The Quantum World

A Rapid Introduction

Reuben R.W. Wang

This is dedicated to my mentors and instructors.

This is currently the **first edition**.
There are likely to be errors.
Send any corrections and comments to `reuben.wang@colorado.edu`.

Contents

Preface **vi**

Introduction:
Why Quantum Mechanics? **x**
0.1 Breaking Classical Law . . . x
0.1.1 Young's Experiment . . . x
0.1.2 Young Revisited . . . xi
0.2 Fighting Fire with Radiation . . . xii
0.3 Classical Deviations . . . xiii
0.3.1 Linearity of Quantum Mechanics . . . xiii
0.3.2 Necessity of Complex Numbers . . . xiv
0.3.3 Loss of Determinism . . . xiv
0.3.4 Superposition . . . xiv
0.3.5 Entanglement (Qualitative Insight) . . . xv

I Understanding the Substrate **1**

1 A Dive into Superposition **2**
1.1 Mach-Zehnder Interferometry . . . 2
1.1.1 Matrix Representation . . . 3
1.2 Elitzur-Vaidman Bombs . . . 5

2 Quantum Promotions **8**
2.1 Matter Waves . . . 8
2.2 Operators . . . 9
2.3 Commutators . . . 12

3 Building Tools for Measurement **14**
3.1 Inner Products . . . 14
3.2 Expectation Values . . . 15
3.3 Uncertainty . . . 16
3.4 Hermiticity and Diagonalization . . . 17
3.5 Measurement . . . 18

4 What Now Schrödinger? **20**
4.1 Stationary States . . . 20
4.2 Modelling Radioactive Decay . . . 21

4.2.1 In the Nuclear Well . . . 23
4.2.2 Classically Forbidden Regions . . . 23
4.2.3 Freed from Nuclear Entrapment . . . 24
4.2.4 Joining the Puzzle Pieces . . . 24
4.2.5 Stuck in a Box! . . . 25
4.3 Dirac's Bras and Kets . . . 27

II Applied Abstractions 32

5 Quantum Computation 33
5.1 TLDR; Classical Computers . . . 33
5.1.1 Byte-Sized Complexity Theory . . . 34
5.2 The Qubit . . . 35
5.3 Pauli Gates . . . 36
5.4 More Qubits; Tensor Products . . . 37
5.5 Quantum Circuits . . . 38
5.6 Spooky Action at a Distance . . . 40
5.7 Beam Me Up, Scotty! . . . 40
5.7.1 Q-Teleportation Analysis . . . 41
5.8 Deutsch–Jozsa's Algorithm . . . 43
5.8.1 2-Qubit Algorithm Analysis . . . 44

6 Bell vs EPR 47
6.1 More on Spin Measurement . . . 47
6.2 Just An Illusion? . . . 48

Appendices 53

A Early Beginnings of QM 54
A.1 Catastrophic Beginnings . . . 54
A.2 Experimental Persuasions . . . 55
A.2.1 The Photoelectric Effect . . . 55
A.2.2 Compton Scattering . . . 56

B Elitzur-Vaidman Probabilistic Improvements 57

C Wave Mechanics 59
C.1 Galilean Transformation of Classical Waves . . . 59
C.2 Matter Waves . . . 60
C.3 Group Velocity . . . 60
C.4 Principle of Stationary Phase . . . 61
C.5 Time-Evolving Wavepackets . . . 61
C.6 Heisenberg Uncertainty Principle (Qualitative) . . . 63
C.7 Interpretation of Waves and Normalization . . . 64

D Quintessential 1D Potentials 65
D.1 Spooky Circles . . . 65
D.2 Quantum Boxes . . . 66
D.2.1 Prove It! . . . 66

D.2.2 Boxes Continued . . . 68
D.3 Infinitely Sharp Wells . . . 73
D.4 Quantum Springs . . . 75

E Spin **78**
E.1 Head Spinning Results . . . 78
E.1.1 Magnetic Moments . . . 79
E.2 Superposition of Spin States . . . 81

F Abstract and Linear Algebra **83**
F.1 Groups, Rings and Fields . . . 83
F.2 Vector Spaces, Hilbert Spaces and Lie Algebras . . . 85
F.2.1 Linear Operators and $\mathscr{L}(V)$ . . . 86
F.2.2 Kernel and Range . . . 87
F.2.3 Hilbert Spaces and Lie Algebras . . . 88

Preface

This handbook is designed as a brief but mathematically rigorous introduction to quantum science and technology for the tech enthusiast. The materials covered in this handbook are intended to be taught/learned over the course of 2 to 4 weeks with no prior knowledge of quantum physics required. In order to appeal to both scientists and engineers, there will be several topics covered with applications as quantum technologies in sufficient but not comprehensive depth so as to gain literacy of the subject matter. Specifically, we will be exploring a simplified model of **radioactive decay** in ionization smoke detectors and the model of **quantum computation**. As a means for appealing to a diverse audience and trying to incorporate the best of both worlds, I have divided the handbook into 2 parent parts. These are namely "*understanding the substrate*" and "*applied abstractions*". This partitioning is to differentiate between content that focuses on quantum theory topics pertaining to describing physical systems vs material that cares only about abstracted utilizable properties (analogous to the distinction between electrical engineering and computer science).

Some prerequisites to understanding the material in this book would be knowledge of **1)** linear algebra **2)** ordinary differential equations **3)** classical mechanics **4)** basic electrodynamics **5)** basic probability theory. I will also occasionally mention relevant words and topics of study that will not be expounded on in this book. This is intentional and meant to encourage the reader to go beyond the contents presented here. Be sure that this will **not** impede the reader's understanding of this book. If you are indeed new to quantum mechanics and learning it from scratch, I would suggest attempting the given proofs, derivations and worked examples yourself as practice before looking up the solutions to ensure mastery of the content. This handbook is organized sequentially and no additional resources are required to understand the material outside the prerequisites. If you are unsure of certain concepts presented in this book, it would be useful to take a look at the appendices. There, I have written up additional notes and elaborations on things I found may be useful to the reader.

If at the end of this handbook you still feel bewildered by the perplexity that is quantum mechanics, rest in the comfort that even the best minds have struggled with attaining a true grasp of this aspect of reality.

"If quantum mechanics hasn't profoundly shocked you, you haven't understood it yet."

– Niels Bohr

Despite this, I am convinced that Quantum mechanics is indeed a beautiful theory of our universe, and I hope this book expresses that to you as much as it does me.

Note to the reader:

In this handbook, there are *worked examples* and *exercises* which are left to the reader. The exercises are given not so much as tricky problems, but to elucidate understanding of the material. Examples tend to be more instructive. All provided problems are a good gauge of understanding and are mostly non-trivial (worth solving). For easy navigation and clarity of presentation,

- Sharp edged black outlined white boxes contain definitions, laws and principles.

  Definition/Principle/Law ...

- Round edged gray outlined white boxes contain theorems.

  Theorem ...

- Round edged gray outlined light gray boxes contain proofs.

  Proof. ...

- Round edged dark gray outlined gray boxes contain important things to note.

  Note: ...

- Rounded edged unlined gray boxes contain worked examples and highlighted segments.

  Example ...

- Round edged black outlined white boxes contain chapter summaries.

  § **SUMMARY** §

- Sharp edged black outlined white double boxes contain exercises.

  Exercises

Acknowledgements

Just as I am passing it to you the readers, much of the content presented in this book was passed to me through the lessons and materials provided by my brilliant instructors. In particular, I would like to show appreciation to *Professors Dario Poletti, Jesse Thaler, Riccardo Comin, Barton Zwiebach, Isaac Chuang, Peter Shor* and *Cris Negron* in no particular order of merit. These professors have shown me and many others their immense dedication to teaching and advancements of work related to the contents of this book. Also, this handbook was funded under the *SUTD UROP funding scheme*, for which outstanding support and resources were provided for its completion.

R. R. W. Wang

Introduction:
Why Quantum Mechanics?

*Quantum Mechanics is a framework that describes the behaviour of matter and energy at very small scales and low temperatures. Despite popular belief, quantum mechanics is a '**deterministic theory of probabilities**', meaning that the mathematical formalisms that describe it are concrete, but it's experimental outcomes are subject to probability. As such, the mechanics of quantum phenomena can be used to develop new technological applications such as the model of quantum computation. This may sound paradoxical, but the chapters ahead will attempt to resolve this apparent contradiction. We embark on this instructive journey by first giving a partial introduction to the discovery of quantum mechanics, and shed light on a common household technology that actually utilizes it.*

§0.1 Breaking Classical Law

§0.1.1 Young's Experiment

In 1801, Thomas Young performed the famous *Young's double-slit experiment*. This experiment proved the that the **classical** theory of light being electromagnetic waves was true, exhibiting interference and superposition effects. The experiment was performed as follows.

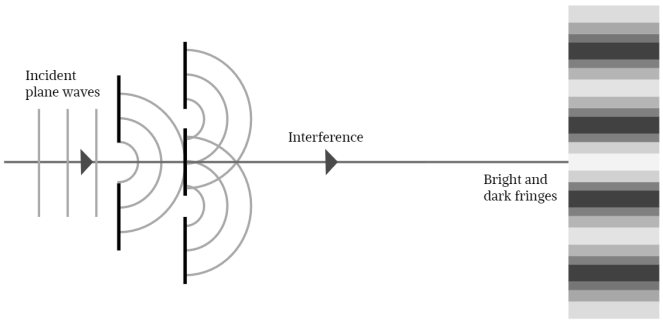


Figure 1: Young's Double Slit Experiment

As seen in figure 1, the set-up consists of 2 barriers having single and double apertures (slits).

A *plane wave* of light is then incident on the 2 consecutive barriers, passing through the single slit then the double slit. Upon transmission through each aperture, the wave-nature of light causes a phenomenon known as *diffraction*[1] to occur. As a result, the outgoing diffracted waves overlap, causing a superposition of wave amplitudes at different points in space. This causes an *interference pattern* of bright and dark fringes to appear on the screen.

Restatement: To emphasize once again, we **expect** this interference pattern classically due to the proposition that **light is described as continuous waves**.

§0.1.2 Young Revisited

In 1927, Clinton Davisson and Lester Germer re-performed the Young's double slit experiment. But instead of light, they had a beam of *electrons* fired at the apertures. At that time, it was believed that electrons were simply point particles with (*semi*)classical behaviour (following the *Bohr model*). This essentially meant that electrons were pretty much believed to be little charged hard spheres, so shooting a bunch of them through slits would have the equivalent result as throwing billiard balls through holes.

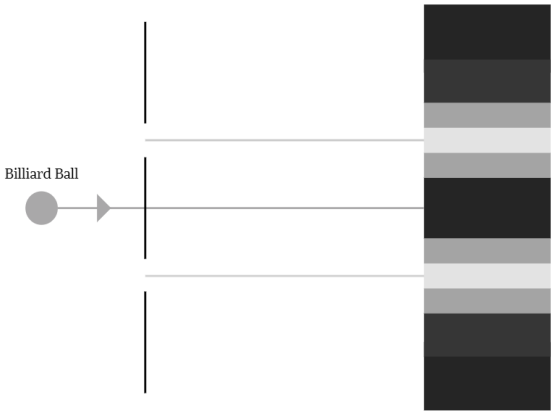


Figure 2: Billiard Ball Double Slit Experiment

The classical expectation of throwing billiard balls through 2 slits would produce a distribution shown in figure 2. In words, these are basically 2 approximately *Gaussian* peaks centered along the slit axes. **But** electrons, as it turns out, are not just your everyday classical objects. What was seen by Davisson and Germer was in fact an interference pattern on the screen, exactly as what Young did for light! Not just that, but they also observed that if a measurement of the electrons was made **at** the slits, the electrons would behave just as the billiard balls would!

Cutting a long story short, this bizarre result gave rise to the notion of *wave-particle duality*. Matter could no longer be thought of deterministic chunks which obeyed physics as these quantum pioneers previously knew it, but existed in this duality of wave and particle states. This

[1] **Definition 0.1.1.** Diffraction: *Diffraction is the phenomenon of waves, which when incident on an edge or aperture will diverge onto its geometrical shadow.*

revelation, along with the postulates by **Einstein** that light comes in discrete packets known as *photons*, and **de Broglie** that all matter possesses an intrinsic wavelength, breathed life into the following equations:

$$\boxed{E = h\nu, \quad p = \frac{h}{\lambda}} \tag{1}$$

Above, $h = 6.62 \times 10^{-34} Js$ is known as the *Planck's constant*, for which its origins are elaborated on in appendix A. It is very common that we instead use $\hbar = \frac{h}{2\pi}$, which is known as the *reduced Planck's constant*.

