}$ to the last one:

$$(4.11) = \begin{vmatrix} -\lambda & 1 & \cdots & 0 \\ \vdots & -\lambda & 1 & \vdots \\ \vdots & \ddots & \ddots & 1 \\ 0 & \frac{1}{\lambda} & \cdots & -\lambda \end{vmatrix}. \tag{4.12}$$

we continue with second, third... and $(n-1)$-th line always multiplied by $\left(\frac{1}{\lambda}\right)^i$, where i is the number of incident line and we get:

$$(4.11) = \ldots = \begin{vmatrix} -\lambda & 1 & \cdots & 0 \\ 0 & -\lambda & \ddots & \vdots \\ \vdots & \ddots & \ddots & 1 \\ 0 & \cdots & 0 & -\lambda + \left(\frac{1}{\lambda}\right)^{n-1} \end{vmatrix}, \tag{4.13}$$

which is determinant of upper-diagonal matrix and the determinant is simply product of the diagonal elements and we get:

$$(-1)^{n-1}(-\lambda)^{n-1}\left(-\lambda + \left(\frac{1}{\lambda}\right)^{n-1}\right) = -\lambda^n + 1, \tag{4.14}$$

and so we see that characteristic equation can be written as:

$$\lambda^n = 1, \tag{4.15}$$

and therefore the spectrum of $\mathcal{P}$ is:

$$\sigma(\mathcal{P}) = \left\{\lambda_i | \lambda_i = e^{i2\pi\frac{j}{n}}, i \in \mathbb{Z}_n = \{0, 1, \ldots n-1\}\right\}. \tag{4.16}$$

Note. The value of $\lambda = 0$ can not be in the spectrum as the only vector that would correspond to it would be a zero vector.

Our next step will be finding corresponding eigenvectors to incident eigenvalues expressed in the computational basis:

$$\begin{pmatrix} -\lambda_j & 1 & \cdots & 0 \\ \vdots & \ddots & & \vdots \\ 0 & & \ddots & 1 \\ 1 & 0 & \cdots & -\lambda_j \end{pmatrix} \begin{pmatrix} \tilde{y}_1 \\ \vdots \\ \vdots \\ \tilde{y}_n \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ \vdots \\ 0 \end{pmatrix}. \tag{4.17}$$

We immediately see that (4.17) is equivalent to recurrence relation for y_k:

$$\tilde{y}_{k+1} = \lambda_j \tilde{y}_k, \tag{4.18}$$

with solution:

$$\tilde{y}_k = (\lambda_j)^{k-1}, k = 1, \ldots n. \tag{4.19}$$

We will require the eigenvectors to be normalized:

$$\left\| \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} \right\| = 1, \tag{4.20}$$

and because the norm of the eigenvectors is:

$$\left\| \begin{pmatrix} \lambda_j^0 \\ \lambda_j^1 \\ \vdots \\ \lambda_j^{n-1} \end{pmatrix} \right\|^2 = \sum_{i=0}^{n-1} \left|\lambda_j^i\right|^2 = \sum_{i=0}^{n-1} 1 = n, \tag{4.21}$$

we see that normalized eigenvectors corresponding to eigenvalue λ_j expressed in the computational basis must be:

$$|y_{\lambda_j}\rangle = \frac{1}{\sqrt{n}} \sum_{\alpha \in \mathbb{S}_n = \{1,2,3,\ldots,n\}} \lambda_j^{\alpha-1} |\alpha\rangle = \frac{1}{\sqrt{n}} \left(1, \lambda_j^1, \ldots, \lambda_j^{n-1}\right), \tag{4.22}$$

hence the spectral representation of $\mathcal{P}$ is:

$$\mathcal{P} = \sum_{\lambda_j \in \sigma(\mathcal{P})} \lambda_j |y_{\lambda_j}\rangle \langle y_{\lambda_j}|. \tag{4.23}$$

From the properties of exponential of operator and using previous equations it is straightforward to construct the first Hamiltonian satisfying equations (4.1) and (4.2) in following manner:

$$\mathcal{H} = \frac{1}{\tau} \sum_{\lambda_j \in \sigma(\mathcal{P})} arg(\lambda_j) |y_{\lambda_j}\rangle \langle y_{\lambda_j}|, \tag{4.24}$$

where $arg(\lambda_j)$ is the phase of the j-th eigenvalue.

Now we can immediately see that this not the only Hamiltonian that leads to permutation (4.10), we can shift each eigenenergy of the Hamiltonian (4.24) by an arbitrary integer multiple of 2π:

$$\begin{aligned} \mathcal{H}_{\vec{l}} &= \mathcal{H} + \sum_{\lambda_{j \in \sigma(\mathcal{P})}} \frac{2\pi l_{\lambda_j}}{\tau} \left|y_{\lambda_j}\right\rangle \left\langle y_{\lambda_j}\right| \\ &= \frac{1}{\tau} \sum_{\lambda_{j \in \sigma(\mathcal{P})}} \left[arg(\lambda_j) + 2\pi l_{\lambda_j}\right] \left|y_{\lambda_j}\right\rangle \left\langle y_{\lambda_j}\right|, \end{aligned} \tag{4.25}$$

where $\vec{l} \in \mathbb{Z}^n \equiv \left\{ \left(l_{\lambda_0}, l_{\lambda_1}, \ldots, l_{\lambda_{n-1}}\right) | l_{\lambda_j} \in \mathbb{Z}, j \in \mathbb{Z}_n \right\}$.

And we see that the whole class of Hamiltonians satisfying (4.1) for the particular one cycle permutation is:

$$\mathfrak{C}_{\mathcal{H}} = \left\{ \mathcal{H}_{\vec{l}} \,|\, \vec{l} \in \mathbb{Z}^n \right\}. \tag{4.26}$$

We can see that the class of Hamiltonians is parametrized by integer vector $\vec{l}$ and therefore there are infinitely many Hamiltonians in the class.

