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# **BASIC PRINCIPLES OF QUANTUM COMPUTING**

Bachelor's Thesis  
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## ABSTRACT

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Quantum mechanics has proven its position as the primary theory for accurately describing microscopic domains. Numerous fields in physics utilize quantum mechanics to great effects, with one prominent application being quantum computing. Quantum computing extends the field of quantum mechanics to information theory, striving to perform computational tasks utilizing quantum phenomena with notably greater efficiency compared to classical alternatives. In this thesis, I will go through the basics required in the field of quantum computing.

To understand quantum computing demands adapting a new type of matrix mechanical view. This involves considering Hilbert spaces, which are linear vector space having a well defined inner product. Hilbert spaces contain state vectors describing quantum states, as well as operators for altering and measuring these states. The dynamics of quantum systems are governed by three quantum postulates. These specify Hilbert spaces and state vectors as the fundamental components of quantum systems, Hermitian operators as providing the physical manifestation of these systems, and finally, the Schrödinger's equation to describe the time evolution of such systems. These notions are required in producing quantum computing.

Quantum computing uses qubits as the computational basis, analogous to classical bits but with the added capability of quantum superposition. Qubits are represented as two-state vectors, and can be physically realized with any quantum-behaving binary-valued system, like the electron spins. Qubits can be combined into higher dimensional states with the use of tensor products, causing the system's Hilbert space to expand as  $2^n$  with  $n$  being the number of qubits, allowing for exponential computational speedup. Computational logic can be constructed by acting on the qubits using unitary operators, known as quantum gates. The combinations of qubits and quantum gates can be visualized as quantum circuits, depicted using specialized circuit diagram notations.

An essential part of quantum computing, and the phenomena enabling exponential computational speedup, is quantum entanglement. Entanglement arises in interacting qubits, intertwining them so that the individual states become correlated. Entanglement can be characterized by being unable to reduce a combined state into its pure constituents. The amount of entanglement in a system can be measured using von Neumann entropy, analogous to Shannon entropy in classical information theory. Entanglement serves various purposes in quantum computing and is a defining feature distinguishing it from the classical domain.

In this thesis, the entanglement properties of a periodic four-qubit circuit with alternating quantum gates were simulated. The simulation was performed computationally, and measured entanglement entropy as a function of the amount of circuit periods. The results demonstrated different characteristics of entanglement depending on the parameters used for the quantum gates, with the entanglement either being periodic, non-occurring or chaotic in nature.

Keywords: quantum computing, qubit, quantum circuit, quantum gate, entanglement, entanglement entropy

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# TIIVISTELMÄ

Santeri Huhtanen: Kvanttilaskennan perusta  
Kandidaatintutkielma  
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Kvanttimekaniikka on vakiinnuttanut asemansa ensisijaisena teoriana mikroskooppisten fysiikan ilmiöiden mallintamiseen. Kvanttimekaniikkaa hyödynnetään nykyisin lukuisilla eri fysiikan osa-alueilla, ja tässä opinnäytetyössä tutustutaan näistä kvanttilaskentaan. Kvanttilaskenta laajentaa kvanttimekaniikan periaatteita klassisen informaatioteorian puolelle ja saavuttaa näin suurempia laskentatehoja klassiseen laskentaan verrattuna. Tämä opinnäytetyö esittelee kvanttilaskentaan tarvittavat perusteet, sekä havainnollistaa kvanttilaskennan käyttöä lomittumissimulaation avulla.

Kvanttilaskennan käsittelemiseksi tutustutaan ensiksi matriisimekaniikkaan. Matriisimekaniikka määrittelee Hilbertin avaruuden, eräänlaisen lineaarisen vektoriavaruuden, jolle on määritelty sisätulon käsite. Kvanttimekaniikassa Hilbertin avaruus pitää sisällään tilavektorit, jotka kuvastavat systeemin mahdollisia kvanttitiloja, sekä operaattorit, joilla voidaan muokata tai mitata kyseisiä tiloja. Kvanttisysteemien dynamiikkaa mallinnetaan kolmen postulaatin avulla. Näistä ensimmäinen omaksuu Hilbertin avaruuden käytön laskentaan, toinen määrittelee systeemin fyysiset ominaisuudet Hermiittisten operaattorien avulla, ja kolmas kertoo tilojen aikaevoluution Schrödingerin yhtälöllä. Näitä käsitteitä hyödynnetään kvanttilaskennassa.

Kvanttilaskennassa käytetään laskennan komponentteina kubitteja, jotka ovat kvanttimekaniikan versioita klassisista biteistä. Kubitteja merkitään kaksitasoisilla tilavektoreilla, joita fyysisesti vastaa mikä tahansa kvanttimekaanisesti käyttäytyvä binäärinen systeemi, kuten elektronien spin. Kubitteja voidaan yhdistellä laajalotteisiksi kokonaisuuksiksi tensoritulon avulla. Tällöin yhdistetyn tilan Hilbertin avaruus kasvaa eksponentiaalisesti suhteessa kubitien lukumäärään, mahdollistaen laskennan eksponentiaalisen nopeutumisen. Varsinainen laskennallinen logiikka toteutetaan kvanttiporttien avulla, joita vastaavat unitaariset operaattorit. Kubitteja ja erilaisia kvanttiportteja yhdistelemällä voidaan rakentaa kvanttipiirejä.

Olenainen osa kvanttilaskentaa, sekä eksponentiaalisen laskentatehon mahdollistava ilmiö, on kvanttilomittuminen. Lomittumista syntyy kubitien vuorovaikutuksessa, jolloin yksittäisten kubitien tilat sekoittuvat ja niistä tulee korreloituvia. Lomittuminen voidaan määritellä yhdistettyjen tilojen avulla, sillä jos tilaa ei voida esittää kahden puhtaan tilan tulona, on systeemi lomittunut. Lomittumisen suuruutta mitataan von Neumannin entropian avulla, jota vastaa Shannonin entropia klassisessa informaatiotieteessä.

Tässä opinnäytteessä, lomittumista simuloitiin jaksollisessa, neljästä kubitista ja erityisistä kvanttiporteista koostuvassa kvanttipiirissä. Lomittumisentropiaa mitattiin jaksojen lukumäärän funktiona, josta haluttiin selvittää lomittumisen käyttäytymistä simuloinnin aikana. Lopputuloksena lomittumisen huomattiin riippuvan kvanttiporteille annetuista parametreista, jolloin lomittuminen käyttäytyi joko jaksollisesti, lomittumista ei esiintynyt ollenkaan tai lomittuminen oli luonteeltaan kaoottista.

Avainsanat: kvanttilaskenta, kubitti, kvanttipiiri, kvanttiportti, lomittuminen, lomittumisentropia

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## 1. INTRODUCTION

Since the discovery of quantum mechanics over a hundred years ago, the quantum theory has solidified its position as the most correct way to describe physics in microscopic levels, overtaking any related classical theories. Even though nowadays being a widely accepted and researched field, quantum mechanics has historically been a largely debated branch of physics due to its non-intuitive and even strange approach with no classical counterparts. It has taken physicists even decades to counterclaim some of the objections pointed against quantum mechanics before any conclusive evidence for their validity could be provided. Most recently, this earned the physics Nobel Prize of 2022 to the laureates Alain Aspect, John F. Clauser and Anton Zeilinger for their work in uncovering the properties of quantum entanglement [1].

One of the more prominent use cases for quantum mechanics since its formulation has been the construction of the theory for quantum computation, which replaces classical computational elements with their quantum mechanical variants. Through introducing quantum mechanics into computational processes, quantum computing is able to supersede classical computation in terms of resources required to perform some calculatory tasks, known as quantum algorithms. Some quantum algorithms, most famously Shor's factorization algorithm and Grover's search algorithm, have been estimated to provide significant advantage over their closest classical equivalents. [2, pp. 1–3] The study and design of similar algorithms remains an active field to the modern day, recently producing papers like finding a quantum algorithm for financial risk analysis [3] and optimization of large quantum circuits [4].

Other aspects of quantum computing have also seen active research, be it the construction of quantum computers or discovering new ways to physically realize quantum processes. The actual development of functioning quantum computers is still on its early stages, with any practical usage being some ways into the future. Some quantum computers are slowly being opened up to the closed public, like Helmi 5-qubit quantum computer recently build in Finland for research purposes [5], but any commercially available solutions are still just a dream. Ongoing research in the these areas is constantly made with fresh solutions and ideas enabling new possibilities. Recently these include finding new ways to physically implement qubits required for quantum computing [6] or researching the intersection between photonics and

superconducting quantum circuits [7].