The equations in 1 essentially paved the way for the development of a quantum theory of our universe. Also, it is relevant to know that the term quantum comes from the idea of quantization (or discretization), which is how real quantum systems manifest themselves. (For a more comprehensive picture of the early beginnings of quantum mechanics, refer to appendix A.)

§0.2 Fighting Fire with Radiation

Fast forward to 1951, where the first ionization smoke detectors were sold. A smoke detector, as implied by its name, is used to detect the presence of smoke caused by fires. But how does it work? Ionization smoke detectors utilize a strange process known as *radioactive decay*. Essentially, there is a region between 2 charged plates where the air is irradiated by a radiation source as shown in figure 3.

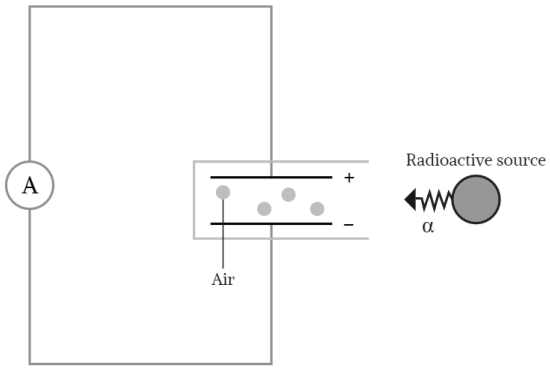


Figure 3: Simplified smoke detector

This causes the air to be ionized, allowing for a small current to flow between the plates. As such, when smoke permeates the air and space between the plates, the ionization of air decreases. This decrease causes a drop in the current, leading to the detection of smoke.

This in itself seems like a rather clear *qualitative* picture of how smoke detectors work as a device. However, can we model radioactive decay *quantitatively*? Understanding the mechanism for which radioactive decay occurs would allow us to make even more precise smoke detectors, along with many other devices. Just from this simple technology, it is evident that classical mechanics

is no longer a sufficient description of our universe, and the study of quantum mechanics is necessary. As such, let's dive into learning some of the fundamentals of quantum theory!

Note: In this handbook, we will be primarily learning what is known as *first quantization*, which is a semi-classical treatment of quantum mechanics where the environment is expressed with classical potentials.

§0.3 Classical Deviations

There are several key features of quantum mechanics which point toward the failure of classical mechanics as a comprehensive theory. These properties are fundamental in the study of quantum mechanics and is essential that we keep them in mind as we progress along.

§0.3.1 Linearity of Quantum Mechanics

Generally, theories in physics consist of 1) *Equations of Motion* and 2) *Dynamical Variables*. These can be broken up into 2 broad categories known as *Linear Theories* and *Non-Linear Theories*.

Linear Theories

Linear theories imply that we can express the equations governing these theories as linear operators acting on solutions of these equations.

Definition 0.3.1. Linearity: *Given an operator $\mathcal{L}$ and a set of solutions $\{u_i\}$, it is linear if it satisfies the following relations*

$$\mathcal{L}(au_i) = a\mathcal{L}(u_i), \quad for\, a \in \mathbb{C} \tag{2}$$

$$\mathcal{L}(u_i + u_j) = \mathcal{L}(u_i) + \mathcal{L}(u_j), \quad for\, i \neq j \tag{3}$$

An example of a linear theory would be *Maxwell's Theory of Electromagnetism*.

Non-Linear Theories

A non-linear by extension, would be theories that cannot be described by linear operators. This means that we **cannot** construct new solutions from arbitrary linear combinations of known solutions. Examples of such theories would be *Classical Mechanics* and *Einstein's Theory of General Relativity*. Non-linear theories tend to be mathematically intricate and highly complex, making solutions difficult to find.

Fortunately, the governing equation in quantum mechanics is built by linear operators, making it **in fact**, a linear theory! *(This however, in no way implies that QM is simple!)*

§0.3.2 Necessity of Complex Numbers

Since quantum dynamics is governed by the famed *Schrödinger's Equation* ($i\hbar\frac{\partial}{\partial t}\Psi = \hat{H}\Psi$), we see that the imaginary number on the left causes the equation to be **innately** complex. We will also later see that the operator $\hat{H}$ on the right is a *Hermitian Operator* with **real** components. Hence, this enforces the necessity of solutions to carry complex numbers within them. As a result, **all** solutions to the *Time-Dependent Schrödinger Equation* are complex.

§0.3.3 Loss of Determinism

This first became an issue when the quantization of light was discovered. The fact that light could be thought of as particles seemed to contradict the results of polarized light. Consider a polarizer aligned along the x-axis, and a ray of light polarized along an axis with an angle α from it passing through. We can describe the electric field associated to the light ray by,

$$\vec{E_\alpha} = E_0\cos(\alpha)\hat{x} + E_0\sin(\alpha)\hat{y} \tag{4}$$

By classical electromagnetic theory, the polarizer would then only pick out the $\hat{x}$ component of the electric field, $E_0\cos(\alpha)\hat{x}$. We also know that the energy, E of light is proportional to $|\vec{E}|^2$, this causes the emitted energy, $E_{emitted}$ to be reduced by a factor $\cos^2(\alpha)$.

However, knowing that the ray of light is also made up of identical photons, classical mechanics tells us that whatever happens to a photon under a set of initial conditions must also happen to all identical photons under the same initial conditions. How then, can only a fraction of the polarized photons enter the polarizer if this is true? This leads to the idea of the loss of determinism! This experiment showed that photons either passed through or they didn't, allowing us to only predict the **probabilities** of these photons passing through the polarizer.

§0.3.4 Superposition

As earlier mentioned, we have shown via experiment that matter does indeed possess a kind of wave-like nature. We will soon come to realize that these wave properties arise from *'Probability Waves'* used in describing *'states'* of a quantum system. These waves of probability do **not** possess all the standard properties of the conventional waves we are familiar with in classical wave mechanics, but **do** possess the property of *superposition*. It is now useful to formally define a *quantum states* to prevent any future misconceptions.

Definition 0.3.2. Quantum State: *A quantum state is defined as an element of a Hilbert space (F.2.14) $\mathcal{H}$, that carries information on the associated quantum system.*

Physicists often refer to quantum states as *vectors* or '*kets*', because we can think of them as having *matrix representations*.

§0.3.5 Entanglement (Qualitative Insight)

Entanglement shows up in quantum mechanics because of the loss of determinism in particle states. This is a weird and unique phenomena that occurs when we allow particles to interact with each other and become *correlated*. This causes the particles to form some kind of *'non-local bond'* between one another, causing them to affect each other **instantaneously** no matter how far apart you make them! Einstein dubbed this *'Spooky Action at a Distance'* and is in fact a very real property of *'quantum states'* as proven by experiment. Entanglement arises also because of superposition and is an essential property utilized for quantum computation.

§ **SUMMARY** §

In this introductory chapter...

- We looked at the Young's double slit experiment and how waves can undergo diffraction and interference.
- We saw the break down of classical mechanics when electrons displayed both wave and particle characteristics, leading to a wave-particle duality.
- We were told that ionization smoke detectors actually utilize radioactive decay (a quantum mechanical process) to function, something we will get to quantitatively study.
- We learned that quantum mechanics has several key features, namely:
  - Linearity
  - Necessity of complex numbers
  - Superposition
  - Entanglement

  Once again, do ensure that you keep these in your back pocket as we traverse through the quantum terrain of this book.

Exercises

1. Given that visible light has a wavelength of $\sim$ 500nm, find the energy and momentum of a photon using the equations in (1).
2. Find the wavelength of a non-relativistic electron moving with velocity 10^5 m/s.
3. Consider the operators $\mathcal{A}$ and $\mathcal{B}$ where they perform the following operations on a continuous function $f(x)$.

$$\begin{aligned} \mathcal{A} &: f(x) \mapsto f'(x) + xf(x) \\ \mathcal{B} &: f(x) \mapsto f(x^2) + 3 \end{aligned} \tag{5}$$

   Are the operators $\mathcal{A}$ and $\mathcal{B}$ linear? Explain why or why not.
4. Write the following complex numbers as $re^{i\theta}$ where r and θ are strictly real.
   (a) $2 + i\sqrt{3}$
   (b) $(\sqrt{5} + i\sqrt{2})(1 + i\sqrt{7})$
   (c) $(\sqrt{3} + i8)/(\sqrt{2} - i5)$
5. Prove *Euler's identity*, $re^{i\theta} = r(\cos\theta + i\sin\theta)$.

Part I

Understanding the Substrate

Chapter 1

A Dive into Superposition

Since superposition is a fundamental and recurring concept in quantum mechanics, it will be the first quantum morsel on the menu. To illustrate and understand this concept, we turn to interferometry. Interferometry is a class of experimental techniques that superimposes electromagnetic waves and exploits the properties of interference to gather information. Interferometry is a widely used experimental technique throughout all of physics, being the platform on which many insightful theories such as Einstein's Theory of Special Relativity have been realized. For what we intend to learn, we will look at one specific example of interferometry as performed by Ernst Mach and Ludwig Zehnder.

§1.1 Mach-Zehnder Interferometry

Consider a set-up of a laser, beam splitters, mirrors and detectors as shown below.

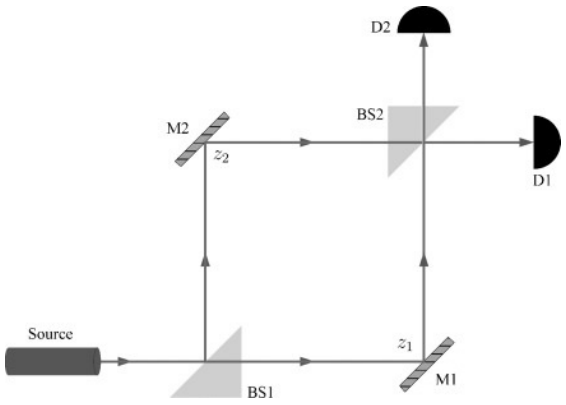


Figure 1.1: Mach-Zehnder Interferometer

As suggested in figure 1.1, a source emits a photon that is split (able to 'choose' a path) by beam splitter 1 (BS1) and 'recombined' at beam splitter 2 (BS2). The resulting outgoing photon is then detected by the either detector, D1 or D2. It turns out that we can model this set-up with a

2-dimensional Hilbert space representation. We define a 2-dimensional basis $\{|u\rangle, |l\rangle\}$, where $|u\rangle$ denotes the state representing the photon occupying the upper beam and $|l\rangle$ denotes the photon occupying the lower beam.

Before we fully formalize these mathematical objects, we have to look at the fact that these states are carriers of **'probabilistic information'**, which for now will just be an assertion. A key feature of *probability theory* is that the sum over probabilities of all possible outcomes must equate to 1. This implies that there must be some *invariant* quantity of the states that is preserved and equal to unity. This quantity is in fact the norm-squared of the state ($\||\psi\rangle\|^2 = 1$) and it will become clear why in the later chapters. For now, we will just take this to be fact and also impose the condition that any operation that maps a quantum state to another quantum state must preserve its norm.

§1.1.1 Matrix Representation

To perform mathematical operations on these states, we can construct a *representation* of these states with vectors of a vector space.

$$|u\rangle = \begin{bmatrix}1\\0\end{bmatrix}, \; |l\rangle = \begin{bmatrix}0\\1\end{bmatrix} \tag{1.1}$$

Because this system is simply a *2-level system*, the representations appear as these elegant finite, 2-dimensional number arrays. This means that an arbitrary state in this Hilbert space is written as,

$$|\psi\rangle = \alpha \begin{bmatrix}1\\0\end{bmatrix} + \beta \begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}\alpha\\\beta\end{bmatrix}, \; \alpha, \beta \in \mathbb{C} \tag{1.2}$$

Note: Given any quantum system, we can always write the state of that system with a vector representation. However, if the state is described by a **continuous** variable (e.g. x position), then the state vector would be an **infinite** dimensional array.

Now, we shall model the action of the beam splitters on input states (light beams). It turns out that these are simply linear transformations on the vectors $|\psi\rangle$ and thus, we can construct this using a 2×2 *matrix representation.*

Definition 1.1.1. Matrix Representation: *Given a linear transformation $T : V \to U$ and the bases for V and U being $B_V = \{\vec{v}_j\}_{j=1}^{|V|}$ and $B_U = \{\vec{u}_j\}_{j=1}^{|U|}$ respectively, then we have:*

$$T(\vec{v}_j) = \sum_i a_{ij}\vec{w}_i \tag{1.3}$$

where a_{ij} are the entries of the matrix representation of T with respect to B_V and B_U.