Next we can mention here that equation (4.25) can be rewritten using the projectors Π_{λ_j} projecting on the eigensubspaces of the permutation $\mathcal{P}$:

$$\mathcal{H}_{\vec{E}} = \sum_{\lambda_j \in \sigma(\mathcal{P})} \varepsilon_{\lambda_j} \left| y_{\lambda_j} \right\rangle \left\langle y_{\lambda_j} \right| \equiv \sum_{\lambda_j \in \sigma(\mathcal{P})} \varepsilon_{\lambda_j} \Pi_{\lambda_j}, \tag{4.27}$$

where the spectrum vector $\vec{E} \in \mathbb{R}^n \equiv \left\{ \left(\varepsilon_{\lambda_0}, \varepsilon_{\lambda_1}, \ldots, \varepsilon_{\lambda_{n-1}} \right) \,|\, \varepsilon_{\lambda_j} \in \mathbb{R}, j \in \mathbb{Z}_n \right\}$.

Using (4.22) we can express the Hamiltonian in the computational basis:

$$\mathcal{H}_{\vec{E}} = \sum_{\alpha,\beta \in \mathbb{S}_n} \sum_{\lambda_j \in \sigma(\mathcal{P})} \frac{1}{n} \varepsilon_{\lambda_j} \lambda_j^{\alpha-\beta} \left| \alpha \right\rangle \left\langle \beta \right|, \tag{4.28}$$

because we see that for the eigenvalues of $\mathcal{P}$ is valid relation:

$$\overline{\lambda_j^{\alpha-1}} = \lambda_j^{1-\alpha}, \tag{4.29}$$

which can be rewritten to more usual form:

$$\mathcal{H}_{\vec{E}} = \mathcal{H}_{\vec{E}}^{(0)} + \mathcal{V}_{\vec{E}}, \tag{4.30}$$

with defining the diagonal part:

$$\mathcal{H}_{\vec{E}}^{(0)} := \sum_{\alpha \in \mathbb{S}_n} E_\alpha \left| \alpha \right\rangle \left\langle \alpha \right|, \tag{4.31}$$

and the interaction part:

$$\mathcal{V}_{\vec{E}} := \sum_{\alpha \neq \beta \in \mathbb{S}_n} G(\alpha, \beta) \left| \alpha \right\rangle \left\langle \beta \right|. \tag{4.32}$$

And so the energies and the couplings are given by

$$E_\alpha = \frac{1}{n} \sum_{\lambda_j \in \sigma(\mathcal{P})} \varepsilon_{\lambda_j}, \tag{4.33}$$

$$G(\alpha, \beta) = \frac{1}{n} \sum_{\lambda_j \in \sigma(\mathcal{P})} \varepsilon_{\lambda_j} \lambda_j^{\alpha-\beta}. \tag{4.34}$$

From (4.33) we can see that Hamiltonians may only lead to PST when involving the same energy level for all the sites. Important case in PST are the NN (nearest-neighbor) interactions, Hamiltonians of which are typically tridiagonal in the computational basis ($G(\alpha, \beta) = 0$ for all $\beta \notin \{\alpha, \alpha \pm 1\}$). It has been previously shown [4] that there are none NN-interaction Hamiltonians that would lead to PST in the framework presented.

Theorem. *For networks of arbitrary dimension ($n > 2$), there exists no nearest-neighbor-interaction Hamiltonian satisfying condition* (4.1) *in the framework of permutation* (4.2).

Proof. See [4]. □

The theorem (4.3) is valid for any one cycle permutation, not only the presented one [4].

4.4 Hamiltonians Associated With Many-Cycle Permutations

In this subsection we would like to find the class of Hamiltonians that lead to a many-cycle permutation of the states of the sites. Such a permutation can be decomposed into several disjoint cycles (see Subsection 4.2 on page na straně 22). Each cycle is of the length $d < n$ and does not involve all the sites in the network, only a subset of them $\mathbb{S}_d \subset \mathbb{S}_n$ and the cycle can be treated separately as one cycle permutation on the subset and therefore we know from previous subsection that its eigenvalues must be:

$$\lambda_j = e^{i2\pi\frac{j}{d}} \; for \; j \in j \in \mathbb{Z}_d, \tag{4.35}$$

and for the projection of the corresponding eigenvectors onto the computational basis we have in analogue way as in (4.22):

$$\left\langle \alpha \middle| v_{\lambda_j}^{(k)} \right\rangle = \begin{cases} \frac{\lambda_j^{\alpha-1}}{\sqrt{d}} & for\, \alpha \in \mathbb{S}_d \\ 0 & otherwise \end{cases}. \tag{4.36}$$

We can see from (4.35) that the spectrum of a many cycle permutation is always degenerate as eigenvalue λ_0 appears as many times as the total number of cycles. We denote the number of distinct vectors corresponding to eigenvalue λ_j by δ_{λ_j}, i.e. the δ_{λ_j} is degeneracy of the value λ_j. And we denote the subspace spanned by the eigenvectors belonging to λ_j by $\mathcal{E}_{\lambda_j}$.

Now using the Gram-Schmidt orthonormalization process we choose in every subspace $\mathcal{E}_{\lambda_j}$ orthonormal basis

$$\left\{ |y_{\lambda_j}^{(k)}\rangle \right\}, \tag{4.37}$$

where $|y_{\lambda_j}^{(k)}\rangle$ are linear combinations of original eigenvectors belonging to λ_j and therefore also eigenvectors with eigenvalue λ_j.