This thesis acts as a literature review to quantum computing and focuses on introducing its mathematical aspects while disregarding the physical obstacles to realize such systems. In chapter 2, the quantum mechanical nomenclature will be briefed alongside the required mathematical basics for working with quantum systems. Chapter 3 will focus on the notions in quantum computing, and the mathematical architecture to produce logic in quantum circuits as well as giving graphical depictions to describe such circuits. Chapter 4 will finalize the look into quantum computation by performing a thorough investigation on quantum entanglement, which culminates on an entanglement entropy measurement project in a simulated periodic circuit. All of the concepts and findings of this thesis will be summarized in the conclusion in chapter 5, as well as a short rundown on possible future subjects to follow this thesis will be given.

## 2. MATHEMATICAL BASICS OF QUANTUM MECHANICS

Understanding the fundamental mathematical principles behind modern quantum mechanics is essential for delving further into the field of quantum computing. This chapter will summarize the mathematical key concepts required to understand the ideas that will be presented in the following chapters.

### 2.1 Quantum states and operations in finite Hilbert space

The exact mathematical machinery for quantum mechanics was first proposed in 1926 by Heisenberg, Born and Jordan, who in their article, "Zur Quantenmechanik II" (eng. On Quantum Mechanics II) [8], founded the matrix mechanical principles of quantum mechanics. The underlying mathematical principles have preserved to the modern age of quantum mechanics, although the outward appearance has changed over time.

The matrix mechanical interpretation of quantum mechanics focuses on complex Hilbert spaces, which are a type of linear vector space. The linearity of the space includes in itself some standard operations for vectors, like the sum of vectors or multiplication by scalar being well defined. The crucial difference why Hilbert spaces are required in quantum mechanics rather than other vector spaces is the definition of vector inner product in the space. [9, pp. 325–353] Inner products of state vectors in Hilbert space have been noticed to give rise to the physical interpretation of quantum mechanics through the inner product's induced concept of norm [10, pp. 35, 61].

Mathematically Hilbert spaces can be expanded to account for infinite dimensional vector spaces, which is important for multiple quantum mechanical applications, like the definition of particle position [10, pp. 123–144]. However, quantum computing only requires finite dimensions for calculations. Thus in this thesis only the notions for the finite case will be inspected.

Complex Hilbert space in quantum mechanics is often denoted by the letter  $\mathcal{H}$ . The complex vectors in this Hilbert space represent the possible quantum states which the system can take. [10, p. 36] These states are written in vector form using bra-ket notation, developed by Dirac in 1939 [11]. A ket-vector corresponds to the standard

column vector as

$$|\psi\rangle = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} \quad (2.1)$$

and a bra-vector respectively represents the conjugate transpose of a similar column vector as

$$\langle\chi| = \left[ b_1^* \quad b_2^* \quad \cdots \quad b_n^* \right]. \quad (2.2)$$

The vector values are generally complex in  $a, b \in \mathbb{C}$  and the upper sign  $*$  represents a complex conjugate of those values. The inner product of two vectors in a complex vector space is then written using this notation as

$$\langle\chi|\psi\rangle = \sum_{i=1}^n b_i^* a_i. \quad (2.3)$$

The norm of a vector is defined to be the square root of the inner product with itself, resulting in the equation form

$$\sqrt{\langle\psi|\psi\rangle} = \sqrt{\|\psi\|^2} = \|\psi\|. \quad (2.4)$$

Quantum states can be altered by acting on them with self-adjoint (Hermitian) matrix operators residing in the complex Hilbert space. The self-adjointness of an operator is defined as the matrix itself after conjugate transpose, as shown by the equation

$$A = A^\dagger = (A^T)^*. \quad (2.5)$$

Applying an operator to a quantum state corresponds to measuring or otherwise interfering with the state. [10, pp. 36–40]

## 2.2 Postulates of quantum mechanics

The general mathematical structure of quantum mechanics follows three axioms formulated from the theories produced by Dirac in 1930 [12] and von Neumann in 1932 [13], now known as the Dirac–von Neumann axioms. These postulates determine the rules on how quantum systems behave in a mathematical sense. The three postulates are presented in a slightly modified form below: [10, pp. 57–58]

1. The state vector  $|\psi(t)\rangle$  residing in complex Hilbert space  $\mathcal{H}$  contains in itself the most complete physical information available on the system.
2. Measurable physical quantities are represented by self-adjoint matrix operators on

the Hilbert space  $\mathcal{H}$ .

3. A system undisturbed by external influences evolves in time according to the Schrödinger equation

$$i\hbar \frac{d|\psi(t)\rangle}{dt} = H(t) |\psi(t)\rangle, \quad (2.6)$$

where  $H$  represents the Hamiltonian of the system.

The first postulate lays the ground work for the mathematical machinery described in section 2.1. The most simple quantum system is often taken to be that of a singular particle, like a single electron. The state vector then gives the most complete information available on this particle, like its position, momentum or spin, depending on the quantities of interest. [10, pp. 58–59]

The second postulate gives ways to interact with the defined quantum systems through self-adjoint (2.5) matrix operators. Possible detectable physical quantities, known as observables, can be recovered from the system by acting on the state vector with the equivalent operator. This action corresponds to conducting a measurement on the system and observing the result. The possible observed values after measurement of a state vector  $|\psi\rangle$  are eigenvalues of the operator  $A$ , and the possible states after the measurement are the eigenvectors of the operator. Mathematically, an operation on the state vector  $|\psi\rangle$  can be denoted as

$$A|\psi\rangle = a|a\rangle, \quad (2.7)$$

where  $a$  is the measured eigenvalue of  $A$  and  $|a\rangle$  is the corresponding eigenvector and the new state of the system. As seen from (2.7), all information of the state before the measurement is completely lost, which is commonly referred to as the measurement principle. [10, pp. 43, 59]

The third postulate determines the available possible states of the system as well as the time evolution of the system through the Schrödinger equation (2.6). A state vector independent of time must still fulfil the conditions set out by the third postulate and the Schrödinger equation. The linearity of the equation results in a phenomena known as the superposition principle, where if there are two or more valid solutions to the Schrödinger equation for a certain system, the linear combination of those solutions is then also a valid solution to the Schrödinger equation. This has been demonstrated in an equation form below

$$|\psi\rangle = \alpha|\chi\rangle + \beta|\theta\rangle, \quad (2.8)$$

where the states  $|\chi\rangle$  and  $|\theta\rangle$  are individually valid solutions to the Schrödinger equation. The complex coefficients  $\alpha$  and  $\beta$  represent the weights of these states and relate to the probability of observing said state when conducting a measurement on the system. The probability of observing any of the states is gained from the squared norm of these

complex coefficients. The probability of observing any one state must amount to unity, meaning we have then for the total probabilities the statement

$$|\alpha|^2 + |\beta|^2 = 1. \quad (2.9)$$

This relation holds for normalized states, which is generally assumed for states in quantum mechanical calculations. [10, pp. 58–60]

The  $H$  in the Schrödinger equation (2.6) refers to the Hamiltonian of the system and represents the system's total energy. Generally, the Hamiltonian is written in the form

$$H = \frac{P^2}{2m} + V(X), \quad (2.10)$$

where  $P$  is the momentum operator,  $m$  is the mass of the particle,  $V$  is the potential affecting the particle and  $X$  is the position operator. This type of Hamiltonian is analogous to its classical form expanded to quantum systems through the canonical quantization. [10, pp. 59–60]

### 3. ARCHITECTURE OF QUANTUM CIRCUITS

This chapter goes through the theoretical structure of quantum circuits and introduces qubits as the computational units for quantum computing. These notions are then expanded in the upcoming chapter considering the entanglement properties between these qubits.