Knowing this, we also have that there are 2 possible input basis states that can enter the beam splitters, and 2 unique outcomes for each of these 2 inputs. This means that we require 4 numbers to fully characterize the action of a beam splitter on an arbitrary input state.

$$BS = \begin{bmatrix}a & b\\c & d\end{bmatrix} \tag{1.4}$$

With the condition,

$$\|(BS)\,|\psi\rangle\|^2 = \left\| \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \right\|^2 = 1 \tag{1.5}$$

$$\Rightarrow ((BS)\,|\psi\rangle)^\dagger (BS)\,|\psi\rangle = (|\psi\rangle)^\dagger (BS)^\dagger (BS)\,|\psi\rangle = 1$$

$$\Rightarrow \boxed{(BS)^\dagger (BS) = \mathbb{I}} \tag{1.6}$$

Property (2.5) is known as *Unitarity* and allows $\||\psi\rangle\|^2$ to be invariant as unity. We have now built-up sufficient formalism to generate valid mathematical models of real physical phenomena.

Example

Consider a *'balanced beam splitter'* defined by, $|a|^2 = |b|^2 = |c|^2 = |d|^2 = \frac{1}{2}$. In order to adhere to condition (2.4), we are allowed to construct BS1 and BS2 as such.

$$BS1 = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix},\ BS2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \tag{1.7}$$

To check that BS1 and BS2 indeed adhere to condition (2.4), consider an arbitrary input state of norm 1.

$$\Rightarrow \||\psi\rangle\|^2 = \left\| \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \right\|^2 = |\alpha|^2 + |\beta|^2 = 1 \tag{1.8}$$

Applying operators BS1 and BS2, we get

$$\|BS1\,|\psi\rangle\|^2 = \left\| \frac{1}{\sqrt{2}} \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \right\|^2 = \left\| \begin{bmatrix} \frac{\beta-\alpha}{\sqrt{2}} \\ \frac{\beta+\alpha}{\sqrt{2}} \end{bmatrix} \right\|^2 = |\frac{\beta-\alpha}{\sqrt{2}}|^2 + |\frac{\beta+\alpha}{\sqrt{2}}|^2 = 1 \tag{1.9}$$

$$\|BS2\,|\psi\rangle\|^2 = \left\| \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \right\|^2 = \left\| \begin{bmatrix} \frac{\alpha+\beta}{\sqrt{2}} \\ \frac{\alpha-\beta}{\sqrt{2}} \end{bmatrix} \right\|^2 = |\frac{\alpha+\beta}{\sqrt{2}}|^2 + |\frac{\alpha-\beta}{\sqrt{2}}|^2 = 1 \tag{1.10}$$

Indeed showing that these beam splitter operators do map the initial quantum state to a new quantum state of norm 1.

Note: Unitarity is an important property of physical operations done on states which evolve them in time (which we refer to as *unitary time evolution*). In fact, any physical operation on a closed system **must** be unitary.

From this (relatively) simple set-up, we have actually implemented a single *qubit* quantum computer! We will revisit quantum computers and quantum computation in greater detail later in the book.

Exercise

For an arbitrary state $|\psi\rangle = \{\alpha, \beta\}^T$, the probability to be in the 'lower' state is $\mathbb{P}(|l\rangle) = |\alpha|^2$ and the probability to be in the 'upper' state is $\mathbb{P}(|u\rangle) = |\beta|^2$. Given the beam splitters presented in the example above,

(a) find the probabilities of detection for D1 and D2 if no amendments are made to the set-up.

(b) find the probabilities of detection for D1 and D2 if a blockage is added to the lower arm after BS1.

§1.2 Elitzur-Vaidman Bombs

In 1993, Avshalom Elitzur and Lev Vaidman conceived a thought experiment that could probabilistically predict whether any *Elitzur-Vaidman bomb* was working. This utilize the properties of quantum mechanics and was notable because any classical approach would fail with 100% certainty. An Elitzur-Vaidman bomb is a bomb with a photo-detector used as its trigger. If the bomb is working, a single photon incident on the photo-detector would cause the bomb to go off. Else, the photon would pass through unaffected. The experimental set-up is as follows.

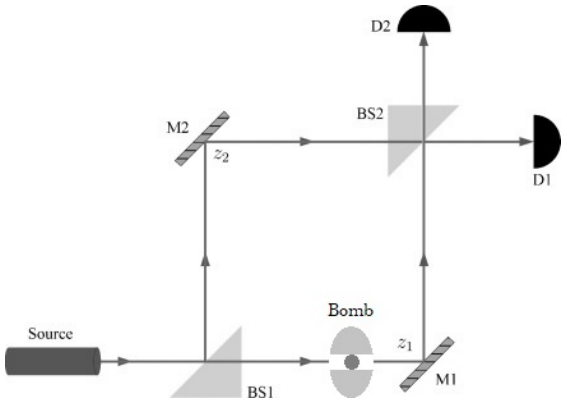


Figure 1.2: Elizur-Vaidman Bomb Detection Set-Up

Let's work through what happens if we use the balanced beam splitter used in the example above ($BS1$). Consider an input beam entering from the upper channel $|u\rangle$. After passing through the first beam splitter,

$$(BS1)\,|u\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}-1 & 1\\ 1 & 1\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix}-1\\1\end{bmatrix} \tag{1.11}$$

From here, let us first assume that the bomb is **not** working. If so, the interferometry experiment would occur as though there were no bomb in the first place. Hence after the result in (1.11),

the split beam continues to pass through BS2.

$$(BS2)(BS1)\,|u\rangle = \frac{1}{2}\begin{bmatrix}-1 & 1\\ 1 & 1\end{bmatrix}\begin{bmatrix}-1\\ 1\end{bmatrix} = \begin{bmatrix}1\\ 0\end{bmatrix} \tag{1.12}$$

The result of a defective bomb is that we will **always** get a reading from D2. Now let us perform the analysis once more with a working bomb. Since the bomb is only present after BS1, the result from (1.11) is exactly the same. This is where things get interesting. Notice that the probabilities of being either an upper or lower beam after BS1 are equal.

$$\mathbb{P}(|u\rangle) = \left|\frac{-1}{\sqrt{2}}\right|^2 = \frac{1}{2}\,, \quad \mathbb{P}(|l\rangle) = \left|\frac{1}{\sqrt{2}}\right|^2 = \frac{1}{2}$$
$$\Rightarrow \quad \mathbb{P}(|u\rangle) = \mathbb{P}(|l\rangle) = \frac{1}{2}$$

Evidently if the beam does in fact enter the lower path, the bomb detonates and the experiment is undoubtedly over (not too great a result). So let us consider instead the case where the beam chooses to enter the upper path. In this scenario, all the probability collapses onto the upper beam hence the state entering BS2 is simply $|u\rangle$.

$$(BS2)\,|u\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}-1 & 1\\ 1 & 1\end{bmatrix}\begin{bmatrix}1\\ 0\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix}-1\\ 1\end{bmatrix} \tag{1.13}$$

Amazingly, we retrieve the same result as in (1.11) with an equal probability for the beams to be detected by D1 and D2! A summary of the results is given in the table below.

Detector outcomes	$\mathbb{P}_{\text{defective}}$	$\mathbb{P}_{\text{working}}$
Photon enters D1	1	1/4
Photon enters D2	0	1/4
Bomb is detonated	0	1/2

Table 1.1: Elitzur-Vaidman Bomb Detection Outcomes

Note that the probabilities to be detected by D1 and D2 for a working bomb set-up are 1/4 and not 1/2 because we had to multiply the initial 1/2 probability of being in the upper beam. In conclusion, we are able to detect a working bomb without detonating it with a 1/4 probability.

§ **SUMMARY** §

In this chapter...

- We were introduced to quantum superposition with Mach-Zehnder interferometry.
- We saw how we could represent quantum states as vectors and have matrix representations for operations on those states.
- We saw that quantum states must necessarily be unit normalized ($\|\psi\|^2 = 1$) and physical operations on those states are required to satisfy unitarity ($U^\dagger U = \mathbb{I}$).
- We saw that we can retrieve the probabilities of being in each state by taking the absolute squares of the corresponding state entries.
- We looked also at how defective Elitzur-Vaidman bombs could be detected without detonation with the help of quantum mechanics.

Exercises

1. Let us now consider the case where the beam splitters for our Mach-Zehnder interferometer do not reflect and transmit photons with equal probability, but instead have reflection and transmission coefficients (R and T respectively). Construct a 2×2 **unitary** matrix that models this with entries being functions of R and T. Use the convention that all entries are real and note that $R + T = 1$.

2. A defective bomb is now inserted as in figure 1.2. Recompute the probabilities of detection for each photon detector, D1 and D2.

3. Now let's say you have a large sample of Elitzur-Vaidman bombs to test for defects. In terms of R and T, what is fraction the of **operational** bombs that can be successfully tested without detonation?

4. Consider an additional apparatus called the phase shifter. It's matrix representation is given by

$$S = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix} \tag{1.14}$$

   We insert this phase shifter into the lower arm of the Mach-Zehnder interferometer after BS1 before a working Elitzur-Vaidman bomb. Compute the new detection probabilities of D1 and D2.

5. Can you think of a scheme/modification such that we can further increase the detection probability of a live Eiltzur-Vaidman bomb? (Refer to appendix B.)

Chapter 2

Quantum Promotions

In quantum mechanics, the notion of physical quantities gets a little fuzzy. There is ***uncertainty*** *in the system that follows not from poor apparatus or human error, but intrinsic properties of nature. Because of this, we can no longer express the evolution in time of a system with definite dynamical variables and equations of motion like we did classically. We instead have to turn to a different mathematical framework.*

In this chapter, we will work through building up this framework (at a highly accelerated pace) through the language of ordinary differential equations and learn how to use it. First, we go back to address the duality between matter possessing both wave and particle-like properties.

§2.1 Matter Waves

As earlier discussed (0.1.2), matter at very small scales exhibit wave-like properties (diffraction and interference). The mathematical answer to why this is is actually that matter exists as *probabilistic waves*. These waves of probability have their own unique dynamics determined by the **Schrödinger's equation** (More information on wave mechanics is given in appendix C).

> **Note:** The most common physical interpretation for this is known as the *Copenhagen interpretation*. This says that the non-deterministic nature of reality is innate, and observation forces the system to *collapse* into a definite state.

Because of this, we no longer look to classical dynamical variables $\{x(t), \dot{x}(t)\}$ to determine the state of a system, but a *wave function* $\Psi(x,t)$ (Note that as a starting point, we are only considering **single particle** systems). Working with a wave function makes extracting information about the system a little less direct, but is something you can build an intuition in doing. With the notion that Ψ is associated to probabilities, we know from probability theory that the integral over all space of some function of Ψ has to equate to unity.

$$\int_{-\infty}^{\infty} f(\Psi(x,t))dx = 1 \tag{2.1}$$

There seems to be no reason to for any restriction on the value of the wavefunction ($\Psi(x,t) \in \mathbb{C}$). This means that $\Psi(x,t)$ could be a purely negative valued function, which would **not** satisfy condition 2.1. So a good quantity to look at would be $|\Psi(x,t)|^2$. Sure enough, this quantity turns out to be the *Probability Density* of the wave function.

Definition 2.1.1. Probability Density: *The probability density $\rho(\vec{x},t)$, of a wavefunction is the probability per unit volume of locating a particle at some position.*

$$\rho(\vec{x},t) = |\Psi(\vec{x},t)|^2 = \Psi^*(\vec{x},t)\Psi(\vec{x},t) \tag{2.2}$$

The definition above considers general systems in possibly more than 1-dimension ($\vec{x}$ vs x). However, we will only work in 1-dimension for the time being. Combining (2.1) and (2.2) at some arbitrary time $t = t_0$ gives us,

$$\int_{-\infty}^{\infty} dx|\Psi(x,t_0)|^2 = 1 \tag{2.3}$$

This is known as the *Normalization Condition* of a wave function.

Note: Notice here how this nicely mirrors the unit-norm condition imposed on quantum states in the Mach-Zehnder interferometry experiment (1.5).