In direct generalization to derivation of (4.25), here we also can shift the phase of each eigenvalue of the Hamiltonian by 2π, however, here we can do it for every vector from every (4.37) and we can write:

$$\begin{aligned} \mathcal{H}_{\vec{l}} &= \frac{1}{\tau} \sum_{\lambda_j} \sum_{k=1}^{\delta_{\lambda_j}} \left[arg(\lambda_j) + 2\pi l_{\lambda_j}^{(k)} \right] \left| y_{\lambda_j}^{(k)} \right\rangle \left\langle y_{\lambda_j}^{(k)} \right| \\ &= \frac{1}{\tau} \sum_{\lambda_j} \sum_{k=1}^{\delta_{\lambda_j}} \varepsilon_{\lambda_j}^{(k)} \left| y_{\lambda_j}^{(k)} \right\rangle \left\langle y_{\lambda_j}^{(k)} \right|, \end{aligned} \tag{4.38}$$

where $\vec{l} \in \mathbb{Z}^n \equiv \left\{ (l_{\lambda_0}^{(1)}, \ldots, l_{\lambda_0}^{(\delta_{\lambda_0})}; l_{\lambda_1}^{(1)}, \ldots, l_{\lambda_1}^{(\delta_{\lambda_1})}; \ldots) \,|\, l_{\lambda_j}^{(\delta_{\lambda_j})} \in \mathbb{Z} \right\}$.

Part III
Application of Fundamentals to Trapping Ions

In this part of this work we will be using some of the basic ideas presented in 3, such as the Zeeman shift, to introduce first some of rather early approaches to quantum computers based on trapped ions [6] and then we will present some ideas from more recent works of experimental physicists [7–10]. We will explain why the development has been taking the path presented and compare the new results to the previous ones.

Several approaches have been developed to building a quantum computer [2, 11] such as computer based on electromagnetic cavities, solid-state systems or macromolecules besides the trapped ions, which we will focus on in this part and this work. The other principles described in detail can be found e.g. in [2, 11] together with their comparison, advantages and disadvantages.

5 Trapping Cold Ions (Paul Traps)

The term cold ions in the title of this subsection could be a little confusing as we will be talking about just a few particles and so this thermodynamical property doesn't really have a good meaning and more appropriate would be to say ions with low energy. The reason ions have been chosen for trapping is that their laws of motion are strongly dependent on external fields present and as experiments have shown, even individual ions can be confined to a very small space into very stable traps [6, 9, 10].

First thing we need to mention here is the Earnshaw theorem that suggests that only static potentials can never trap charged particles in all three dimensions in a limited area. We can see that from the condition which every potential $V(r)$ must obey in the empty space

$$\nabla^2 V(r) = 0, \tag{5.1}$$

which implies that there cannot be any extreme value in the region, the only place where extremes could happen is at the edges of the area, but that is where electrodes are placed and therefore stable trapping by static potentials truly isn't possible. We will try to find trapping potentials amongst rapidly oscillating electric fields. If we look at the equation of motion in one dimension

$$m\ddot{x} = \lambda x \cos(\omega t)\,. \tag{5.2}$$

at the first glance there seems to be no trapping happening as we cannot see any stable solution because the force acting on the object averages to zero over longer periods of time. However, for large frequencies ω (i.e. in the limit for ω) it is justifiable to separate the quick motion of the object that follows the oscillations of the field and the slower drift relevant for longer periods of time. We will be calling these a *micromotion* $\xi(t)$ and a *smooth motion* $X(t)$

$$x(t) = X(t) + \xi(t). \tag{5.3}$$

After we put (5.3) into (5.2) we get

$$m\ddot{X} + m\ddot{\xi} = \lambda X \cos\omega t + \lambda\xi \cos\omega t. \tag{5.4}$$

We now need to add one more condition on ξ and X and that is relations between them and their second derivatives

$$\xi \ll X, \tag{5.5}$$

$$\ddot{\xi} \gg \ddot{X}. \tag{5.6}$$

that will allow us to compare the lowest order in Taylor series of (5.3) to get

$$m\ddot{\xi} = \lambda X \cos\omega t, \tag{5.7}$$

solution of which is well known

$$\xi(t) = -\frac{\lambda X(t)}{m\omega^2}\cos\omega t. \tag{5.8}$$

If we insert this into remaining part of (5.4), we get

$$m\ddot{X} = \lambda\xi\cos\omega t = -\frac{\lambda^2 X}{m\omega^2}\cos^2\omega t, \tag{5.9}$$

which is an equation for the smooth motion. Now comes the time for using the separation of motion as we will replace the $\cos^2\omega t$ with its time average and get equation

$$\ddot{X} = -\Omega^2 X, \tag{5.10}$$

which is commonly referred to as to the equation of harmonic oscillator with frequency

$$\Omega = \frac{\lambda}{\sqrt{2}m\omega}. \tag{5.11}$$

This shows us how we can trap charged objects with rapidly varying electric fields with vanishing average. This kind of traps is called the Paul traps named after German physicist Wolfgang Paul.

5.1 Commonly Used Trapping Potential

The example given in the previous paragraph isn't the one that is the most commonly used, the most common trap is usually a quadrupole field of the type

$$V(x, y, z) = V_0(x^2 + y^2 - 2z^2)\cos\omega t, \tag{5.12}$$

that can be simply put into (5.1) to see that the condition is fulfilled. And what is important is that this potential gives equation of motion similar to (5.10) in every direction. Electrode configuration that is capable of creating such a potential is on Figure 5.1. The resulting potential barrier is in

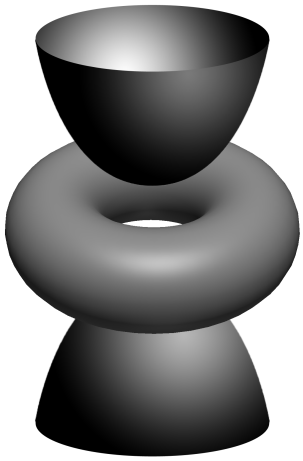

Figure 5.1: Electrodes for potential (5.12)

the order of couple of electron volts and therefore quite stable. The frequencies on which the ions oscillate in the trap (5.10) is in the range from 100 kHz to 10MHz, with the driving field on the frequencies of the order of 100 MHz (from that we can see that the separation of the micromotion really was justified).