#### 3.1 Qubits and two qubit systems

Qubits are the computational units in quantum computing and relate analogously to the bits in classical computers. As classical computers perform calculations by changing and comparing the values of bits through logic gates, so do quantum computers act on qubits through quantum gates. However, the crucial differences between classical and quantum mechanical bits are the quantum properties qubits exhibit. These properties enable the utilization of the superposition principle in calculations, which through entanglement permits an exponential speedup for making calculations. [14, pp. 8–9, 17, 69–70]

A qubit is a binary quantum state residing in two dimensional Hilbert space. There are multiple valid physical realizations for qubits, which just have to conform to the constraints of being binary valued and possessing quantum properties. Some possible examples of binary quantum systems include the polarization of light, excitations of atomic states and the most commonly used spin value of the electron. Each of these systems fulfil the necessary constraints. Quantum mechanically, this type of binary state is represented by the state vectors

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad (3.1)$$

referred to as the *computational basis*. In the case of spin states, the state vectors can also be referred to as  $|\uparrow\rangle$  and  $|\downarrow\rangle$  correspondingly. This thesis will mainly utilize the notation given by the computational basis (3.1). [14, pp. 8–9, 17]

As previously stated in 2.2, the superposition principle claims that two possible states of the system solving the Schrödinger equation (2.6) can also form a superposition state, which is also a legitimate solution to this equation. This way it is possible for the qubits to

achieve superposition states represented by

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle \quad (3.2)$$

where the complex coefficients  $\alpha$  and  $\beta$  follow the probability realization given by equation (2.9). [14, pp. 9–11]

Two single qubit systems can be combined to form an expanded Hilbert space, which encompasses the vector spaces of both qubits. This is required in order to construct multi-qubit systems for performing operations and computing. The combining of Hilbert spaces is done through a tensor product between the individual spaces. In equation form, this can be presented as

$$\mathcal{H}_1 \otimes \mathcal{H}_2 = \mathcal{H}_\psi, \quad (3.3)$$

where  $\mathcal{H}_1$  and  $\mathcal{H}_2$  represent the Hilbert spaces of the original single qubit states and the  $\mathcal{H}_\psi$  represents the resulting combined Hilbert space. The tensor product between two qubits residing in the spaces  $\mathcal{H}_1$  and  $\mathcal{H}_2$  respectively, results in a vector state  $|\psi\rangle$  in this combined Hilbert space  $\mathcal{H}_\psi$ . As an example, taking the qubits  $|0\rangle$  and  $|1\rangle$  to be the starting states results in a combined state

$$|0\rangle \otimes |1\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = |01\rangle \quad (3.4)$$

residing in the Hilbert space  $\mathcal{H}_\psi$ . Notably, the dimensions of this new space are  $n_1 \times n_2$ , where  $n_1$  and  $n_2$  are the dimensions of the original Hilbert spaces  $\mathcal{H}_1$  and  $\mathcal{H}_2$  respectively. [15, pp. 45–46]

## 3.2 Quantum logic gates

Quantum gates are quantum equivalent to classical logic gates. Quantum gates are mathematically implemented as unitary operators acting on qubits, either preserving or changing the state depending on the operator's type. Like with classical logic gates, there are multiple quantum gates for different computational operations, with many analogous to the classical logic gates. Some commonly used gates include the identity gate  $I$ , which preserves the state of the qubit, or the NOT-gate  $X$ , which inverts the state of a qubit. These are presented in operator form as

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad (3.5)$$

where the NOT-gate  $X$  can also be seen to be the Pauli  $x$ -matrix. Acting on an example spin-up state  $|0\rangle$  with the NOT gate reverses it to the spin-down state as seen from the following equation:

$$X |0\rangle = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = |1\rangle. \quad (3.6)$$

The example operation above is similar to the classical NOT logic gate acting on a bit. However, the given example state can also be a superposition of the qubit states  $|0\rangle$  and  $|1\rangle$  as presented in the equation (3.2). Operations on this type of superpositioned state consider the probabilities given by the complex coefficients and preserve or modify them accordingly. [14, pp. 69–72]

Single qubit quantum gates demonstrate the mathematical constructs of quantum computing. However, single qubit systems by themselves are not capable enough to produce high complexity algorithms for meaningful computational task. Instead, multiple qubits and their interactions through quantum gates are required for proper computing. As with the single state systems, combined states, like the one presented in equation (3.4), can also be acted on with unitary operators residing in the combined Hilbert space  $\mathcal{H}_\psi$ , resulting in a new operated state in  $\mathcal{H}_\psi$ . These quantum gates act on a select number of qubits at once and intertwine them to produce results depending on the combination of the states.

With the combined quantum gates, it is possible to create conditional gates that take into consideration the state of *control* qubits, changing the state of the *target* qubits accordingly. One such gate is the controlled NOT-gate, CNOT, that reverses the state of the second qubit if the first qubit is in the state  $|1\rangle$ . In matrix form, this gate is presented as

$$\text{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \quad (3.7)$$

where the CNOT-gate can be noticed to resemble block matrix combination of  $I$  and  $X$  gates on the diagonal. We can demonstrate the effect of CNOT-gate on the combined

state  $|11\rangle$  as

$$\text{CNOT}(|11\rangle) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = |10\rangle. \quad (3.8)$$

We can see that in the resulting state, the second state has been changed to its opposite. However, if the first state would have been  $|0\rangle$  instead, the equation would result in

$$\text{CNOT}(|01\rangle) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = |01\rangle, \quad (3.9)$$

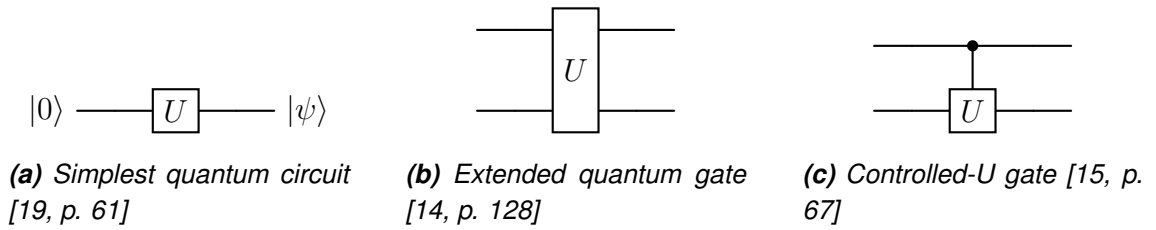
where we can notice the state of the second qubit being the same compared to the one at the beginning. [14, pp. 62, 83–85]

As with singular qubits, combined quantum gates also take into account the superposition of the singular states and their corresponding complex coefficients. For the case of the CNOT-gate, if the first qubit would be a superposition state presented as (3.2), then the second qubit would be flipped according to the probabilities given by the complex squared norms of the coefficients.

### 3.3 Graphical depictions of quantum circuits

Quantum computing partly adopts the graphical customs utilized in depicting classical logic circuits. In classical circuit diagrams, an electrical current is travelling along wires through logic gates and producing output based on the used gate and the input [16, pp. 98–100]. In quantum mechanics, there might not be any moving particles to "carry the current" but the computational units might stay stationary and only be affected by outside interferences. The "current" is thus instead realized by replacing the classical current by qubit states, and classical logic gates with quantum gates [15, p. 61]. This new type of form for quantum circuit diagrams was introduced by Feynman in 1986 [17] and later modified by Barenco *et al.* in 1995 [18]. This notation given by Barenco *et al.* represents the current modern format for depicting quantum circuits and will be gone over in this chapter.

The state of a qubit in a quantum circuit is imagined to travel along a wire from left to right. This wire might contain quantum gates that act on the qubit, meaning that the leftmost



**Figure 3.1.** Three graphical depictions for basic quantum circuits.

gate is the first one to operate on the qubit, then the second gate etc. [14, pp. 123–124] A simplest possible quantum circuit is given in the figure 3.1a, where  $|0\rangle$  is the starting state,  $U$  is the quantum gate operating on the qubit and  $|\psi\rangle$  is the resulting operated state. Quantum gate  $U$  represents a general unitary operator

$$U = \begin{bmatrix} u_{00} & u_{01} \\ u_{10} & u_{11} \end{bmatrix}, \quad (3.10)$$

where  $u_{ij}$  values are chosen so that the gate respects unitarity. In the given case, the operator  $U$  could for example be replaced by the NOT-gate (3.5), which would then give the resulting state as  $|1\rangle$ . [14, p. 71]

As mentioned previously in section 3.2, singular qubit operations are not enough to produce meaningful computation. Rather, many qubit operations are required to perform relevant tasks. In quantum circuit diagrams, these are presented in a couple of different ways depending on the desired result. For an operator acting similarly to many qubits at once, the quantum gate is extend to encompass all of the affected qubits, as presented in figure 3.1b. In matrix form this type of extended gate would be designated as

$$U \otimes U, \quad (3.11)$$

where each of the unitary operators are seen to act on their respective wires. This extension of quantum gates is treated similarly even for higher qubit systems. [14, pp. 127–128]