This means that if $\int_{-\infty}^{\infty} dx|\Psi(x,t_0)|^2 = C \neq 1$, the mathematically coherent version of the wave function needs to be $\frac{1}{\sqrt{C}}\Psi(x,t_0)$ (where an **overall** complex phase does **not** make a difference to the physics).

§2.2 Operators

We will now see that physically observable quantities will be 'promoted' to what are known as *operators* in quantum mechanics. First consider the simplest classical wave solution, a *1-dimensional plane wave.*

Definition 2.2.1. 1-Dimensional Plane Wave: *A 1D plane wave travelling in the positive x-direction with parameters $\{k,\omega\}$ (k being the wave vector and ω being the angular frequency), has the form*

$$\Psi(x,t) = e^{i(kx-\omega t)} \tag{2.4}$$

Now, consider a derivative with respect to x on this plane wave.

$$\begin{aligned} & \frac{\partial}{\partial x}\Psi(x,t) = ike^{i(kx-\omega t)} \\ \Rightarrow \quad & -i\hbar\frac{\partial}{\partial x}\Psi(x,t) = \hbar ke^{i(kx-\omega t)} \\ \Rightarrow \quad & \boxed{-i\hbar\frac{\partial}{\partial x}\Psi(x,t) = p\Psi(x,t)} \end{aligned} \tag{2.5}$$

(We used the fact that $p = \hbar k$ in the above derivation, which was proposed by Max Planck.) We have found something interesting here. It is as though acting on this wave function with a '*differential operator*' has pulled out the **momentum** of this wave function. As such we present the following definition.

Definition 2.2.2. Momentum Operator: *The momentum operator (denoted with a hat) which acts on a wave function described in the position basis is defined as,*

$$\hat{p} = -i\hbar\frac{\partial}{\partial x} \tag{2.6}$$

Remember that in quantum mechanics, we work with Hilbert spaces (appendix F.2.14). Elements of these Hilbert spaces are known as quantum states and thus any quantum state that when acted on by an operator remains unchanged up to a scale factor is known as an *eigenstate* (appendix F.2.13). The scale factor is called the associated *eigenvalue*. Thus, we see that **1D plane waves are *momentum eigenstates***! It is important to note that momentum eigenstates are *non-normalizable* states and hence are **not** physically realizable. However, the linearity of quantum mechanics allows us to use these eigenstates to construct physically allowed states known as *wave packets* (C.3) via linear combination.

We can now use what we have learned to further develop more of such operators. We know from classical mechanics that the kinetic energy of a particle is given by $E = \frac{p^2}{2m}$. Using this, we extend our classical intuition and define the following.

Definition 2.2.3. Kinetic Energy Operator: *The kinetic energy operator which acts on a wave function described in the position basis is defined as,*

$$\hat{E} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \tag{2.7}$$

To double check that our intuition has not failed us, we try applying this operator on the 1D plane wave function.

$$\begin{aligned} \hat{E}\Psi(x,t) &= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}e^{i(kx-\omega t)} = -\frac{\hbar^2}{2m}(-k^2)e^{i(kx-\omega t)} = \frac{p^2}{2m}\Psi(x,t) \\ \Rightarrow\ \hat{E}\Psi(x,t) &= E\Psi(x,t) \end{aligned} \tag{2.8}$$

Thus this indeed works out! Seeing that the wave function is both a function of space **and time**, what if we instead take a time derivative on $\Psi(x,t)$?

$$\begin{aligned} &\frac{\partial}{\partial t}\Psi(x,t) = -i\omega e^{i(kx-\omega t)} \\ \Rightarrow\ &i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hbar\omega e^{i(kx-\omega t)} \\ \Rightarrow\ &\boxed{i\hbar\frac{\partial}{\partial t}\Psi(x,t) = E\Psi(x,t)} \end{aligned} \tag{2.9}$$

(We used the fact that $E = \hbar\omega$ from 1.) Strangely enough, the time derivative operator also extracts the wave energy just as the kinetic energy operator does. Thus combining the 2 results from (2.2.3) and (2.9), we effectively derived the *Free Particle Schrödinger Equation*.

$$\boxed{i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t)} \tag{2.10}$$

Note that partial differentials acting on continuous wave functions are ***linear*** *endomorphisms* on the Hilbert space. This implies that equation (2.10) holds for $\Psi(x,t)$ being wave packets. But what if the particle in question is not 'free'? Meaning that there is a non-zero potential that interacts with the particle ($V(x,t) \neq 0$). From equation (4.8) and by *analytic continuity*, we can extend the kinetic energy operator into what is known as the *Hamiltonian*.

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hat{E}\Psi(x,t) \;\rightarrow\; i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hat{H}\Psi(x,t) \tag{2.11}$$

Taking from classical *Hamiltonian Mechanics*, we know that the Hamiltonian of a non-dissipative system is always conserved. As such, we will use the Hamiltonian in quantum mechanics as well, where we promote the conjugate variables to operators.

$$\boxed{\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)} \tag{2.12}$$

With this *quantum Hamiltonian*, we arrive at the **full** *Time-Dependent Schrödinger Equation*.

$$\boxed{i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \Big(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\Big)\Psi(x,t)} \tag{2.13}$$

Which by extension, we can generalize to 3 dimensions.

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{x},t) = \Big(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})\Big)\Psi(\vec{x},t) \tag{2.14}$$

Finally, we introduce the *position operator*. Because we have been working in the *'position basis'*, the position operator seems trivial but is useful to ensure a full picture of important operators when working with different bases.

Definition 2.2.4. Position Operator: *The position operator which acts on a wave function described in the position basis is defined as,*

$$\hat{x} = x \tag{2.15}$$

In quantum mechanics, these operators that represent physically measurable quantities are known as *observables*.

Note: A special property of obsevables is that they are always *Hermitian* (will be further elaborated on).

§2.3 Commutators

Having introduced operators that act on the quantum states of a given Hilbert space, we will now equip the $\mathbb{C}$-vector space of operators acting on the Hilbert space ($\mathscr{L}(\mathcal{H})$, appendix F.2.1) with an additional structure called the *commutator*. This makes the $\mathbb{C}$-vector space into a *Lie algebra* (appendix F.2.16).

Definition 2.3.1. Commutator: *Given 2 operators $\hat{A}$ and $\hat{B}$, the commutator of $\hat{A}$ with $\hat{B}$ is defined as*

$$\Big[\hat{A},\hat{B}\Big] = \hat{A}\hat{B} - \hat{B}\hat{A} \tag{2.16}$$

We will continue to look at and utilize commutator relations throughout this book so it is important to get accustomed to the use of them. Below is a list of useful commutator identities.

1. $\Big[\hat{A},\hat{A}\Big] = 0$
2. $\Big[\hat{A},\hat{B}\Big] = -\Big[\hat{B},\hat{A}\Big]$
3. $\Big[\hat{A},\hat{B}\pm\hat{C}\Big] = \Big[\hat{A},\hat{B}\Big] \pm \Big[\hat{A},\hat{C}\Big]$
4. $\Big[\hat{A}\hat{B},\hat{C}\Big] = \hat{A}\Big[\hat{B},\hat{C}\Big] + \Big[\hat{A},\hat{C}\Big]\hat{B}$
5. $\Big[\hat{A},\hat{B}\hat{C}\Big] = \hat{B}\Big[\hat{A},\hat{C}\Big] + \Big[\hat{A},\hat{B}\Big]\hat{C}$
6. $\Big[\hat{A},\Big[\hat{B},\hat{C}\Big]\Big] + \Big[\hat{C},\Big[\hat{A},\hat{B}\Big]\Big] + \Big[\hat{B},\Big[\hat{C},\hat{A}\Big]\Big] = 0$

The last identity is known as the *Jacobi identity* and is necessary for Lie algebras.

Example

Consider the commutator between the $\hat{x}$ operator and $\hat{p}$ operators. To compute this in the representations we have presented them in thus far, we require that the commutator act on some test function $\psi(x)$.

$$\begin{aligned}
[\hat{x},\hat{p}]\psi(x) &= \left[x, i\hbar\frac{\partial}{\partial x}\right]\psi(x) = i\hbar\left[x,\frac{\partial}{\partial x}\right]\psi(x) \\
&= i\hbar\Big(x\frac{\partial}{\partial x}\psi(x) - \frac{\partial}{\partial x}\big(x\psi(x)\big)\Big) = i\hbar\Big(x\frac{\partial}{\partial x}\psi(x) - \psi(x) - x\frac{\partial}{\partial x}\psi(x)\Big) \\
&\Rightarrow [\hat{x},\hat{p}]\psi(x) = i\hbar\psi(x) \\
&\Rightarrow \boxed{[\hat{x},\hat{p}] = i\hbar}
\end{aligned}$$

It would be good for you to remember this relation as it will come in handy as we move along.

§ **SUMMARY** §

In this chapter...

- We looked at a new mathematical object known as the *wave function* $\Psi(x,t)$, from which we can extract probabilistic information about the quantum system.
- We learned that physically measurable quantities are now encoded in *operators* known as *observables* which can act on wave functions.
- 3 operators have been formally introduced with the following representations in *position space*,

$$\begin{cases} \hat{x} = x \\ \hat{p} = -i\hbar\frac{\partial}{\partial x} \\ \hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x) \end{cases} \tag{2.17}$$

- We learned about commutators as a binary operation on operators $\left[\hat{A},\hat{B}\right] = \hat{C}$, and saw some common commutator identities.

Exercises

1. Given some function $\Psi(x,t)$ that spreads over all space and solves the Schrödinger equation, what boundary condition is necessary for the function to be normalizable (integrates to a finite value)?
2. Normalize the following functions (i.e. find $\mathcal{N}$),
   - $\psi(x) = \mathcal{N}\exp\left(-\frac{x^2}{2\sigma}\right)$ where $\sigma \in \mathbb{R}$.
   - $\psi(x) = \mathcal{N}\sin\left(\frac{n\pi x}{L}\right), \quad |x| \leq L, \quad (n \in \mathbb{Z})$
   - $\psi(x) = \begin{cases} \mathcal{N}\sinh(\kappa x) & , -\frac{L}{2} < x < 0 \\ -\mathcal{N}\sinh\left(\kappa(x-L)\right) & , 0 \leq x < \frac{L}{2} \end{cases}$
3. Consider a wave function $\Psi(x,t)$. If we are concerned with the wave function at some fixed time $t = t_0$, we can drop the time dependence to give $\Psi(x)$. Prove that we can get a momentum space wave function $\Phi(p)$ from the position space wave function $\Psi(x)$ via a Fourier transform. *(Hint: recall the relation $p = \hbar k$.)*
4. Consider a set of wave functions $\{\psi_1(x), \psi_2(x), ..., \psi_N(x)\}$, all of which solve the time-dependent Schrödinger equation (2.13). Prove that an arbitrary linear combination of these wave functions also solves the time-dependent Schrödinger equation.
5. Compute the following commutators.
   $\left[\hat{x},\hat{H}\right], \left[\hat{p},\hat{H}\right], \left[\hat{x}\hat{p},\hat{H}\right]$
   (Hint: $[\hat{x}, f(\hat{x})] = [\hat{p}, g(\hat{p})] = 0$ for arbitrary functions f, g.)

Chapter 3

Building Tools for Measurement

In this chapter, we will be addressing the notion of measurements and how it fits into the mathematical picture of quantum theory. At this juncture, it is essential to introduce several important mathematical tools and address key properties of operators associated to observables. These may vary in appearance depending on the representation of the theory we choose, but rarely is there any ambiguity once we understand the underlying concepts.

§3.1 Inner Products

We first define an inner product between 2 continuous functions in an infinite-dimensional complex vector space. This makes the vector space a Hilbert space.

Definition 3.1.1. Continuous Function Inner Product: *For 2 continuous, complex functions $f(x)$ and $g(x)$, the inner product of $f(x)$ with $g(x)$ is defined as,*

$$\langle f(x), g(x)\rangle = \int_{-\infty}^{\infty} dx f^*(x) g(x) \tag{3.1}$$

The inner product of 2 wave functions tell us their *overlap*, or colloquially speaking, how much 2 states have in common. If the states are exactly the same, then their overlap is 1 by the normalization condition. Hence we have the inequality

$$0 \leq |\langle \psi, \phi\rangle| \leq 1 \tag{3.2}$$

where ψ and ϕ are normalized wave functions.