Using results from quantum mechanics [2] such as calculation of the probability of laser induced energy transitions of the ion in the trap (we're using the external laser fields for cooling the ion) - let $A_\pm$ be the transition rates up/down - we can assign an effective temperature to the trap

$$\frac{A_+}{A_-} = \exp\left(-\frac{\hbar\Omega}{k_B T}\right), \tag{5.13}$$

where k_B is the Boltzmann constant ($k_B \doteq 1.3806504 \cdot 10^{-23} JK^{-1}$), and using the Planck distribution we could find the final energy of the cooling [2]

$$E_f = \hbar\Omega\left(\frac{1}{\exp\left(\frac{\hbar\Omega}{k_B T}\right) - 1} + \frac{1}{2}\right). \tag{5.14}$$

It is clear that the condition on the transition rates

$$A_+ < A_-, \tag{5.15}$$

is a condition equal to saying that cooling of the ion is prevailing. And if the cooling is very efficient

$$A_+ \ll A_-, \tag{5.16}$$

we can find that

$$k_B T = \frac{\hbar\Omega}{\log\left(\frac{A_-}{A_+}\right)} \ll \hbar\Omega. \tag{5.17}$$

And we see that (5.16) is a condition for cooling to cool the ion into its ground state.

5.2 Multiple Ions and Collective Motion

When multiple ions get into the trap, strong repulsive Coulombic forces start acting between them and they tend to form a linear structures, preferably linear chain (Figure 5.2) [2]. Because of the

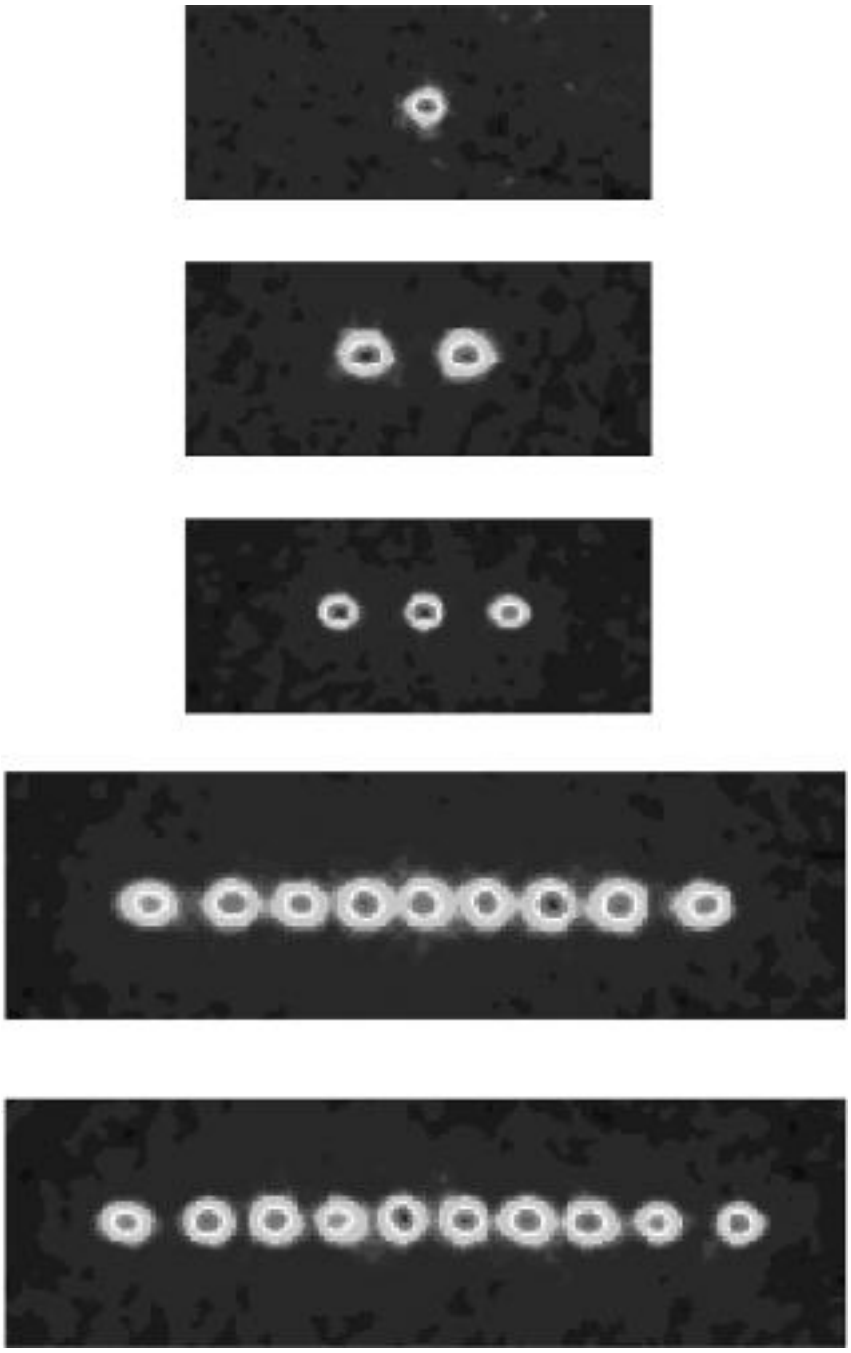

Figure 5.2: Multiple Ions in the Trap (From [2], originaly from work of Rainer Blatt's group.)

repulsive force the distance between the ions in the trap is rather large, however, the Coulombic

forces are still strong enough to induce collective modes of motion. If the transverse trapping is very effective, the simplest mode the ions can oscillate in is a uniform oscillation with the center of their mass along the trap with frequency Ω. Another mode is the breathing mode similar to the breathing mode of linear chain of pendulums connected by springs (Figure 5.3), the frequency of this mode is higher then Ω (See Figure 5.4).