However, in the case of conditional gates, like the one given by CNOT (3.7), the circuit diagram is drawn like in the figure 3.1c. Here the mark connecting the first wire with the second one represents the control unit for gate  $U$ . In this presentation form, the qubit travelling along the second wire is only operated on with the unitary gate  $U$  (not necessarily NOT-gate as is for CNOT) if the qubit traveling on the control wire is at state

[1]. This kind of general controlled operator would be given in matrix form as

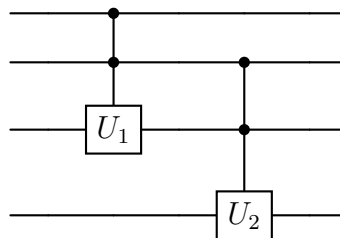
$$CU = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & u_{00} & u_{01} \\ 0 & 0 & u_{10} & u_{11} \end{bmatrix}. \quad (3.12)$$

The CU-gate can be seen as consisting of block matrices  $I$  and  $U$  on the diagonal. [14, pp. 87–88] The control qubit is not necessarily the qubit travelling on the uppermost wire, but can be arranged to be any of the qubits in the system. This formulation then just changes the order of the block matrices appearing in the operator. [14, pp. 85–86, 88] [15, pp. 66–68]

### 3.4 Expanding to many qubit systems

Including an increasing amount of qubits into the system follows the same principles previously illustrated in 3.1. The total combined state consists of the tensor products of all the individual qubits, increasing the size of the state two fold for each qubit. Similarly, the combined Hilbert space  $\mathcal{H}_\psi$  consists of the tensor products of all the individual Hilbert spaces. The resulting space has dimensions of  $2^n$  where  $n$  is the number of qubits included in the system, resulting in an exponential expansion of the  $\mathcal{H}_\psi$  space. This feature is utilized in achieving exponential speedup of quantum processes, alongside quantum entanglement. [2, p. 2] [20, pp. 16–17, 202]

The circuit diagrams for multi-qubit systems follow the principles laid out in 3.3. The qubits are added to the diagrams as additional wires, which can be operated on with quantum gates. This allows for more complex circuits to be build, for example enabling multiple qubits to act as control units for operations. Example of this type of multi-qubit-controlled circuit is given in the figure 3.2.



**Figure 3.2.** Multi-controlled  $U$  gates for four qubit quantum system.

In the figure, each of the quantum gates consider the controlled input of the two previous qubits similar to the CNOT-gate. [14, pp. 91–92]

## 4. QUANTUM ENTANGLEMENT

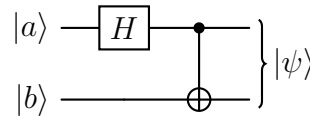
This chapter introduces the concept of quantum entanglement through common examples. It then proceeds to expand the notion to general mathematics and use cases in quantum computation. The chapter culminates on a quantum circuit simulation project which demonstrates the fluctuation of entanglement entropy in a periodic system.

### 4.1 Introduction to entanglement via Bell states

Entanglement is a purely quantum mechanical phenomena with no classical counterpart. It has been described by Schrödinger to be "*the* characteristic trait of quantum mechanics" [21], and can generally be found in systems that have had previous interactions with other quantum systems, often due to spatial proximity.

Quantum entanglement in its essence intertwines quantum-behaving systems—such as particles—resulting in correlated observable values. A simple example of this correlation is given by the decay of subatomic particles: a high-energy photon can decay into a pair of an electron and a positron [22]. The general conservation law applies to the system, meaning that various observable quantities must remain unchanged between the starting and the resulting particles. One such type of quantity is the spin of the particles, which is zero for a photon and one half for electrons and positrons. After the decay event, the spin of one of the resulting particles can be measured along some axis, which immediately tells the spin of the other particle must be opposite (along the same axis) due to the conservation of spin in the system. In quantum terms, this means that the total wave function of the system must be correlated so that a measurement on one particle collapses the wave function of the whole system and gives information on the other particle.

This type of application of quantum entanglement has created a seemingly paradoxical situation. The entangled particles are not required to be in a spatial proximity for the described correlation to be valid, leading to the possibility of instantaneous traversal of information. This in turn would result in breaking the rules of special relativity where according to Einstein [23] (translated recreation, for original work see [24]), no information can travel faster than the speed of light. For this reason, quantum entanglement has been one of the most controversial subjects in quantum mechanics, Albert Einstein famously



**Figure 4.1.** Quantum circuit for preparing an arbitrary Bell state  $|\psi\rangle$  by the selection of states  $|a\rangle, |b\rangle \in \{|0\rangle, |1\rangle\}$ . [15, p. 75]

claiming it as "spooky action at a distance". This dissent culminated in Einstein, Podolsky and Rosen releasing an article in 1935 insisting that quantum mechanics as a whole must contain some local hidden variables to explain the behaviour, an assertion now known as the EPR-paradox [25]. However, these claims were debased by Bell in 1964, when Bell proved the formulation of quantum mechanics is unable to hold such local hidden qualities [26]. This proof has since come to be known as the Bell's Inequality.

Generally entanglement in quantum computing is introduced through examples using Bell states (also known as EPR pairs). Bell states are a set of four two-qubit orthonormal states residing in a four dimensional Hilbert space. They are regarded as maximally entangled two-qubit states and are presented as [19, p. 88] [27, p. 1]

$$\begin{aligned} |\Phi^\pm\rangle &= \frac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle) \\ |\Psi^\pm\rangle &= \frac{1}{\sqrt{2}}(|01\rangle \pm |10\rangle). \end{aligned} \quad (4.1)$$

Bell states can be constructed by using the circuit shown in figure 4.1, where the states  $|a\rangle$  and  $|b\rangle$  can be either of the computational basis states (3.1) and the gate  $H$  is a Hadamard gate with a matrix form realization

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \quad (4.2)$$

A Hadamard gate acting on a computational basis maps it to a superposition state. This is demonstrated in the following equation

$$H|0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle). \quad (4.3)$$

The superposed state is then acted on with CNOT-gate (3.7), which flips the state of the second qubit based on the value of the first one. As the first qubit is in a superposed state, this "transfers" the superposition to the other state of the system. With different combinations of the computational basis vectors for the original states  $|a\rangle$  and  $|b\rangle$ , the circuit results in one of the four Bell states. [14, pp. 74–76, 431] [15, pp. 70–71, 75] [20, pp. 19, 25]

The system described by Bell states entangles the individual qubits together so that they cannot be separated into individual states without collapsing the system. This is commonly described by the following example:

One of the Bell states is prepared, chosen to be  $|\Psi^+\rangle$  for this example, and the individual qubits are given to Alice and Bob without identifying the states at any point. Alice and Bob take off with the qubits, travelling to different directions. After a set amount of time, Alice and Bob decide to measure their qubits along the axis  $x$ ,  $y$  or  $z$ , chosen randomly. By conducting the measurement, they receive either of the states  $|0\rangle$  or  $|1\rangle$  as result. Upon repeating this process multiple times and coming together to compare the results, Alice and Bob notice that after each measurement where the axis has been the same the results are precisely anticorrelated and otherwise have no correlation. [10, p. 375] [28, p. 7] [29, pp. 3–8]

This observation can be made due to the measurement process actually measuring the entangled Bell state  $|\Psi^+\rangle$  rather than the individual states, and collapsing this state to be either  $|0\rangle_A |1\rangle_B$  or  $|1\rangle_A |0\rangle_B$  respectively. However, this is only applicable if Alice and Bob prepare their measurement in the *same basis*, namely measuring along the same axis. Preparing a measurement along the same axis, Alice and Bob are able to precisely determine the state of the other qubit even across large distances and without being in direct interaction. [10, p. 375][29, pp. 3–8]

## 4.2 General mathematics of entangled systems

Next we must ask the question, how can we determine if a system is entangled? To answer this question, we must first expand some basic concepts related to how quantum states are addressed in advanced quantum mechanics.