Example

Consider the functions $f(x) = \exp\left(-\frac{x^2}{2}\right)$ and $g(x) = x^2$. The inner product of $f(x)$ with $g(x)$ would thus be

$$\begin{aligned}\langle f(x), g(x)\rangle &= \int_{-\infty}^{\infty} dx f^*(x) g(x) \\ &= \int_{-\infty}^{\infty} x^2 \exp\left(-\frac{x^2}{2}\right) dx \\ &= \sqrt{2\pi}\end{aligned}$$

Note here that both $f(x)$ and $g(x)$ are real, hence the order of which we arrange the functions in the inner product is of little significance ($\langle f(x), g(x)\rangle = \langle g(x), f(x)\rangle$).

§3.2 Expectation Values

Quantum mechanics relies heavily on probability theory for mathematical structure. As such, we can use this to our advantage and adopt probability tools to help us better grasp quantum systems. *Expectation values* or simply *expectation*, gives us a weighted average of all the possible values of an observable upon *measurement*.

Definition 3.2.1. Expectation Value: *Given an operator $\hat{Q}$ and an arbitrary quantum state Ψ, the expectation value of that operator on Ψ is defined as*

$$\langle \hat{Q} \rangle_\Psi = \langle \Psi, \hat{Q}\Psi \rangle = \int_{-\infty}^{+\infty} dx \left(\Psi^* \hat{Q} \Psi\right) \tag{3.3}$$

Note that expectations can be taken on any operator (not just observables), so in general,

$$\langle \hat{Q} \rangle_\Psi \in \mathbb{C} \tag{3.4}$$

where Q is some arbitrary linear operator.

Example

Given the wave function $\psi(x) = \exp\left(-\frac{x^2}{2\sigma}\right)$ and operator $\hat{p} = -i\hbar\frac{\partial}{\partial x}$, the expectation of $\hat{p}$ on $\psi(x)$ is given by

$$\begin{aligned}\langle\hat{p}\rangle_\psi &= \int_{-\infty}^{\infty} \psi^*(x)\hat{p}\psi(x)dx \\ &= -i\hbar\int_{-\infty}^{\infty} \psi^*(x)\frac{\partial}{\partial x}\psi(x)dx \\ &= i\hbar\int_{-\infty}^{\infty}\left(\frac{x}{\sigma}\right)\exp\left(-\frac{x^2}{\sigma}\right) = 0\end{aligned}$$

A fast means of arriving at the result is noticing that $\psi(x)$ is an even function whereas x is odd. Hence their product would be odd and the integral over all space would vanish. Because of their vanishing inner product, $\psi(x)$ and x are called *orthogonal* (F.2.15).

§3.3 Uncertainty

Another commonly employed tool in classical probability theory is known as the *standard deviation*, usually denoted as σ. In quantum mechanics, we take the standard deviation of an observable with respect to a given quantum state as the *uncertainty*. For 2 observables $\hat{A}$ and $\hat{B}$ which do **not** commute ($\left[\hat{A},\hat{B}\right] \neq 0$), there is an uncertainty when measuring the 2 quantities simultaneously. This is known as the *Heisenberg uncertainty principle*. The statement of this principle is as follows.

Heisenberg Uncertainty Principle

Given 2 observables $\hat{A}$ and $\hat{B}$ that do not commute, there will be an uncertainty relation when measuring the 2 observables on a quantum state ψ given by

$$\sigma_{\hat{A}}^2\sigma_{\hat{B}}^2 \geq \left|\frac{1}{2i}\langle\psi,\left[\hat{A},\hat{B}\right]\psi\rangle\right|^2 \tag{3.5}$$

where σ is the uncertainty of an observable defined by $\sigma_{\hat{A}} = \sqrt{\langle\hat{A}^2\rangle_\psi - \langle\hat{A}\rangle_\psi^2}$.

Example

Consider the 2 observables $\hat{x}$ and $\hat{p}$. We have already seen that their commutation relation is given by $[\hat{x},\hat{p}] = i\hbar$. This means that there is an uncertainty relation between these 2 variables which can be computed as follows.

$$\begin{aligned}\sigma_{\hat{x}}^2\sigma_{\hat{p}}^2 &\geq \left|\frac{1}{2i}\langle\psi,[\hat{x},\hat{p}]\psi\rangle\right|^2 \\ &\geq \left|\frac{1}{2i}\langle\psi,i\hbar\psi\rangle\right|^2 = \frac{\hbar^2}{4}\end{aligned} \tag{3.6}$$

This is the widely known position-momentum uncertainty relation and is more commonly

written as $\triangle\hat{x} \triangle \hat{p} \geq \hbar/2$.

§3.4 Hermiticity and Diagonalization

Hermiticity is a property of all observables and ensures that measured values associated to *Hermitian observables* are guaranteed to be *real*. This is essential in making quantum mechanics a valid theory of nature.

Definition 3.4.1. Hermiticity: *Given an operator A acting on a Hilbert space $\mathcal{H}$, the operator is said to be* ***Hermitian*** *if*

$$\langle \Psi, A\Psi \rangle = \langle A\Psi, \Psi \rangle \tag{3.7}$$

for Ψ being some arbitrary element of the Hilbert space.

At this juncture, it is appropriate to introduce the notion of *diagonlizing* an operator. This will allow us to move between different *'spaces'* (or bases) and tells us the possible states a system can be in.

Theorem 3.4.1. *A linear operator Q on a Hilbert space $\mathcal{H}$ is* ***diagonalizable*** *iff there exists an ordered set of eigenstates $\{\psi_i\}$ with corresponding eigenvalues $\{\alpha_i\}$ such that these eigenstates* ***span*** *the Hilbert space.*

To make use of this theorem and understand its utility, we require the following theorems on Hermitian operators. The proofs are also presented below.

Theorem 3.4.2. *All the Eigenvalues of a Hermitian operator $\hat{A}$, are real ($\mathbb{R}$).*

Proof. Consider an eigenstate (Φ_a) of $\hat{A}$ with Eigenvalue a. Then since $\hat{A}$ is Hermitian,

$$\begin{aligned}
&\Rightarrow (\Phi_a, \hat{A}\Phi_a) = (\hat{A}\Phi_a, \Phi_a) \\
&\Rightarrow (\Phi_a, a\Phi_a) = (a\Phi_a, \Phi_a) \\
&\Rightarrow a(\Phi_a, \Phi_a) = a^*(\Phi_a, \Phi_a) \\
&\Rightarrow a^* = a \\
&\therefore a \in \mathbb{R}
\end{aligned}$$

□

Hence, if all observables can be described by Hermitian operators, we have resolved the issue of possibly having complex measurement values! Another useful property of Hermitian operators we will come to use time and time again is the *orthogonality* of its *non-degenerate* eigenstates.

Theorem 3.4.3. *The eigenstates of a Hermitian operator form an orthogonal set of states. (This is in fact an orthogonal basis that spans the observables' state space.)*

Proof. Consider 2 different eigenstates Φ_a and Φ_b, of $\hat{A}$ with different eigenvalues a and b respectively. Then using the Hermiticity of $\hat{A}$,

$$\begin{aligned}
&\Rightarrow (\Phi_a, \hat{A}\Phi_b) = (\hat{A}\Phi_a, \Phi_b) \\
&\Rightarrow (\Phi_a, b\Phi_b) = (a\Phi_a, \Phi_b) \\
&\Rightarrow b(\Phi_a, \Phi_b) = a(\Phi_a, \Phi_b) \\
&\Rightarrow (b-a)(\Phi_a, \Phi_b) = 0 \\
&\Rightarrow b = a \quad \text{or} \quad (\Phi_a, \Phi_b) = 0
\end{aligned}$$

Since we already established that a and b are different eigenvalues, this leads us to conclude that $(\Phi_a, \Phi_b) = 0$. Hence the eigenstates are orthogonal. □

The 2 proofs above constitute what is known as the *Spectral Theorem*, and in summary tells us that any Hermitian operator can be diagonalized to give an **orthogonal** set of eigenstates with **real** eigenvalues which span the Hilbert space. This means that **any** arbitrary quantum state can be written as a linear combination of an observable's eigenstates!

§3.5 Measurement

So far, we have seen that quantum systems are described by wave functions and no longer adhere to regular classical descriptions. However when we perform a measurement, we don't obtain these quantum waves of probability but instead the classical notion of physical quantities. So what is actually happening and how do we incorporate this into our theory? The answer comes from a phenomenon known as the *'collapse of the wave function'* and is presented in the ***measurement postulate*** below.

Postulate 3.5.1. *Given a diagonalizable Hermitian observable $\hat{Q}$ and an arbitrary quantum state expressed as the superposition of $\hat{Q}$ eigenstates $\Psi = \sum_j \alpha_j \psi_j$, performing a measurement of $\hat{Q}$ on Ψ would cause it to collapse into one of the eigenstates ψ_j with probability $|\alpha_j|^2$. The measurement outcome would be the eigenvalue q_j associated to ψ_j.*

So realize now that every observable has it's own set of eigenstates and eigenvalues, which allows us to use different bases of eigenstates as different but equivalent descriptions of a system. Wave function collapse again, nicely goes hand in hand with the Copenhagen interpretation.

Note: Because measurements are also physical operations on a system, many have asked how this satisfies the unitarity condition. Some interesting reads which discuss this issue are given in the bibliography [1], [2].

§ **SUMMARY** §

In this chapter,

- We were introduced to *inner products* with it's structure elevating a $\mathbb{C}$-vector space to a Hilbert space.
- We learned the definition of *expectation* values in the context of quantum mechanics.
- The commutator between 2 observables can tell us if they are complementary variables, or measurable simultaneously without any uncertainty.
- We saw that observables are represented as *Hermitian operators* and looked at several properties to do with Hermiticity.
- We learned how to *diagonalize* an operator to give the *spectrum of the theory*.
- We learned about measurement and how it reconciles the wave function formalism with our observable reality.

Exercises

1. Find the inner product between the following functions in position space:
   - $f(x) = \exp\left(-\frac{x^2}{2}\right)$ and $g(x) = x$
   - $f(x) = x^2 e^{-x}$ and $g(x) = \begin{cases} \sin(x) & , x \in [0, 2\pi] \\ 0 & , \text{otherwise} \end{cases}$
2. Find the expectation value of $\hat{x}$ and $\hat{p}$ on all 4 wave functions from the previous question in position space.
3. An operator $\hat{A}$ is called *anti-Hermitian* if it satisfies the following relation.
$$\langle \Psi, \hat{A}\Psi \rangle = -\langle \hat{A}\Psi, \Psi \rangle \tag{3.8}$$
Prove that all eigenvalues of an *anti-Hermitian* operator are strictly imaginary.
4. Derive the following identities.
$$\frac{d}{dt}\langle \hat{x} \rangle = \frac{1}{m}\langle \hat{p} \rangle, \quad \frac{d}{dt}\langle \hat{p} \rangle = -\langle V'(x) \rangle \tag{3.9}$$
These identities constitute the *Ehrenfest theorem* and are the quantum analog to Newton's classical laws of motion.
5. Starting from the time-dependent Schrödinger equation (2.13), convince yourself that for any **time-independent** Hamiltonian, the general solution is given by
$$\psi(x;t) = e^{-\frac{i\hat{H}t}{\hbar}}\psi(x;0) \tag{3.10}$$
Also prove that this time-evolution operator $\hat{U}(t) = \exp\left(-\frac{i\hat{H}t}{\hbar}\right)$, is unitary ($\hat{U}(t)^\dagger \hat{U}(t) = \mathbb{I}$).

Chapter 4

What Now Schrödinger?

Earlier, we arrived at the famous Schrödinger's equation (2.13) which is the wave equation that governs all of quantum dynamics. That said, how do we actually find solutions to this differential equation? Well, we can simplify things by first looking at objects known as ***stationary states****. From there, we will finally be able to build and solve a simplified model of radioactive decay as introduced through smoke detectors at the start of this handbook. We will also see a key feature of quantum mechanics known as* ***quantization*** *emerge.*

§4.1 Stationary States

Thus far, we have explored eigenstates and seen many wonderful properties that these states exhibit. Knowing the usefulness of eigenstates, we will now explore a specific kind of eigenstate known as *stationary states*.