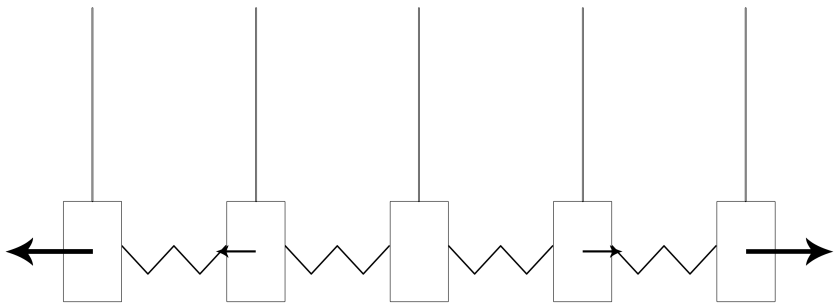

Figure 5.3: The Breathing Mode

The collective motion becomes one of the main tools for quantum computation on the ion chain as it couples the internal motions of each ion. One would ask how we could imprint the information onto the internal motion of each ion and the answer to that lies in the large distances between the ions, the distances are large enough to focus lasers on each ion separately and we can use the laser to drive each ion [2]. This approach, although experimentally achievable, is not the most efficient one for the real experiments and alternative path of driving each ion has been developed [7–10], which relies on applying an additional magnetic field to the trap which allows for driving using rf or microwave radiation, but this time the focusing on each ion does not have to take place and we can illuminate even the whole chain. We will discuss the alternative approach later, in this subsection we will be discussing only the laser driving and we will try to explain the simplest operations using lasers.

5.3 Quantum Logic in an Ion Trap

Neglecting the external couplings we may write the Hamiltonian in the form [2]

$$H = \hbar \left(\omega_e \left| e \right\rangle \left\langle e \right| + \omega_g \left| g \right\rangle \left\langle g \right| + \Omega a^\dagger a \right), \tag{5.18}$$

here $a^\dagger$ and a act on the vibrational level of the collective vibrational level and e stands for the excited and g for the ground levels. Transition between the ground state and the excited state ($\left|g, n_i\right\rangle \longleftrightarrow \left|e, n_f\right\rangle$) happens whenever the laser frequency is given by

$$\omega_0 = \omega_e - \omega_g + \Omega \left(n_f - n_i \right), \tag{5.19}$$

where n_f and n_i represent the $i$nitial and the $f$inal state of the collective oscillation. This gives us the possibility to drive each ion if we do not take into consideration the off-resonant excitations; however, as mentioned before, we have to focus each ion separately with frequency that depends on the collective motion state. The resonant laser is assumed to affect the coupling

$$\Sigma = a \left| e \right\rangle \left\langle g \right| + a^\dagger \left| g \right\rangle \left\langle e \right|, \tag{5.20}$$

where a and $a^\dagger$ act on the oscillation states of the motion. The laser therefore generates the transformation [2]

$$U_\theta = e^{-i\theta\Sigma}, \tag{5.21}$$

where the parameter θ is proportional to the coupling strength times the interaction time. And so we get

$$U_\theta \left| g, 0 \right\rangle = \left| g, 0 \right\rangle. \tag{5.22}$$

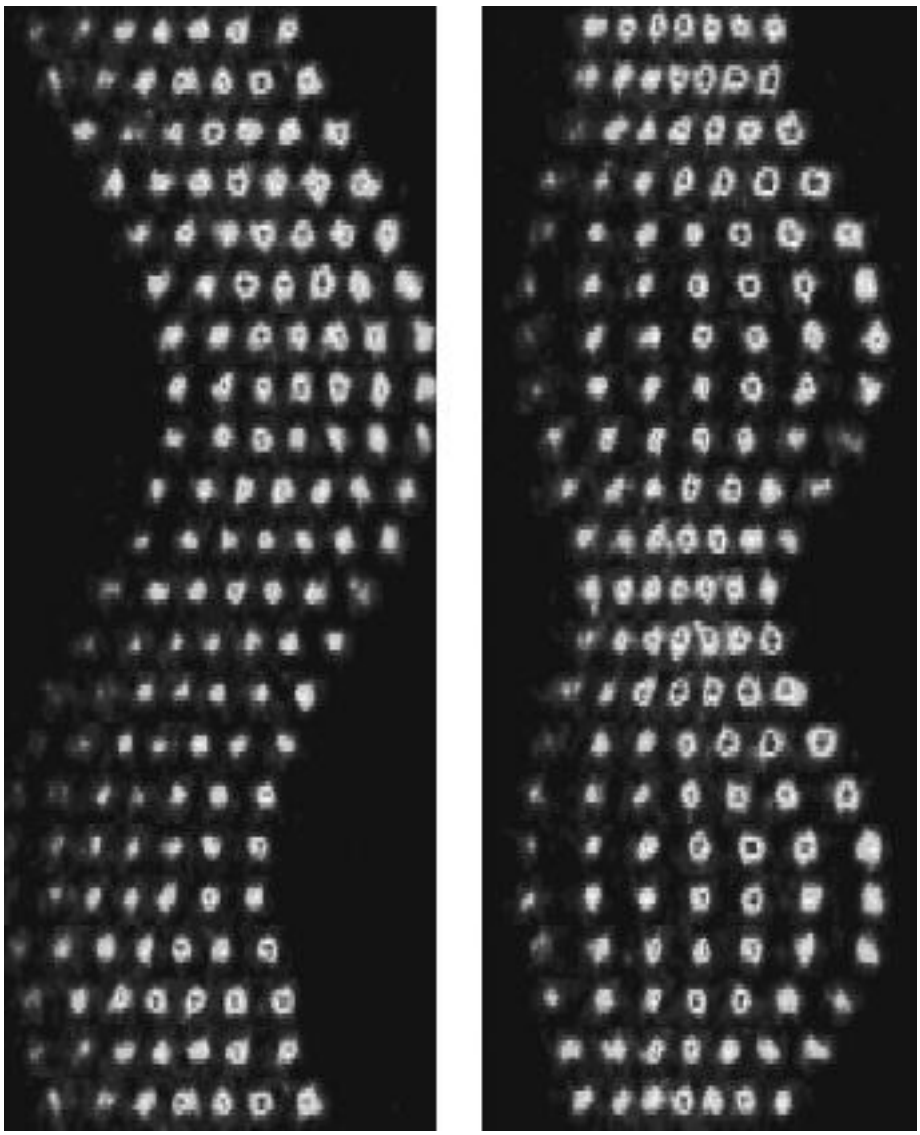

Figure 5.4: The Modes of the String, the vertical axis represents the time; the breathing mode is mixed with the left uniform motion (From [2], originaly from work of Rainer Blatt's group.)