Until this point, the state of our Hilbert space has been addressed by a definite state vector  $|\psi\rangle$  which has been known to precisely describe our quantum system. These types of states are known as *pure states*. However, often times it is found out that the state of the system cannot be definitely described by a singular pure state vector, but instead a collection of such states with some probability of finding the system in said state. This ensemble of states is known as a *mixed state*. A set of  $n$  such states can generally be written as

$$\left\{ (|\psi_1\rangle, p_1), (|\psi_2\rangle, p_2), \dots, (|\psi_n\rangle, p_n) \right\}, \quad (4.4)$$

where  $|\psi_k\rangle$  represents the  $k$ :th pure state that can be found with probability  $p_k$  upon measurement. [15, p. 53]

To generalize our inspection of quantum states, we also take on a new approach in treating our quantum systems. Instead of using state vectors like  $|\psi\rangle$  to describe our system, we adopt the use of Hermitian *density operators* for similar results, which reside

in their own Hilbert space  $\mathcal{H}$ . A density operator for a pure state  $|\psi\rangle$  is realized through a *density matrix* given by [15, p. 53]

$$\rho = |\psi\rangle \langle\psi|. \quad (4.5)$$

The density operators gives a concise form for describing mixed states with a matrix representation [20, p. 99] [28, p. 6]

$$\rho = \sum_i^n p(i) |\psi_i\rangle \langle\psi_i|. \quad (4.6)$$

An operator  $U$  acting on pure state  $|\psi\rangle$  would result in a new state  $U|\psi\rangle$ . With this new form of notation, we would have as the density matrix for this system [15, p. 54] [20, p. 99]

$$\rho = U |\psi\rangle \langle\psi| U^\dagger. \quad (4.7)$$

For density matrices, the trace of a matrix (sum of diagonal elements) becomes the tool for tracking important quantities. For this matter, we give here the multiplication of a pair of tensor products and the cyclicity of the trace as helpful algebraic tools for solving upcoming systems: [15, p. 54] [28, p. 5]

$$\begin{aligned} (A \otimes B)(C \otimes D) &= AC \otimes BD \\ \text{Tr}(ABC) &= \text{Tr}(CAB) = \text{Tr}(BCA). \end{aligned} \quad (4.8)$$

The trace of a density matrix should amount to unity, as seen by [20, p. 101][28, p. 7]

$$\text{Tr}(\rho) = \sum_i^n p(i) \text{Tr}(|\psi\rangle \langle\psi|) = \sum_i^n p(i) \langle\psi|\psi\rangle = \sum_i^n p(i) = 1, \quad (4.9)$$

where the probabilities must amount to 1 (for pure states this holds automatically). An example use for the trace is finding the probability of measuring some state, for this case  $|0\rangle$ , given by the equation [15, p. 55]

$$\text{Tr}(\langle 0| \rho |0\rangle) = \text{Tr}(|0\rangle \langle 0| \rho) = \text{Tr}(P_0 \rho), \quad (4.10)$$

where  $P_0$  is the projection operator to state  $|0\rangle$ .

The trace of the combined system's density operator serves as a useful tool for qualifying entanglement. Entanglement in a system is overall defined through being unable to reduce a combined system to the contributing pure states. If the combined state  $|\psi\rangle$  cannot be written as the product state of the pure states  $|\psi_A\rangle \otimes |\psi_B\rangle$  for any  $|\psi_A\rangle, |\psi_B\rangle$ , then the system is determined to be entangled. Density operators enable the possibility to reduce the system to density matrices of its components using *partial traces*, which

trace over/remove the contribution of one of the systems. For the composite Hilbert space (3.3) of partial systems  $A$  and  $B$  and the case of pure states, tracing over one of the systems  $A$  or  $B$  would only result in the density matrix description of the other state. For the case of entangled states, tracing over one of the contributing systems would result in a mixed state density matrix description for the other state, and thus the system can be concluded to be entangled. [14, pp. 22, 417–419] [15, p. 56]

These two occasions are gone over in the following examples. For the non-entangled case, we take our initial system to be in the combined state  $|01\rangle$  (3.4) consisting of the pure states  $|0\rangle \in \mathcal{H}_A$  and  $|1\rangle \in \mathcal{H}_B$ . The density matrix for this combined states is then given as

$$\rho^{AB} = |01\rangle \langle 01|. \quad (4.11)$$

We can now trace over the system  $B$  and gain the *reduced density operator* of system  $A$  as a result.

$$\begin{aligned} \rho^A &= \text{Tr}_B(\rho^{AB}) \\ &= \text{Tr}_B(|01\rangle \langle 01|) \\ &= \text{Tr}_B((|0\rangle \otimes |1\rangle)(\langle 0| \otimes \langle 1|)) \\ &= \text{Tr}_B(|0\rangle \langle 0| \otimes |1\rangle \langle 1|) \\ &= |0\rangle \langle 0| \text{Tr}_B(|1\rangle \langle 1|) \\ &= |0\rangle \langle 0| \langle 1|1\rangle \\ &= |0\rangle \langle 0| \end{aligned} \quad (4.12)$$

The resulting reduced density operator is for a pure state  $|0\rangle$ , which is expected from a non-entangled state.

For the entangled case, let's take the previously considered Bell state  $|\Psi^+\rangle$  (4.1) as our combined state for the example. The density matrix for the system then is

$$\rho^{AB} = \frac{1}{2}(|01\rangle \langle 01| + |01\rangle \langle 10| + |10\rangle \langle 01| + |10\rangle \langle 10|). \quad (4.13)$$

Tracing out the system  $B$ , we then get

$$\begin{aligned}
\rho^A &= \text{Tr}_B(\rho^{AB}) \\
&= \text{Tr}_B\left(\frac{1}{2}(|01\rangle\langle 01| + |01\rangle\langle 10| + |10\rangle\langle 01| + |10\rangle\langle 10|)\right) \\
&= \text{Tr}_B\left(\frac{1}{2}(|0\rangle\langle 0| \otimes |1\rangle\langle 1| + |0\rangle\langle 1| \otimes |1\rangle\langle 0| + |1\rangle\langle 0| \otimes |0\rangle\langle 1| + |1\rangle\langle 1| \otimes |0\rangle\langle 0|)\right) \\
&= \frac{1}{2}(|0\rangle\langle 0| \text{Tr}_B(|1\rangle\langle 1|) + |0\rangle\langle 1| \text{Tr}_B(|1\rangle\langle 0|) + |1\rangle\langle 0| \text{Tr}_B(|0\rangle\langle 1|) + |1\rangle\langle 1| \text{Tr}_B(|0\rangle\langle 0|)) \\
&= \frac{1}{2}(|0\rangle\langle 0| \langle 1|1\rangle + |0\rangle\langle 1| \langle 0|1\rangle + |1\rangle\langle 0| \langle 1|0\rangle + |1\rangle\langle 1| \langle 0|0\rangle) \\
&= \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|).
\end{aligned} \tag{4.14}$$

We can notice the resulting state being a mixed state of  $\rho_0$  and  $\rho_1$  with probabilities  $p_0 = p_1 = 1/2$ . With our previous claims, this leads to the Bell states being entangled. [15, p. 57]

### 4.3 Schmidt decomposition and von Neumann entropy

Next we want to know, is there a way to track the amount of entanglement in a system? As previously stated in 4.1, Bell states have been mentioned to be maximally entangled states, meaning there is a qualitative scale for entanglement. In order to measure this amount of entanglement, we'll need to introduce the mathematical concepts of Schmidt decomposition and von Neumann entropy.

Generally, any combined state  $|\psi\rangle$  in  $\mathcal{H}$  can be written as a combination of orthonormal basis states  $|i^A\rangle$  and  $|j^B\rangle$  in  $\mathcal{H}_A$  and  $\mathcal{H}_B$  respectively, as

$$|\psi\rangle = \sum_{i,j} a_{ij} |i^A\rangle |j^B\rangle, \tag{4.15}$$

where  $a$  is a complex matrix with matrix elements  $a_{ij}$ . Further, it is possible to carry out a singular value decomposition (SVD for short) for this matrix to reduce it into three simplified matrices  $a = u d v$ , where  $u$  and  $v$  are unitary matrices and  $d$  is a diagonal matrix with non-negative real elements. We can absorb the unitary  $u$  into the state  $|i^A\rangle$ , giving us the state  $|\phi^A\rangle$ , and similarly absorb the unitary  $v$  to  $|j^B\rangle$  in order to get  $|\phi^B\rangle$ . These orthogonal states are generally known as the Schmidt basis. Thus we are left with the diagonal  $d$  and an orthonormal basis, in which we can write our system as

$$|\psi\rangle = \sum_i \alpha_i |\phi_i^A\rangle |\phi_i^B\rangle, \tag{4.16}$$

where  $\alpha_i$  represent the non-negative diagonal elements of  $d$ , known as the Schmidt coefficients. This procedure represents the Schmidt decomposition, and it tells us that

we can always find an orthogonal basis in  $\mathcal{H}_A$  and  $\mathcal{H}_B$  to describe our combined state with only summing over one set of indices. [14, pp. 433–434] [15, p. 35] [19, pp. 94–95] [20, p. 109]