Definition 4.1.1. Stationary States: *Stationary states are energy eigenstates constructed by finding* ***separable solutions*** *to the Schrödinger's equation.*

Note that *energy eigenstates* are eigenstates of the Hamiltonian. From this definition, we see that stationary states require us to write our solution to the Schrödinger's equation as

$$\Psi(x,t) = \psi(x)f(t) \tag{4.1}$$

plugging this into Schrödinger's equation, we get

$$\begin{aligned} i\hbar\frac{df(t)}{dt}\psi(x) &= \Big(\hat{H}\psi(x)\Big)f(t) \\ \Rightarrow\ i\hbar\frac{1}{f(t)}\frac{df(t)}{dt} &= \frac{1}{\psi(x)}\hat{H}\psi(x) \end{aligned} \tag{4.2}$$

We notice that the left-hand side is solely dependent on t whereas the right-hand side is solely dependent on x. Hence, the only way these 2 sides could be equal is if they were both equal to a constant. Checking the dimensions, we see that both the LHS and RHS have units of energy

making it convenient to label the seperation constant as E. As such, we arrive at the following 2 equations.

$$\begin{cases} i\hbar\frac{df(t)}{dt} = Ef(t) \\ \hat{H}\psi(x) = E\psi(x) \end{cases} \tag{4.3}$$

Looking first at the time dependent equation,

$$\begin{aligned} \frac{df(t)}{dt} &= -\frac{iE}{\hbar}f(t) \\ \Rightarrow\ f(t) &= f(0)e^{-\frac{iE}{\hbar}t} \end{aligned} \tag{4.4}$$

That was simple enough to solve. With this result, we can write our stationary state as

$$\boxed{\Psi(x,t) = \psi(x)e^{-\frac{iE}{\hbar}t}} \tag{4.5}$$

Notice that in the above representation of the stationary state, we have absorbed the initial condition factor from solving the time equation into $\psi(x)$. Additionally, we can show that the stationary state is indeed an energy eigenstate as follows.

$$\begin{aligned} \hat{H}\Psi(x,t) &= \hat{H}\psi(x)e^{-\frac{iE}{\hbar}t} \\ &= e^{-\frac{iE}{\hbar}t}\hat{H}\psi(x) \\ &= e^{-\frac{iE}{\hbar}t}E\psi(x) = E\tilde{\Psi}(x,t) \end{aligned}$$

Hence, we have shown that $\Psi(x,t)$ indeed satisfies the energy eigen-equation and is thus an energy eigenstate with energy eigenvalue E.

Having proven this fact, recall that any arbitrary quantum state can be constructed from a superposition of eigenstates via the spectral theorem. Hence, we can construct any quantum state from a superposition of stationary states as well!

$$\boxed{\Psi(x,t) = \sum_{n=1}^{\infty}\alpha_n\Psi_n(x,t) = \sum_{n=1}^{\infty}\alpha_n\psi_n(x)e^{-\frac{iE_n}{\hbar}t}} \tag{4.6}$$

§4.2 Modelling Radioactive Decay

Having solved the temporal portion of the separated Schrödinger's equation, we are now ready to look for explicit forms of $\psi(x)$ (in 1-dimension).

> **Note:** Unfortunately, a general analytic solution to arbitrary $V(x,t)$ in the Schrödginer's equation has **not** been found. We will be looking at solutions to specific 1D potentials.

This means we are finally ready to build a quantitative picture of radioactivity used in smoke detectors! We will only be solving a **simplified** model for radioactive decay, but it will be enough for us to extract some insightful physics. In particular, we will be considering *alpha-decay* from a larger nucleus. The mechanism for radioactive decay is as follows.

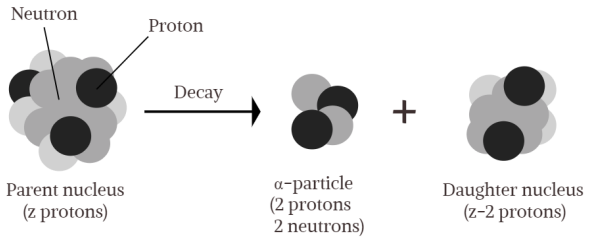


Figure 4.1: α-Particle Decay

During α-decay, the α-particle spontaneously *tunnels* out of the *nuclear potential* barrier. When the α-particle is no longer in tact with the other nucleons, it feels only the electrostatic repulsion due to the charged daughter nucleus. It thus accelerates away, acquiring the kinetic energy of a few million electron volts. The approximate *radial* potential during this process is illustrated below.

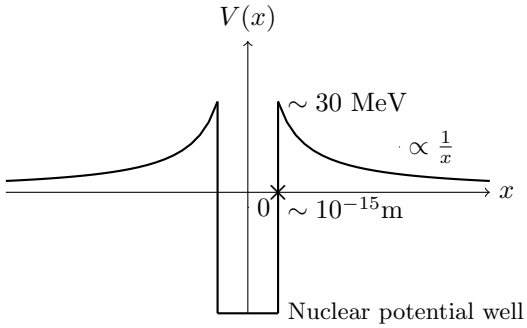


Figure 4.2: Radioactive Decay Radial Potential

As seen in figure 4.2, there is a deep nuclear potential well where the α-particle lives before decay. Without any excitation, the α-particle would have insufficient energy to **classically** overcome the nuclear force barrier. But we know that quantum mechanics often breaks classical intuition, so let's see what Schrödinger's equation has to say about this. First, we make one further simplification to the potential shown in the figure below.

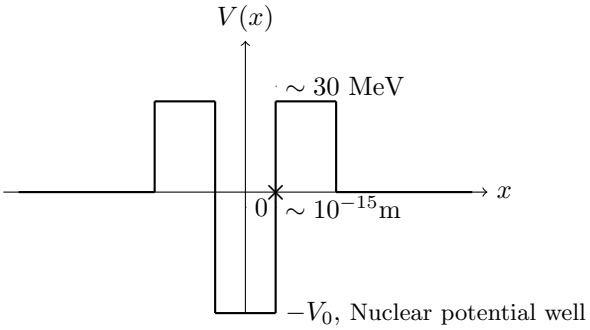


Figure 4.3: Simplified Radioactive Decay Radial Potential

Now, we systematically partition the system into spatial segments, solving for the wave function within each segment then 'stitching' them together afterward.

§4.2.1 In the Nuclear Well

Looking first at region $x \in [-R, R]$, the Schrödinger equation here is

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) - V_0\psi(x) &= E_\alpha\psi(x) \\ \Rightarrow \quad \frac{d^2}{dx^2}\psi(x) &= -\frac{2m(E_\alpha + V_0)}{\hbar^2}\psi(x) \end{aligned} \tag{4.7}$$

Much like a finite-square well. To simplify things, we define

$$k^2 \equiv \frac{2m(E_\alpha + V_0)}{\hbar^2} \tag{4.8}$$

where k is known as the *wave number*. From our knowledge of ordinary differential equations, we see that the solution to this ODE is as follows.

$$\boxed{\psi(-R < x < R) = Ae^{ikx} + Be^{-ikx}} \tag{4.9}$$

(a linear combination of plane-wave solutions with momentum to the left and right) where A and B are arbitrary complex coefficients to be solved via boundary conditions.

§4.2.2 Classically Forbidden Regions

We now look at the region $x \in [R, R_c]$ (the $x \in [-R_c, -R]$ region also has a very similar solution). Here, we note that the energy of the α-particle is lower than the strength of the nuclear potential barrier V_n. The Schrödinger equation is thus

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V_n\psi(x) &= E_\alpha\psi(x) \\ \Rightarrow \quad \frac{d^2}{dx^2}\psi(x) &= \frac{2m|V_n - E_\alpha|}{\hbar^2}\psi(x) \end{aligned} \tag{4.10}$$

Again, we define a wave number parameter κ for this (*classical forbidden*) region,

$$\kappa^2 \equiv \frac{2m|V_n - E_\alpha|}{\hbar^2} \tag{4.11}$$

Taking special care to keep track of our negative signs, we arrive at the following solution.

$$\psi(R < x < R_c) = Ce^{-\kappa x} + De^{\kappa x} \tag{4.12}$$

Actually, we can see that $D = 0$ because we cannot have the probability amplitude exponentially increase in a classically forbidden region. Try to reason this to yourself! (The opposite result is true for $x \in [-R_c, -R]$). This renders our wave function simply as

$$\boxed{\psi(R < x < R_c) = Ce^{-\kappa x}} \tag{4.13}$$

§4.2.3 Freed from Nuclear Entrapment

Finally, we consider the region $x \in [R_c, \infty)$. It definitely seems classically unorthodox to even consider this region having a solution, but well, things are unintuitive in the quantum world. Here, we essentially have a free-particle Schrödinger's equation. So we again get plane-wave solutions with wave number $k'^2 \equiv \frac{2mE_\alpha}{\hbar^2}$.

$$\boxed{\psi(x > R_c) = Ee^{ik'x}} \tag{4.14}$$

The difference here, is that we know the decayed particle would only have escape momentum away from the parent nucleus, hence we only considering outward moving plane-wave solutions.

§4.2.4 Joining the Puzzle Pieces

Now, we have 3 separate solutions for 3 separate regions. In fact, we can utlize symmetry and extend this solution to the entire x space to give

$$\psi(x) = \begin{cases} Ee^{-ik'x}, & -\infty < x < -R_c \\ Ce^{\kappa x}, & -R_c < x < -R \\ Ae^{ikx} + Be^{-ikx}, & -R < x < +R \\ Ce^{-\kappa x}, & +R < x < +R_c \\ Ee^{-ik'x}, & +R_c < x < +\infty \end{cases} \tag{4.15}$$

What about the complex coefficients (A,B,C,E)? We know we need a continuous solution because the Schrödinger's equation is a second order differential equation, hence requiring $\psi(x)$ **and** $\psi'(x)$ to be continuous. We can utilize these continuity conditions to aid us in our solution. A visualization of the continuous solution is given below (figure 4.4).

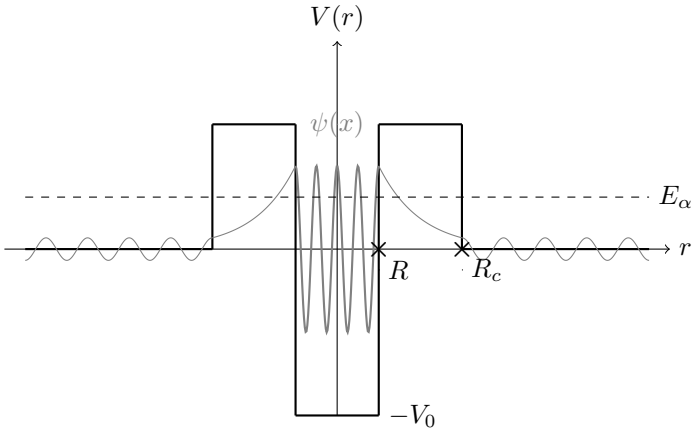


Figure 4.4: Visualization of the Wave Function

Firstly, at the $x = R$ boundary we have

$$\psi(x = R) : Ae^{ikR} + Be^{-ikR} = Ce^{-\kappa R} \tag{4.16}$$

A valid approximation to employ is that there is a very small amount of the wave which propagates through the barrier. Hence, most of the wave is reflected off, causing the amplitudes A and B to be largely similar ($A \approx B$). As such, we get

$$\begin{aligned} & 2A\cos(kR) = Ce^{-\kappa R} \\ \Rightarrow\ & C = 2Ae^{\kappa R}\cos(kR) \end{aligned} \tag{4.17}$$

Now looking at the $x = R_c$ boundary, we have

$$\begin{aligned} & Ce^{-\kappa R_c} = Ee^{-ik'R_c} \\ \Rightarrow\ & 2Ae^{\kappa R}\cos(kR)e^{-\kappa R_c} = Ee^{-ik'R_c} \\ \Rightarrow\ & E = 2Ae^{-ik'R_c}e^{\kappa(R-R_c)}\cos(kR) \end{aligned} \tag{4.18}$$

From here, we can immediately extract valuable information relating to the likelihood of the trapped α-particle escaping. We use a metric known as the *transmission coefficient* T to measure this, where T is then the ratio of the outgoing flux from a barrier to the incoming flux (probability of transmission through a boundary).

$$T = \frac{k'|\psi(x > R_c)_{\text{outgoing}}|^2}{k|\psi(-R < x < R)_{\text{incoming}}|^2} \tag{4.19}$$

So from our solutions earlier, we get a transmission coefficient as follows.

$$\begin{aligned} T &= \frac{k'|E|^2}{k|A|^2} \\ &= \frac{k'}{k} \cdot \frac{\left|2Ae^{-ik'R_c}e^{\kappa(R-R_c)}\cos(kR)\right|^2}{|A|^2} \\ &= 4\sqrt{\frac{E_\alpha}{E_\alpha + V_0}} \cdot e^{2\kappa(R-R_c)} \cdot \cos^2(kR) \end{aligned}$$

Which explicitly written, is

$$\boxed{T = 4\sqrt{\frac{E_\alpha}{E_\alpha + V_0}} \cdot \cos^2\left(\frac{R\sqrt{2m(E_\alpha + V_0)}}{\hbar}\right) \cdot \exp\left\{-\frac{\sqrt{8m|V_n - E_\alpha|}}{\hbar}(R_c - R)\right\}} \tag{4.20}$$

Hence, we see that the transmission coefficient depends heavily on the width of the barrier ($R_c - R$), the strength of the potential well and barrier (V_0 and V_n respectively) and of course the energy of the α-particle E_α. But in any case, there is still a **non-zero**, significant probability that the α-particle could sneak its way out of the nuclear potential well! This phenomena is known as *quantum tunneling*, and is in fact an essential process for the existence of our universe.