It is also easy to see that

$$\Sigma^2 = aa^\dagger \left|e\right\rangle \left\langle e\right| + a^\dagger a \left|g\right\rangle \left\langle g\right| . \tag{5.23}$$

Letting Σ^2, Σ act on states $\{\left|e,0\right\rangle, \left|g,1\right\rangle\}$ we get

$$\Sigma^2 \left|e,0\right\rangle = \left|e,0\right\rangle ; \Sigma \left|e,0\right\rangle = \left|g,1\right\rangle , \tag{5.24}$$

$$\Sigma^2 \left|g,1\right\rangle = \left|g,1\right\rangle ; \Sigma \left|g,1\right\rangle = \left|e,0\right\rangle . \tag{5.25}$$

If we now expand the transformation, we will get

$$\begin{aligned} U_\theta = e^{-i\theta\Sigma} &= \sum_{k=0}^{\infty} \frac{(-i\theta)^k}{k!} \Sigma^k \\ &= \sum_{\nu=0}^{\infty} \frac{(-i\theta)^{2\nu}}{(2\nu)!} \Sigma^{2\nu} + \sum_{\nu=0}^{\infty} \frac{(-i\theta)^{2\nu+1}}{(2\nu+1)!} \Sigma^{2\nu+1}. \end{aligned} \tag{5.26}$$

If we now use the relations (5.24), (5.25), we can get

$$U_\theta \left|g,1\right\rangle = \cos\theta \left|g,1\right\rangle - i \sin\theta \left|e,0\right\rangle , \tag{5.27}$$

$$U_\theta \left|e,0\right\rangle = \cos\theta \left|e,0\right\rangle - i\sin\theta \left|g,1\right\rangle . \tag{5.28}$$

And so we can see that a π-pulse ($2\theta = \pi$) affects the system in a following way

$$\left|g,1\right\rangle \to -i \left|e,0\right\rangle , \tag{5.29}$$

$$\left|e,0\right\rangle \to -i \left|g,1\right\rangle . \tag{5.30}$$

And a 2π-pulse ($\theta = \pi$) affects the ion as follows

$$\left|g,1\right\rangle \to - \left|g,1\right\rangle , \tag{5.31}$$

$$\left|e,0\right\rangle \to - \left|e,0\right\rangle . \tag{5.32}$$

Using these pulses we could introduce a two-quibit logical gate [2]. Let two ions in the trap be indexed 1 and 2. Now we can use two two-level systems to encode four numbers into their internal states (see Subsection (1.1)):

$$\{\left|g\right\rangle_1 \left|g\right\rangle_2 , \left|g\right\rangle_1 \left|e\right\rangle_2 , \left|e\right\rangle_1 \left|g\right\rangle_2 , \left|e\right\rangle_1 \left|e\right\rangle_2\} \longleftrightarrow \{\left|00\right\rangle , \left|01\right\rangle , \left|10\right\rangle , \left|11\right\rangle\} . \tag{5.33}$$

We denote by U_π^k a π-pulse applied to k-th ion ($k = 1, 2$) and $U_{2\pi}^k$ similarly a 2π-pulse and by $\tilde{U}_{2\pi}^k$ a 2π-pulse transforming $\left|g\right\rangle_2 \to - \left|g\right\rangle_2$ without affecting anything else. Using these operations we can achieve a fundamental logical gate [2].

6 Modified Ion Traps

In this section of this work we will discuss an alternative approach to driving the ions in the Paul traps which may be considered better than that in Sec. 5, from an experimental point of view. In the above we mentioned driving the ions and their oscillation levels with lasers focused on each ion, this approach is experimentally achievable [6–10], but with growing number of ions in the trap is still more difficult and "expensive", also the technology allowing experimentalists to focus each ion is not a common commercial technology and therefore all the procedures are very difficult to achieve. And so instead of focusing each ion with rare technology, another and rather simple method that uses rf or microwave radiation for driving all the ions at once instead of optical lasers has been developed. Advantage in using radiation in these regions lies in many decades of development commercially available technologies such as nuclear magnetic resonance, which are now on very high level of sophistication. In this part we will talk about why it is necessary to use the optical radiation/lasers without the new approach, then we will modify the ion trap using additional magnetic field.

6.1 Coupling Strength Between Internal and Motional Dynamics

In this subsection the variable called Lamb-Dicke parameter will be discussed. This variable usually labeled η is a way of determining the coupling strength between internal and motional dynamics of ions in the trap that depends on the mass of the ion m, the wave-vector of driving light k and the frequency of trapping potential ν_1 [2, 7–10]:

$$\eta = \sqrt{\frac{(\hbar k)^2}{2m\hbar\nu_1}} = \Delta z_1 \, k, \tag{6.1}$$

Where $\Delta z_1 = \sqrt{\frac{\hbar}{2m\nu_1}}$ signifies the spatial extent of the oscillator ground function. The physical meaning of the Lamb-Dicke parameter is that a square of it gives the ratio between the change of kinetic energy of the ion after the absorption or emission of the photon of the driving field and the energy spacing of the harmonic trapping potential with frequency ν_1. Only for significant (non-vanishing) values of η can the absorption or emission of photon be accompanied by a change of the motional state of the ion. For example trapping a $^{171}\mathrm{Yb}^+$ ion with $\nu_1 = 2\pi\,100\mathrm{kHz}$ gives $\Delta z \approx 17\mathrm{nm}$ and 6.1 unfolds that the Lamb-Dicke parameter is non-vanishing only for frequencies from optical regime [2]. This example is very good illustration of why optical radiation has to be used in order to couple the internal and motional states of the ions.