Adopting our previous approach to combined states using density operators (4.5), we can construct the density matrix for the Schmidt decomposition:

$$\begin{aligned}
 \rho^{AB} &= \left( \sum_i \alpha_i |\phi_i^A\rangle |\phi_i^B\rangle \right) \left( \sum_j \alpha_j \langle \phi_j^A| \langle \phi_j^B| \right) \\
 &= \sum_{i,j} \alpha_i \alpha_j |\phi_i^A\rangle |\phi_i^B\rangle \langle \phi_j^A| \langle \phi_j^B| \\
 &= \sum_{i,j} \alpha_i \alpha_j |\phi_i^A\rangle \langle \phi_j^A| \otimes |\phi_i^B\rangle \langle \phi_j^B|.
 \end{aligned} \tag{4.17}$$

A density operator gained through Schmidt decomposition has some useful qualities, like providing an easy way to solve partial traces for the system. This is demonstrated below, where the partial traces over both of the systems  $A$  and  $B$  have been derived into a simple form:

$$\begin{aligned}
 \rho^A &= \text{Tr}_B(\rho^{AB}) & \rho^B &= \text{Tr}_A(\rho^{AB}) \\
 &= \sum_{i,j} \alpha_i \alpha_j |\phi_i^A\rangle \langle \phi_j^A| \text{Tr}_B(|\phi_i^B\rangle \langle \phi_j^B|) & &= \sum_{i,j} \alpha_i \alpha_j \text{Tr}_A(|\phi_i^A\rangle \langle \phi_j^A|) |\phi_i^B\rangle \langle \phi_j^B| \\
 &= \sum_{i,j} \alpha_i \alpha_j |\phi_i^A\rangle \langle \phi_j^A| \langle \phi_j^B| \phi_i^B\rangle & &= \sum_{i,j} \alpha_i \alpha_j \langle \phi_j^A| \phi_i^A\rangle |\phi_i^B\rangle \langle \phi_j^B| \\
 &= \sum_{i,j} \alpha_i \alpha_j |\phi_i^A\rangle \langle \phi_j^A| \delta_{ij} & &= \sum_{i,j} \alpha_i \alpha_j |\phi_i^B\rangle \langle \phi_j^B| \delta_{ij} \\
 &= \sum_i \alpha_i^2 |\phi_i^A\rangle \langle \phi_i^A| & &= \sum_i \alpha_i^2 |\phi_i^B\rangle \langle \phi_i^B|.
 \end{aligned} \tag{4.18}$$

We can see that for both of these cases, the squares of the Schmidt coefficients are the same, meaning the combined system is independent of which partial trace was originally taken. [15, pp. 58–59] [20, pp. 110–111]

The amount of quantum entanglement in a system is measured through *von Neumann entropy* (or *entanglement entropy*) given via

$$S = -\text{Tr}(\rho \log_2 \rho) = -\sum_i \lambda_i \log_2 \lambda_i, \tag{4.19}$$

which corresponds to the quantum version of Shannon entropy from classical information theory (with definition  $0 \log_2(0) = 0$ ). Here  $\log_2$  is in base two due to the entropy gauging binary values of information, and the values  $\lambda_i$  correspond to the observation probabilities  $p(i)$  in (4.6). [14, pp. 421–422] [20, p. 510] [28, p. 15]

For pure states given by (4.5), for which the observation probability is  $p(i) = 1 \vee 0$ , the

von Neumann entropy can be seen to give  $S = 0$  as a result, meaning the total entropy of the system is unchanged. This holds true for reduced density operators of systems that can be decomposed to the product states of pure states (like the one given in (4.14)), as is expected from non-entangled systems. For mixed states, the knowledge on the probabilities  $p(i)$  for observing the system in some state  $|\psi_i\rangle$  would be required to solve the system's entropy, which can often prove difficult. However, for entangled systems where the combined pure states are known (like for Bell states), the  $\lambda_i$  values in (4.19) for the reduced density operators can be gained from the Schmidt decomposition as the Schmidt coefficients (4.16). For a combined systems consisting of two qubits, these coefficients are independent of the system being traced over as was proven previously in (4.18). For entropy, this means that  $S(A) = S(B)$ , and after solving a proper Schmidt basis for the system, the observation probability corresponds to  $\lambda_i = p(i) = \alpha_i^2$ . This way, the entanglement entropy for the component systems can be calculated. The entanglement entropy is always positive for entangled systems with a maximal value of  $S = \log_2(N)$  where  $N$  is the dimensions of the reduced state spaces  $\mathcal{H}_{A,B}$ . [14, pp. 421–422] [19, pp. 232–251] [30]

#### 4.4 Significance on quantum computing

Lastly we must ask the question, is there any way to harness entanglement for use in computation? Entanglement can be said to be *the* primary benefactor for quantum computing, as entanglement is the phenomena that enables exponential speed-up of quantum processes compared to classical one. As the Hilbert space  $\mathcal{H}$  grows in dimensions  $2^n$  for  $n$  qubits, the resource cost to represent the superposition of such system is linear for quantum mechanics due to entanglement, whereas to simulate this kind of space in classical mechanics would require resource cost increasing exponentially in size  $n$ . [2, pp. 1–3] There are also multiple other use cases for entanglement in quantum computing, which some, namely superdense coding and quantum teleportation, will be gone through in this chapter.

Superdense coding is the procedure of producing two classical bits of information from a shared entangled state and transferral of one qubit of information. The procedure starts similarly to the examples given in 4.1, where a Bell state has been produced beforehand and the individual qubits have been distributed to Alice and Bob. For this example, the prepared Bell state is taken to be the state  $|\Phi^+\rangle$  as presented in (4.1). Now, Alice's goal is to send Bob a message consisting of two bits of classical information by only sharing the one qubit she is in possession of. In order to do this, Alice acts on her qubit with one

of the four Pauli gates

$$\begin{aligned} I &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} & X &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ Y &= \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} & Z &= \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \end{aligned} \quad (4.20)$$

depending on the message she would want to transmit to Bob. Each of the two bit messages, their respective two-qubit operations and the resulting entangled states have been listed in the table 4.1. Thus it can be seen that Alice's operation just orients the original Bell state to one of the other Bell basis states or keeps it the same. After operating on her qubit, Alice sends it to Bob through a quantum channel. Bob can then measure the state of the total system in the Bell basis (details of this are omitted in this thesis) to accurately determine Alice's message. [15, p. 79] [16, pp. 129–132] [20, pp. 97–98]

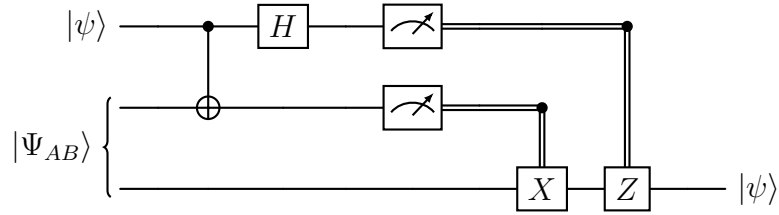
**Table 4.1.** Options for the classical two bit message and the corresponding operations required to produce the respective information. [15, p. 79]

Information	Operation	Resulting state
00	$I \otimes I :$	$\frac{1}{\sqrt{2}}( 00\rangle +  11\rangle) \mapsto \frac{1}{\sqrt{2}}( 00\rangle +  11\rangle) = \Phi^+$
01	$X \otimes I :$	$\frac{1}{\sqrt{2}}( 00\rangle +  11\rangle) \mapsto \frac{1}{\sqrt{2}}( 01\rangle +  10\rangle) = \Psi^+$
10	$Z \otimes I :$	$\frac{1}{\sqrt{2}}( 00\rangle +  11\rangle) \mapsto \frac{1}{\sqrt{2}}( 00\rangle -  11\rangle) = \Phi^-$
11	$iY \otimes I :$	$\frac{1}{\sqrt{2}}( 00\rangle +  11\rangle) \mapsto \frac{1}{\sqrt{2}}( 01\rangle -  10\rangle) = \Psi^-$

Quantum teleportation can be seen as the opposite computational task compared to superdense coding, where a qubit of information is gained from a shared entangled state and transferral of two classical bits of information (in contrast to gaining two classical bits of information from a transferral of a qubit). The process again starts from Alice and Bob being in possession of individual qubits of a Bell state, be it  $|\Phi^+\rangle$ . Alice wants to send Bob a qubit of information, a general state  $|\psi\rangle$ , but only has access to classical channels. Describing the state perfectly in classical terms would require an infinite amount of information, as the complex amplitudes (3.2) of the state are continuous. However, utilizing the shared EPR-pair enables Alice to provide the necessary information concerning her qubit by only using two classical bits. [20, pp. 26–27] [31]