§4.2.5 Stuck in a Box!

Apart from quantum tunnelling, this simple system promises some very insightful new physics. We will now explore the case where the α-particle doesn't even have enough energy to tunnel

out, rendering it stuck forever in the nuclear potential well. Our potential can thus be effectively modelled as an infinite square well. This system is also often referred to as the *particle in a box* problem. Mathematically, we write the potential as

$$V(x) = \begin{cases} 0 & -R < x < R \\ \infty & \text{otherwise} \end{cases} \tag{4.21}$$

Because the particle is trapped within the region $x \in [-R, R]$ region, the wave function **must** vanish at $x = -R$ and $x = R$. As such, we set-up solving our problem with our knowledge of differential equations as follows.

$$\begin{aligned} & -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x), \quad x \in [-R, R] \\ \Rightarrow \quad & \psi(x) = Ae^{ikx} + Be^{-ikx} \end{aligned}$$

Applying the boundary conditions.

$$\begin{aligned} & \psi(-R) = 0 \quad \Rightarrow \quad A + Be^{2ikR} = 0 \\ & \psi(R) = 0 \quad \Rightarrow \quad A + Be^{-2ikR} = 0 \\ \Rightarrow \quad & 2iB\sin(2kR) = 0 \\ \Rightarrow \quad & \boxed{k_n = \frac{n\pi}{2R}}, \quad n \in \mathbb{N}\backslash\{0\} \end{aligned} \tag{4.22}$$

So we see that there is a quantization of the wave number! Recalling that $p = \hbar k$ and $E = p^2/2m$, we find that the associated momenta and energies of the particle are

$$\boxed{p_n = \frac{n\pi\hbar}{2R}, \quad E_n = \frac{\hbar^2 n^2 \pi^2}{8mR^2}} \tag{4.23}$$

Hence we get a *quantization* of both momentum and energy of the particle, indexed by the parameter n. A visualization of the wave functions with the lowest 3 energies are illustrated in figure 4.5.

Exercises

1. By applying the normalization condition, show that the normalized wave functions of an infinite square well of width $2R$ are given by $\psi(x; n) = \frac{1}{2\sqrt{R}}\sin\left(\frac{n\pi}{R}x\right)$.
2. Give an explanation as to why we ignore negative and trivial values of the wave vector k_n.

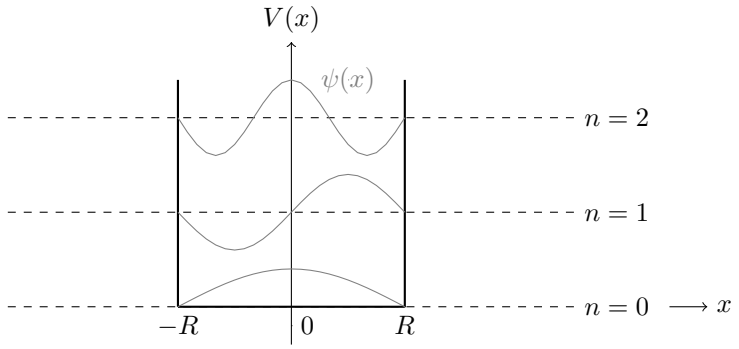


Figure 4.5: $n = 1, 2, 3$ Infinite Square Well Wave Functions

The solution of the infinite square well gives rise to 2 theorems on 1D potentials. These theorems are listed below.

Theorem 4.2.1. *There are **no** degenerate[1] 1D bound states.*

Theorem 4.2.2. *For a 1D bound state, the number of nodes[2] increases linearly with the 'quantization index' n following the relation*

$$\text{number of nodes} = (n-1), \quad \text{for } n = 1, 2, 3... \tag{4.24}$$

Of course, just solving one potential is not sufficient as a proof for these 2 theorems. The proof for these theorems can be found in appendix D.2.1. I would highly recommend reading through these proofs or even trying them for yourselves for maximum take away.

§4.3 Dirac's Bras and Kets

Earlier in chapter 1, we saw how we could write quantum states as vector and the matrix representation of operators acting on these states. But since the start of chapter 2, we have been dealing with these continuous function objects we call wave functions. How do we resolve these 2 seemingly unrelated mathematical objects? Well, firstly we have to be clear about what difference caused us to use these different objects.

In the Mach-Zehnder interferometer, we saw that the states were intrinsically confined to 2 possible configurations $\{|u\rangle, |d\rangle\}$, so there was no need to provide a representation with any

[1] **Definition 4.2.1.** Degeneracies: *An energy level is called degenerate if there exists 2 or more energy eigenstates that are associated to this same energy.*

[2] **Definition 4.2.2.** Node: *For a wave function in one spatial dimension x, a node is a point away from spatial boundaries where the wave function $\psi(x)$ crosses the x axis on a $\psi(x)$ vs x plot.*

more than 2 complex numbers (All probabilistic information of the system could be encoded with these 2 complex numbers). But when we introduced the wave function formalism, we required mathematical objects that were labelled by a continuous variable x (position). This continuous variable makes it way harder to track the probabilistic information of the entire system (tracking $\psi(x)$ for all values of x simultaneously). Despite this, it is still theoretically possible to have a vector analog for systems with continuous labels. We write this abstract **infinitely** long vector as $|\psi\rangle$, known as a '*ket*' (as per in Mach-Zehnder interferometry).

> **Note:** What is written inside the ket is simply a label which indicates the significance of that state with respect to a system. Generally, we write $|\psi\rangle$ when referring to some arbitrary state.

Writing this out explicitly,

$$\psi(x) \to |\psi\rangle = \begin{bmatrix} \vdots \\ \psi(-2\epsilon) \\ \psi(-\epsilon) \\ \psi(0) \\ \psi(\epsilon) \\ \psi(2\epsilon) \\ \vdots \end{bmatrix} \tag{4.25}$$

where ϵ is an infinitesimally small slice of space. To define an inner product on a complex vector space, we require a definition of *conjugate transposition*. The notation that Dirac proposed for the conjugate transpose of a ket is called the '*bra*', given by

$$\langle\psi| = \left(|\psi\rangle^*\right)^T = |\psi\rangle^\dagger \tag{4.26}$$

The symbol we use for conjugate transposition (†) is called the *dagger*. With this, we can formally introduce *inner products* by simple closing the '*bra-ket*', $\langle\psi|\phi\rangle$. *Expectations* are performed in the same way with the observable wedged in-between, $\langle\psi|\,\hat{Q}\,|\psi\rangle$.

> **Note:** Mathematically speaking, bra vectors live in the *dual space* of the ket Hilbert space in accordance to the *Riesz representation theorem*[3].

. Additionally, operators like $\hat{H}$ and $\hat{p}$ will also adopt matrix representations, where the ij^{th} entry is given by

$$[\hat{Q}]_{ij} = \langle\psi_i|\,\hat{Q}\,|\psi_j\rangle \tag{4.27}$$

In equation (4.27) above, the $|\psi_j\rangle$ states are eigenstates of some operator (not necessarily $\hat{Q}$) acting on that Hilbert space. We know from the spectral theorem (3.4.2 and 3.4.3) that Hermitian observables are diagonalizable with real eigenvalues and a spanning set of eigenstates. Hence, it is imperative to **specify which basis** we are working with in order to construct the matrix representation of an operator. To be explicit, given some basis

$$\mathcal{B} = \{|\psi_1\rangle, |\psi_2\rangle, ..., |\psi_n\rangle\} \tag{4.28}$$

[3]The Riesz representation theorem essentially says that for every Hilbert space $\mathcal{H}$, there exists a dual Hilbert space $\mathcal{H}^*$ such that every $|\psi\rangle$ in $\mathcal{H}$ has a $\langle\psi|$ in $\mathcal{H}^*$

and an operator $\hat{Q}$, the matrix representation of $\hat{Q}$ in the $\mathcal{B}$ basis is given as

$$\hat{Q} = \begin{bmatrix} \langle\psi_1|\hat{Q}|\psi_1\rangle & \langle\psi_1|\hat{Q}|\psi_2\rangle & \dots & \langle\psi_1|\hat{Q}|\psi_n\rangle \\ \langle\psi_2|\hat{Q}|\psi_1\rangle & \langle\psi_2|\hat{Q}|\psi_2\rangle & \dots & \langle\psi_2|\hat{Q}|\psi_n\rangle \\ \vdots & & \ddots & \vdots \\ \langle\psi_n|\hat{Q}|\psi_1\rangle & \langle\psi_n|\hat{Q}|\psi_2\rangle & \dots & \langle\psi_n|\hat{Q}|\psi_n\rangle \end{bmatrix} \tag{4.29}$$

Note: Given some observable Q, working in the Q basis would ensure that the matrix representation of $\hat{Q}$ is *diagonal*.

It also follows that in some *countable basis*, the property of *completeness* asserts the following relation:

$$\sum_j |\psi_j\rangle\langle\psi_j| = \mathbb{I} \tag{4.30}$$

This is sometimes referred to as the '*resolution of the identity*'. A simple case to check this would be the 2-level system we saw in the Mach-Zehnder interferometry experiment. For this basis ($\{|u\rangle, |l\rangle\}$), we get the sum to be explicitly written as:

$$\begin{aligned} \sum_j |\psi_j\rangle\langle\psi_j| &= |u\rangle\langle u| + |l\rangle\langle l| \\ &= \begin{bmatrix} 1 \\ 0 \end{bmatrix}\begin{bmatrix} 1 & 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix}\begin{bmatrix} 0 & 1 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \mathbb{I} \end{aligned} \tag{4.31}$$

Indeed giving us a resolution of the identity operator.

Note: For bases that cannot be enumerated (*non-enumerable bases*), the identity is given by an integral. For instance, the resolution of the identity in the position basis is given as:

$$\int_{-\infty}^{\infty} dx\, |x\rangle\langle x| = \mathbb{I} \tag{4.32}$$

This will not be further elaborated on in this handbook, so as to prevent information overload to the learner (more on this can be read about in [5]).

Example

Let's say that we are working in the *momentum basis* for the infinite square well system (of width L) with quantized momentum. It is then useful to write the eigenstates of the $\hat{p}$ operator as $\{|p_n\rangle\}$. In this basis, $\hat{p}$ is diagonal with entries computed by

$$[\hat{p}]_{ij} = \langle p_i|\hat{p}|p_j\rangle = p_{i,j}\delta_{i,j} \tag{4.33}$$

The matrix would thus look something like

$$\hat{p} = \begin{bmatrix} p_{1,1} & & & & 0 \\ & \ddots & & & \\ \vdots & & p_{j,j} & & \vdots \\ & & & p_{j+1,j+1} & \\ 0 & & & & \ddots \end{bmatrix} \tag{4.34}$$

We can also easily see that the j^{th} eigenvector (eigenstate) is a vector with 1 in the j^{th} position and 0 everywhere else.

$$|p_j\rangle = \begin{bmatrix} \vdots \\ 0_{j-1} \\ 1_j \\ 0_{j+1} \\ \vdots \end{bmatrix}, \quad p_{j,j} = \frac{j\pi\hbar}{L} \tag{4.35}$$

This satisfies the relation in 4.33. Make sure to check for yourself that this works and get familiar with the correspondence between kets and number array vectors.

§ **SUMMARY** §

In this chapter,

- We solved for the time dependence of separable wave function solutions.
- We learned about stationary states as separable solutions to the time-independent Schröinger equation.
- We saw how radioactive α-decay from a parent nucleus could be modelled as a 1-dimensional potential problem.
- We saw that quantum tunnelling is the main mechanism which allows for radioactive α-decay to occur.
- We saw energy and momentum quantization naturally arise due to boundary conditions of a 1-dimensional potential.
- We learned how to express general quantum states and operators in their matrix representations, coupled to the use of Dirac notation.