6.2 Adding Axial Magnetic Field Gradient to Ion Trap

Let there be N singly ionized two-level ions in a harmonically trapped ion chain. The electronic part of the total Hamiltonian can be solved independently for each ion by virtue of the distances between the ions as spatial extent of their wave-functions is much lower then the distances [2]. Let us now denote the two Zeeman states of n-th ion corresponding to energies E_0 and E_1 by $|E_{0n}\rangle$ and $|E_{1n}\rangle$, $n = 1 \dots N$. In correspondence with previous text we will think of each ion as of one qubit. The global electronic state of the ions has to agree with:

$$H_{el}\phi_a(z) = E_{el,a}(z)\,\phi_a(z)\,, \tag{6.2}$$

where

$$H_{el} = \frac{1}{2}\hbar\sum_{n=1}^{N}\omega_n(z_n)\,\sigma_{z,n}, \tag{6.3}$$

and

$$\phi_a(z) = \prod_{n=1}^{N}|E_{cn}(z_n)\rangle\,; \tag{6.4}$$

with

$$a = 1\dots 2^N,\ c = 0, 1. \tag{6.5}$$

The z_n here denotes the axial position of n-th ion and $\sigma_{z,n}$ is the usual Pauli matrix, the n here denotes that it is an operator acting in a non-trivial way only on the n-th ion and in the other subspaces it acts as identity (which follows our previous definition of how we will consider a system of quantum particles). The

$$\omega_n = \frac{E_{1n} - E_{2n}}{\hbar},$$

is similarly to previous sections the transition frequency of n-th ion. If we now apply a non-zero magnetic field gradient in the axial direction to the trap ($\vec{B} = bz\cdot\vec{z} + \vec{B_0}$, with $\vec{z}$ being the unity vector in z direction), the qubit states $|E_{cn}\rangle$ will get shifted; and the extension of the shift will depend on the position of each ion in the chain. We will now denote the general Hamiltonian by

$$\begin{aligned} H &= H_{el}(z) + T_A(z) + V_A(z) \\ &= H_{el}(z) + \frac{1}{2m}\sum_{n=1}^{N}p_{z,n}^2 + \frac{m}{2}\sum_{n=1}^{N}\nu_1^2 z + \frac{e^2}{8\pi\epsilon_0}\sum_{n,l;n\neq l}^{N}\frac{1}{|z_n - z_l|}. \end{aligned} \tag{6.6}$$

The parts of potential energy that are acting in a way that affects the motion of the ions can be found from

$$\langle\phi_a|\,(H_{el} + V_A(z))\,|\phi_a\rangle = E_{el,a} + V_A(z)\,. \tag{6.7}$$

With zero field gradient ($b = 0$ in magnetic field), the electronic energy does not depend on the position of each ion and it simply gives additive constant and only V_A and T_A have to be taken into consideration. We can now expand the V_A around the equilibrium positions $z_{0,n}$ of each ions in terms of

$$q_n := z_n - z_{0,n}, \tag{6.8}$$

up to second order. That gives us similarly to classical case of small oscillations the dynamical matrix $\hat{A}$, where

$$A_{ln} = \partial_{z_l}\partial_{z_n}V_A, \tag{6.9}$$

which can be indirectly used to get Hamiltonian of a harmonic oscillator:

$$T_A + V_A = \frac{1}{2m}\sum_{n=1}^{N}P_{Q,n}^2 + \frac{m}{2}\sum_{n=1}^{N}\nu_n^2 Q_n, \tag{6.10}$$

with N uncoupled vibrational modes. The normal coordinates $\vec{Q}$ are connected with the local ones $\vec{q}$ by relation

$$\vec{q} = S\vec{Q}, \tag{6.11}$$

where S is a unitary matrix that diagonalizes A (that is the reason for saying indirectly in previous text). Also the following relation is valid

$$P_{Q,n} = m\dot{Q}_n. \tag{6.12}$$

Much more helpful for our problems with lasers and optical regime is to use the magnetic field with $b \neq 0$. Now a new term in the electronic energy arises for the j-th ion:

$$\langle\phi_a| H_{el,j}(z) |\phi_a\rangle = E_{cj}(z_{0,j}) + \underbrace{\frac{\hbar}{2}\left.\frac{\partial\omega_j}{\partial z_j}\right|_{z_{0,j}} q_j (-1)^{c+1}}_{V_B}. \tag{6.13}$$

We can get an estimate of the ratio between the additional potential energy V_B and the ground energy of unperturbed lowest oscillator mode to see the significance of V_B by inserting substitution

$$q_j \approx \Delta z_1, \tag{6.14}$$

into the previous equation. By that we achieve

$$\varepsilon := \frac{|V_B|}{\hbar\nu_1} = \frac{\left|\frac{\partial\omega_j}{\partial z}\right| \Delta z_1}{\nu_1}. \tag{6.15}$$