Quantum teleportation can be implemented using the circuit in figure 4.2. Mathematically the system starts in a state

$$|\psi\rangle |\Phi^+\rangle = \frac{1}{\sqrt{2}} \left[ \alpha |0\rangle (|00\rangle + |11\rangle) + \beta |1\rangle (|00\rangle + |11\rangle) \right]. \quad (4.21)$$



**Figure 4.2.** A circuit configuration for producing quantum teleportation. [20, p. 27]

As can be seen from the figure, the message state  $|\psi\rangle$  is first coupled to Alice's qubit using the reversed Bell circuit 4.1, taking the system to a total state

$$|\psi_{\text{tot}}\rangle = \frac{1}{\sqrt{2}} \left[ \alpha |0\rangle (|00\rangle + |11\rangle) + \beta |1\rangle (|10\rangle + |01\rangle) \right], \quad (4.22)$$

after which the message state is acted on with a Hadamard gate and the different terms reordered to obtain

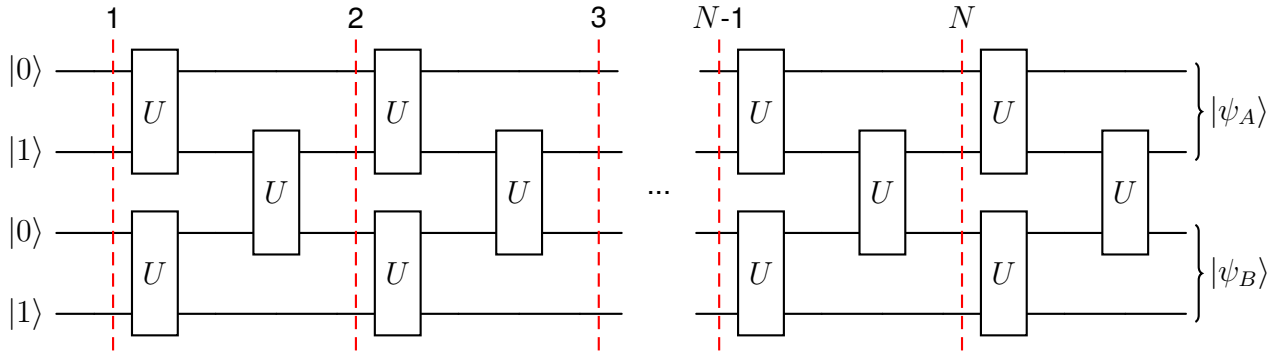
$$|\psi_{H,\text{tot}}\rangle = \frac{1}{2} \left[ |00\rangle (\alpha |0\rangle + \beta |1\rangle) + |01\rangle (\alpha |1\rangle + \beta |0\rangle) \right. \\ \left. + |10\rangle (\alpha |0\rangle - \beta |1\rangle) + |11\rangle (\alpha |1\rangle - \beta |0\rangle) \right]. \quad (4.23)$$

Here the first two qubits of each term refer to the qubits in Alice's possession and the last superpositioned qubit is the one Bob has hold of. With this, Alice can perform a measurement on her two qubits to collapse the system into one of the four terms, and send the measurement results to Bob. From the two bits, Bob can perform an analogous operation to the ones in table 4.1 in order to determine the state his qubit is in and measure the complex coefficients to reproduce the original message. This way, Alice has successfully transferred a qubit of information through classical channels by using up the entanglement of the system and two classical bits of information. [19, pp. 167–171] [20, pp. 26–27]

#### 4.4.1 Simulation of entanglement entropy

The previous notions for quantum entanglement culminate on this simulation of entanglement entropy in a periodic circuit. The goal of the simulation is to inspect the effects of specifically constructed unitary operators applied repeatedly to a circuit to gauge the changes in entanglement. We measure the amount of entanglement in the system using von Neumann entropy 4.3 as the function of the periods  $N$ . The project was designed and overseen by the examiner.

We begin with a circuit depicted in figure 4.3 where we have four qubits in  $|0\rangle$  or  $|1\rangle$  states. These qubits are operated on with the unitary operator  $U$  cyclically, first to the pairwise states and then acting on to the two middle states. The process is repeated  $N$



**Figure 4.3.** Periodic quantum circuit to demonstrate the behaviour of entanglement entropy as a function of periods  $N$ . The circuit consists of four input qubits and unitary quantum gates  $U$  acting on two qubits at a time in cyclical manner. A measurement is conducted on the system between each cycle to gauge the current entanglement.

times and the entanglement between the two pairwise terms, represented as  $|\psi_A\rangle$  and  $|\psi_B\rangle$ , is measured after each iteration. As we have a circuit consisting of four qubits, the dimension of the corresponding Hilbert space is  $2^4 = 16$ . The unitary operator considered for this case has been taken to be

$$U_{j,j+1} = e^{i(a\sigma_x^j\sigma_x^{j+1} + b\sigma_y^j\sigma_y^{j+1} + c\sigma_z^j\sigma_z^{j+1})}, \quad (4.24)$$

where  $j$  represents the index of the qubit being acted on (counting from top to bottom in the circuit),  $a$ ,  $b$  and  $c$  are real coefficients and  $\sigma_i$  are the  $i \in x, y, z$  Pauli matrices (previously seen in gate form at (4.20)) [10, p. 275]

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \quad (4.25)$$

The notion to use matrix exponentials is common practice for operator representation and can be realized with Taylor expansions. The notation of successive Pauli matrices can be interpreted as their Tensor products

$$\sigma_i^j\sigma_i^{j+1} = \sigma_i^j \otimes \sigma_i^{j+1}, \quad (4.26)$$

again  $i \in x, y, z$  and  $j$  being the index of the qubit being acted on. All the individual components of  $U$  are unitary, resulting in  $U$  being a  $4 \times 4$  unitary matrix that acts on two qubits at a time. The operations on the total state can be then be implemented as the composite operators  $U \otimes U$  for the first pairwise states and  $I \otimes U \otimes I$  for the two middle qubits (with  $I$  being  $2 \times 2$  dimensional identity matrix).

The act of measurement is carried out with a modified Schmidt decomposition using the

form

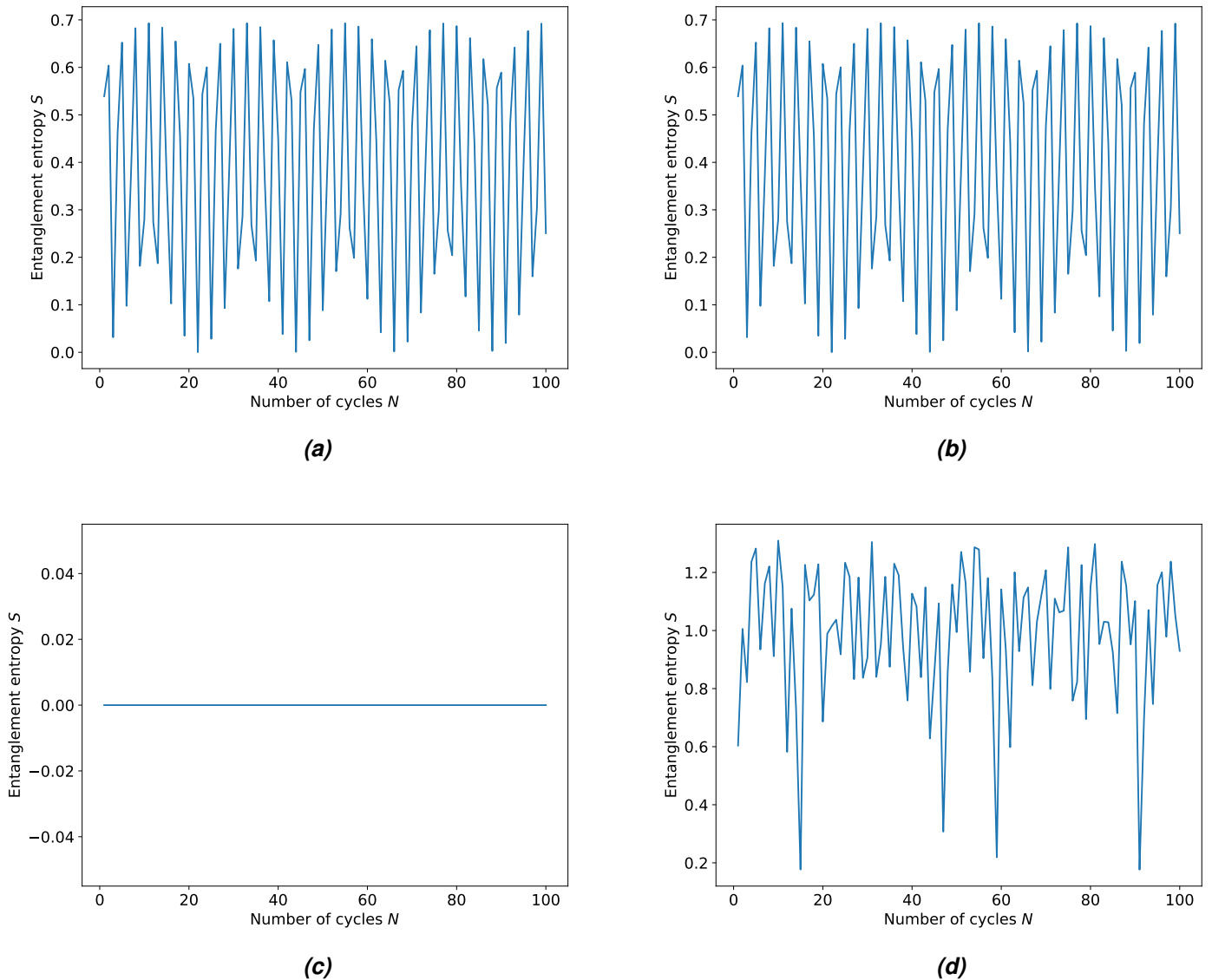
$$|\psi_N\rangle = \sum_{i,j} M_{ij} |i^A\rangle \otimes |j^B\rangle, \quad (4.27)$$

where  $|i^A\rangle, |j^B\rangle$  are the respective orthogonal basis states of  $|\psi_A\rangle, |\psi_B\rangle$ , meaning  $|i^A\rangle, |j^B\rangle \in \{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$  and alongside matrix  $M_{ij}$  these construct the total state  $|\psi_N\rangle$ . This form directly relates to the equation (4.15), where the SVD procedure has not yet been carried out to gain the final form (4.16). Instead the task of directly finding the Schmidt coefficients  $\alpha_i$  has been transformed into finding the matrix elements of  $M_{ij}$  and carrying out SVD to solve the diagonal matrix, from which the Schmidt coefficients can be evaluated. These coefficients are then used in calculating the entanglement entropy between the two qubit pairings  $|\psi_A\rangle$  and  $|\psi_B\rangle$  using modified von Neumann entropy

$$S = - \sum_i \alpha_i \ln(\alpha_i), \quad (4.28)$$

where the logarithm basis has been changed from  $\log_2$  to  $\ln$ , which corresponds to the thermodynamic realization of entropy instead of the informational uncertainty.

The results for the simulations have been shown in figure 4.4. In this case, all of the simulations are for  $N = 100$  iterations and entanglement entropy was measured after each block of operations. The differing figures correspond to different selections of constant values  $a, b$  and  $c$ , belonging to  $\{0, 0.5\}$ .



**Figure 4.4.** Entanglement entropy as a function of cycles  $N = 100$  for different coefficient values  $a$ ,  $b$  and  $c$ . **(a)** Coefficients set as  $a = 0.5$ ,  $b = 0$  and  $c = 0$ . The entanglement entropy can be seen to fluctuate periodically, often reaching even 0 meaning a state of no entanglement. **(b)** Coefficients set as  $a = 0$ ,  $b = 0.5$  and  $c = 0$ . The figure can be seen to be identical to figure (a), with the entanglement fluctuating periodically. **(c)** Coefficients set as  $a = 0$ ,  $b = 0$  and  $c = 0.5$ . With only contribution from  $c$ , the entropy stays at 0 and no entanglement can be observed in the system. **(d)** Coefficients set as  $a = 0.5$ ,  $b = 0.5$  and  $c = 0.5$ . With contribution from all the components, the entanglement seems to behave chaotically and overall reach higher entanglement entropy values. Periodicity cannot be determined within current amount of iterations.

From the top row figures, it can be observed that the simulations dependent on only the coefficients  $a$  or  $b$  have fluctuating periodic structure with well defined entanglement entropy within cycles. At periods of around 22 iterations, the value for entanglement entropy seemingly becomes zero, meaning that the pairwise states  $|\psi_A\rangle$  and  $|\psi_B\rangle$

become orthogonal to each other before beginning a new cycle of operations. It can also be observed that the two figures 4.4a and 4.4b are identical to each other, signalling that the corresponding Pauli matrix combinations for  $\sigma_x$  and  $\sigma_y$  entangle the system in equal steps.

For the figure 4.4c only dependent on coefficient  $c$ , it can be seen that the entropy of the system remains zero during the whole simulation, indicating no entanglement appearing in the system. This results from the geometry of the corresponding Pauli matrix  $\sigma_z$ . The operator from combined Pauli  $\sigma_z$  matrices only has diagonal elements of either  $-1$  or  $1$ , meaning that for the simplistic states like  $|01\rangle$  or  $|10\rangle$ , the operator can only change the sign of the state (direction in Hilbert space). The coefficient  $c$  introduces a multiplier to the state which scales it in the said  $\mathcal{H}$  space, but after normalization this scaling is removed. Thus the states can only get reversed in  $\mathcal{H}$  but no mixing can happen between the individual states. However, the orthogonal elements in the composite operators of  $\sigma_x$  and  $\sigma_y$  introduce mixing between the states and thus entanglement, which also would change the effect of coefficient  $c$  on the states (produce effects other than scaling).

The final figure 4.4d is then a combination of all of the previous coefficients  $a$ ,  $b$  and  $c$ , and can be seen to be rather chaotic in nature with the highest observed value for entanglement entropy. No seeming periodicity can be observed with this amount of iterations, although there are some regions of lower entropy values. The graph can be interpreted as the states being highly entangled/entangled for longer amount of periods, and a higher total count of iterations would be required to notice any repeating patterns.

## 5. CONCLUSION

This thesis was a literature review acting as a short dive into the world of quantum computing. This thesis started out by introducing the mathematical basics of quantum mechanics through presenting the matrix mechanical approach. This contained the notions of finite Hilbert spaces, which define quantum states as vectors and gives them mathematical properties, like the inner product. Matrix mechanics also contains in itself the operator calculus, where matrix operators residing in similar Hilbert spaces can be used to alter quantum states. After introducing matrix mechanics, the first chapter shortly summarized the postulates of quantum mechanics, these being the definition of the state vectors and Hilbert spaces, operators as representatives of physical quantities and time-evolution through the Schrödinger equation.

The second chapter moved on to formulate quantum circuits by first proposing qubits, realized as binary quantum vector states, to be our computational basis units similar to classical bits. To form larger computational systems, the singular qubit states can be combined through the use of tensor products, which expands the dimensions of this new formed conjugate Hilbert space to be  $2^n$ ,  $n$  being the amount of qubits. Following the notions for qubits, we introduced the quantum gates, correspondingly realized as unitary operators, for performing computational operations and showcased the graphical depictions for quantum circuits consisting of qubits and such gates.

Finally, we thoroughly inspected the meaning of entanglement in a quantum system by first giving common examples on the topic, like introducing the concept of Bell states, followed by an introduction to density operators, from which the entanglement could unambiguously be defined. We then conceptualized the measurement of entanglement with von Neumann entropy, which qualitatively tracks the amount of entanglement in a system. This was done by first performing a Schmidt decomposition on a quantum state, seen as the reducing the state to its orthonormal components multiplied by factors known as Schmidt coefficients. These coefficients could then be used in calculating von Neumann entropy, similar to classical Shannon entropy in information theory. After presenting the theory for quantum entanglement, some tangible use cases for entanglement in quantum computation were demonstrated. The chapter culminated the thesis on a quantum circuit simulation project, which illustrated intriguing properties for entanglement entropy in a periodic quantum system. Among these were the

observations of a periodic nature of entanglement when performed transformations in some defined directions, no observable entanglement in the system when transformed in a certain direction and chaotic behaviour when all directional transformations were combined.

Further steps for studying quantum computation would be to lean towards the concepts of quantum algorithms, quantum error correction and the physical actualization of quantum computers (like facing many-body problems). These topics were excluded from this thesis due to limited time and space constraints and thus could not be included in extensive manner.

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