If ε is much smaller then 1, the eigenfrequencies of the oscillator modes will be only slightly dependent on the additional potential term induced by the Zeeman shift and we can approximate the global motional state of the ion string with unperturbed harmonic oscillator and write the complete Hamiltonian as:

$$\begin{aligned} H =& \frac{\hbar}{2}\sum_{n=1}^{N}\omega_n(z_{0,n})\sigma_{z,n} + \frac{1}{2m}\sum_{n=1}^{N}P_{Q,n}^2 + \frac{m}{2}\sum_{n=1}^{N}\nu_n^2 Q_n^2 \qquad (6.16)\\ &+ \frac{\hbar}{2}\sum_{n=1}^{N}\left[\left.\frac{\partial\omega_n}{\partial z_n}\right|_{z_{0,n}}\sigma_{z,n}\sum_{l=1}^{N}S_{ln}Q_l\right] \\ =& \frac{\hbar}{2}\sum_{n=1}^{N}\omega_n(z_{0,n})\sigma_{z,n} + \frac{1}{2m}\sum_{n=1}^{N}P_{Q,n}^2 \qquad (6.17)\\ &+ \frac{m}{2}\sum_{l=1}^{N}\nu_l^2\left[Q_l + \frac{\hbar}{2m\nu_l^2}\sum_n\left.\frac{\partial\omega_n}{\partial z_n}\right|_{z_{0,n}}\sigma_{z,n}S_{ln}\right]^2 \\ &\underbrace{- \frac{\hbar}{4m}\sum_{l=1}^{N}\frac{1}{\nu_l^2}\left[\sum_n\left.\frac{\partial\omega_n}{\partial z_n}\right|_{z_{0,n}}\sigma_{z,n}S_{ln}\right]^2}_{H_{SS}}, \end{aligned}$$

with the electronic part expanded up to first order in q_n. It would be easy to see that a unitary transformation of the form

$$U = e^{-i\sum_l\left(\frac{1}{2m\nu_l^2}\sum_n\left.\frac{\partial\omega_j}{\partial z_j}\right|_{z_{0,j}}\sigma_{z,n}S_{ln}\right)P_{Q,l}}, \tag{6.18}$$

would give for

$$\tilde{H} = U^\dagger H U, \tag{6.19}$$

the result:

$$\tilde{H} = \frac{\hbar}{2}\sum_{n=1}^{N}\omega_n(z_{0,n})\sigma_{z,n} + \sum_{n=1}^{N}\frac{P_{Q,n}^2}{2m} + \frac{m}{2}\nu_n^2 Q_n^2 - H_{SS}. \tag{6.20}$$

If we now define

$$\varepsilon_{nl} := S_{nl}\frac{\frac{\partial\omega_l}{\partial z}\Delta z_n}{\nu_n}, \tag{6.21}$$

	$b(\mathrm{T/m};\ N=10)$	$b(\mathrm{T/m};\ N=20)$	$b(\mathrm{T/m};\ N=40)$
$\omega_z/2\pi = 100\mathrm{kHz}$	9,89	22,1	54,7
$\omega_z/2\pi = 1\mathrm{kHz}$	459,0	1030,0	2540,0

Table 6.2: Magnetic field gradients required to separate the driving frequencies of the ions of $^{171}\mathrm{Yb}^+$ (taken from [8]).

$$J_{nl} := \sum_{j=1}^{N} \nu_j \varepsilon_{jn} \varepsilon_{jl}, \tag{6.22}$$

and insert these into (6.20) together with using the creation and annihilation operators $a_n^\dagger, a_n$ and dropping the constant terms, we will get:

$$\tilde{H} = \frac{\hbar}{2} \sum_{n=1}^{N} \omega_n \left(z_{0,n}\right) \sigma_{z,n} + \sum_{n=1}^{N} \hbar \nu_n \left(a_n^\dagger a_n\right) - \frac{\hbar}{2} \sum_{n,l;n<l}^{N} J_{nl} \sigma_{z,n} \sigma_{z,l}. \tag{6.23}$$

The $\tilde{H}$ we have derived is a description of linear string of ions, but what is very remarkable, is that each ion is accessible on its own frequency, different from the other ions. This allows for us not to have to focus each ion with laser, but rather we can now illuminate the whole trap (both experiments and numerical simulations have shown that off-resonant excitations do not occur with this model), or at least even the neighboring ions of the one we want to drive, without affecting the other ions [6].

If we now wrote the Hamiltonian of the j-th ion in the trap that is illuminated with driving electromagnetic wave, using rotating wave approximation and experimental results, we would find that resonant frequency of each ion almost does not depend on the internal motion of each ion and that there is a constant shift in qubits resonant frequency related to the order of the ion in the trap [6, 8].

There is one more benefit in using the additional magnetic field gradient; if applied, it enables driving with mw or rf radiation instead of lasers [7–10], which is very good for experiments as working with radiation in these regions is very well-developed and accessible. One could ask what field gradients are experimentally achievable, according to [8], the gradient can go up to 8000T/m. For comparison there is a table of field gradients necessary to separate the resonant frequencies of the $^{171}\mathrm{Yb}^+$ ions (Table 6.2).

Conclusion

We have summarized the results of recent research that influences the perfect state transfer on trapped ions and we have laid down the main direction in which we should continue in finding the configurations of ions that would allow for the perfect state transfer to happen. The next step will be to find the Hamiltonians of trapped ions that would belong to the classes of Hamiltonians derived in 4.3 and 4.4.

To find configurations for PST it will be necessary to use many parts of perturbation theory both with its experimental verification similarly to what we have done and commented in 6.2, and afterwards verify that the Hamiltonian found is a member of the classes derived. There are several questions that need to be answered by future research, there is a heating problem with the trapped ions that can disturb the long decoherence times of the ion trap, caused by many factors [6, 7, 9, 10]. The heating problem is yet not fully understood, however it seems to be solvable because very stable and long lived ground states of $^{171}\mathrm{Yb}^+$ in the traps have been presented [7]. Furthermore, there has been part of the theory developed for optimizing the fidelity of the network once the Hamiltonian is found by optimizing the parameters of the interactions [4], that could be of great use for designing an actual experiment and improving it. Similar tasks as perfect state transfer on trapped ions have been solved on other systems as mentioned in the introduction to Part II. It seems that PST on trapped ions is a viable possibility.

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