Exercises

1. (a) Using the node theorem, sketch the ground state ($n = 0$) wave function for the simplified radioactivity model (figure 4.3) where $E_\alpha < 0$.

   (b) Using the intuition from your sketch, solve for an analytic solution.

2. Consider again an infinite square well but now positioned at $x \in [0, L]$. Re-derive the n^{th} bound state wave function along with its quantized momentum and energy.

3. Prove that a non-trivial wave function can never vanish along with its first spatial derivative (cannot have both $\psi(x)$ and $\psi'(x)$ being simultaneously 0 at any x).

4. In the position basis, find the matrix representations of $\hat{x}$ and $\hat{p}$. (Hint: Use the limit definition of a derivative to find $\hat{p}$).

5. Given some arbitrary state $|\psi\rangle$ and a position eigenstate $|x\rangle$, write $\psi(x)$ in terms of these abstract ket vectors. Write $\int_{-\infty}^{\infty} dx|\psi(x)|^2$ in terms of $|\psi\rangle$ and $|x\rangle$.

Part II

Applied Abstractions

Chapter 5

Quantum Computation

So far we have learned that our world works in strange and unintuitive ways at small scales. This advent of quantum mechanics has granted us access to a plethora of previously unimaginable technologies. In this chapter, we take a closer look at an aforementioned emerging quantum technology, one of which could shape our future drastically. This is the technology of quantum computers. Quantum computation is an entirely new model of computation that sprung out of the work by Paul Benioff and Yuri Manin in 1980, Richard Feynman in 1982 and David Deutsch in 1985. We are about to learn the workings of this new computational engine. Strap-up.

§5.1 TLDR; Classical Computers

There are currently many models of classical computation, some of which are what we call, *universal* while others are not. This idea of *universal computation* was proposed by Alan Turing in 1936, saying that any 'reasonable' computation can be solved by a *universal machine*. Below is a list of some of these computational models, whether or not they are universal is indicated.

1. Turing Machines (Universal)
2. Finite Automata (Not Universal)
3. λ-calculus (Universal)
5. Coin Tosses (Not Universal)
6. Circuit Models (Universal)

Out of these, the **circuit model** is what I will be touching briefly on because it will pave the way for the model of quantum computation. What you need to know about the circuit model is that it has the following structure.

Figure 5.1: The Circuit Model (Computer Science)

Note: Circuits are only designed for **finite** sized inputs. The formal mathematical definition of the circuit model requires knowledge of *graph theory*, in which the circuit is a *finite directed acyclic graph*. We will neither learn nor require this formal definition.

The circuit model is a generalization of the common *boolean circuitry* with universal gates $\{\text{AND}, \text{NOT}\}$ (for instance). Also, the description of a circuit should be the output of a classical computer program.

§5.1.1 Byte-Sized Complexity Theory

It would be useful for us to know a little bit of complexity theory as a step to the appreciation of quantum computing.

Disclaimer: Bear in mind that the information on complexity theory provided here is minimal and relatively informal.

Many problems in computer science can be expressed as *decision problems*. Examples of these are the *primality* (is m prime?) and *factoring* (given $m, l \in \mathbb{Z}$ with $l < m$, does m have a non-trivial factor less than l?). For such problems, if the number of operations ($\sim$ time of computation) is a polynomial function of the size of the input n, we call these class of problems *polynomial hard*, or simply $\in P$. Also, if 'yes' instances of these problems are easily verified with the aid of a 'witness', then we say that the problem is contained in the bigger class of NP-hard problems (nondeterministic polynomial time). On the other hand, if 'no' instances are easily verifiable by the witness, the problem $\in$ co-NP.

Finally, there is a special class of problems which are known as NP-complete. What makes it special is that solving NP-complete problems will allow for us to solve **all** NP problems! A set visualization of the classes is given below.

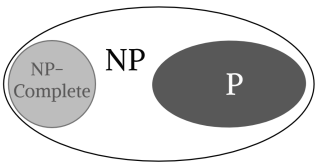


Figure 5.2: Complexity Classes

Of course, these 3 classes of problems are not nearly an exhaustive list of complexity classes being studied by computer scientists. In fact, quantum decision problems solvable in polynomial time are also specially categorized, with the class being known as BQP (bounded-error quantum polynomial time).

§5.2 The Qubit

The fundamental constituent of a quantum computer is a quantum bit, otherwise known as a *qubit*. In theory, any 2-level quantum system can be realized as an implementation of a qubit. Take for instance the previously explored Mach-Zehnder interferometer (1.1). Upon passing the photon through the beam splitters, we effectively created a qubit state in superposition ($|\psi\rangle = \frac{|u\rangle+|d\rangle}{\sqrt{2}}$)!

Another intrinsic 2-level system is the *spin* of spin-$\frac{1}{2}$ particles. A more rigorous treatment of spin is discussed in appendix E but for all intends and purposes, we can think of quantum spin as the 2-level quantized version of the classical spin for a charged sphere. This quantization allows us to represent the *orthogonal* states of our spin qubit as follows.

$$|0\rangle = \begin{bmatrix}1\\0\end{bmatrix}, \quad |1\rangle = \begin{bmatrix}0\\1\end{bmatrix} \tag{5.1}$$

Here, we have adopted the notation used by quantum information scientists, where the 2 qubit states are labelled by 0 and 1. Since spin is an observable quantity, quantum mechanics promotes it to a Hermitian operator denoted as $\hat{S}_z$ with eigenvalues $\pm\frac{\hbar}{2}$. The subscript z on the spin operator denotes the *canonical basis*, where we take the default axis of measurement to be along z in 3D space. A keen observer would have noticed that there is a subtlety here. We have 2 vector spaces in which one seems to be 'embedded' in the other. These vector spaces are

1. The **2D** vector space of **spin states** (quantum state space)
2. The **3D** vector space of **rotations** (real space)

This means that in any arbitrary direction in real space, there lives a 2D complex vector space. Formally, we have a smooth sphere of rotations called the *Lie group* with a tangent vector space known as the *Lie algebra* (appendix F.2.16). The *Pauli matrices* (introduced soon) multiplied with an i are solutions to this Lie algebra, and they can then be *exponentiated* with a continuous **real** parameter to generate the Lie group. A bastardized visualization of this for our context is shown below (figure 5.3).

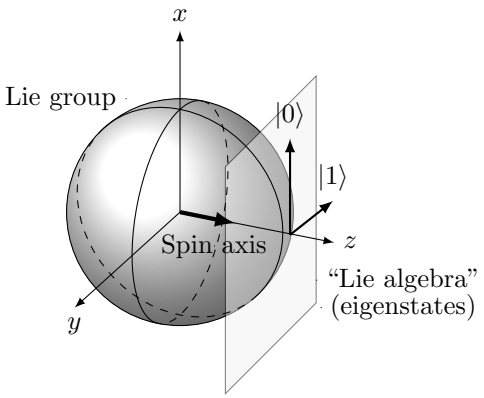


Figure 5.3: Visualization of Spin Rotations

A similar method of visualization is known as the *Bloch sphere* geometric representation. This will not be covered but can be read about in [6].

§5.3 Pauli Gates

There is actually a *bijective map*[1] ($\mathbf{so}(3) \cong \mathbf{su}(2)$)[2] from the *generators* of 3D rotations over an $\mathbb{R}$-vector space to 2D Pauli matrices over the complexes. The matrix representation of the solutions to this algebra ($\mathbf{su}(2)$) are as follows:

$$\mathbb{I} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{5.2}$$

where σ_x, σ_y and σ_z are known as the *Pauli matrices* and the identity matrix is added to form a basis for all 2×2 Hermitian matrices (but not part of the algebra). The Pauli matrices conveniently correspond to spin operators in the x, y and z axes (up to a scale factor of $\frac{\hbar}{2}$). Explicitly, the spin matrices are

$$\hat{S}_x = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \hat{S}_y = \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \hat{S}_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{5.3}$$

each of which are spin observables along specified axes (x, y, z) written in the z basis representation. The eigenstates of each of these operators are given below.

$$\begin{aligned} \hat{S}_x: &\quad |+\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad |-\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix} \\ \hat{S}_y: &\quad |\uparrow\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ i \end{bmatrix}, \quad |\downarrow\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -i \end{bmatrix} \\ \hat{S}_z: &\quad |0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \end{aligned} \tag{5.4}$$

Or written in the canonical basis,

$$\hat{S}_z : \{|0\rangle, |1\rangle\}, \quad \hat{S}_y : \{\frac{|0\rangle + i\,|1\rangle}{\sqrt{2}}, \frac{|0\rangle - i\,|1\rangle}{\sqrt{2}}\}, \quad \hat{S}_x : \{\frac{|0\rangle + |1\rangle}{\sqrt{2}}, \frac{|0\rangle - |1\rangle}{\sqrt{2}}\} \tag{5.5}$$

The spin matrices follow a set of cyclic commutation relations known as the *algebra of angular momentum* (recall the definition of a commutator from 2.3.1).

$$\left[\hat{S}_x, \hat{S}_y\right] = i\hbar\hat{S}_z, \quad \left[\hat{S}_y, \hat{S}_z\right] = i\hbar\hat{S}_x, \quad \left[\hat{S}_z, \hat{S}_x\right] = i\hbar\hat{S}_y \tag{5.6}$$

The Pauli operators follow a similar algebra but with a factor of $2/\hbar$. The wonderful thing about Pauli matrices is that they are all *unitary*, *Hermitian* and *involutory* (squares to identity). Unitarity makes them realizable as physically implementable operations on qubits, so we can use them to construct quantum gates (analogous to logic gates for classical circuits)!

> **Note:** When we refer to the Pauli matrices in the context of gates, we drop the σ and simply label them as $\{X, Y, Z\}$.

[1] Refer to appendix F.2.12 for more information on bijectivity.

[2] $\mathbf{so}(3)$ and $\mathbf{su}(2)$ are Lie algebras of the 3D special orthogonal and 2D special unitary groups, SO(3) and SU(2).

§5.4 More Qubits; Tensor Products

Clearly, having a computer (even a quantum one) with one bit (qubit) isn't very useful. The beauty of quantum computers is that the addition of more qubits doesn't scale in the same way that adding more bits to a C-computer does. For multi-particle (many-body) quantum systems, we require the use of *tensor products*. I will be presenting tensor products in their matrix representation, also known as *Kronecker products*. Given 2 vectors

$$|\psi\rangle = \begin{bmatrix} \vdots \\ \psi_j \\ \psi_{j+1} \\ \vdots \end{bmatrix}, \quad |\phi\rangle = \begin{bmatrix} \vdots \\ \phi_j \\ \phi_{j+1} \\ \vdots \end{bmatrix} \tag{5.7}$$

with $|\psi\rangle \in V$ and $|\phi\rangle \in W$, the Kronecker product of $|\psi\rangle$ and $|\phi\rangle$ is given by

$$|\psi\rangle \otimes |\phi\rangle = \begin{bmatrix} \vdots \\ \psi_j |\phi\rangle \\ \psi_{j+1} |\phi\rangle \\ \vdots \end{bmatrix} \tag{5.8}$$

> **Note:** A common shorthand notation is to drop the $\otimes$ symbol and merge the kets $|\psi\rangle \otimes |\phi\rangle \to |\psi\phi\rangle$.

This new $|\psi\rangle \otimes |\phi\rangle$ state is part of the tensor-ed Hilbert space $V \otimes W$. The dimensions of this larger Hilbert space is given by $\dim(V \otimes W) = \dim(V) \cdot \dim(W)$. We also require the operators acting on these states to have a defined action on the tensor-ed Hilbert space. As such, we also define a Kronecker product for matrices as such. Given 2 matrices,

$$\hat{A} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix}, \quad \hat{B} = \begin{bmatrix} b_{11} & b_{12} & \dots & b_{1nm} \\ b_{21} & b_{22} & \dots & b_{2m} \\ \vdots & & \ddots & \vdots \\ b_{m1} & b_{m2} & \dots & b_{mm} \end{bmatrix} \tag{5.9}$$

the Kronecker product of $\hat{A}$ and $\hat{B}$ is defined as

$$\hat{A} \otimes \hat{B} = \begin{bmatrix} a_{11}\hat{B} & a_{12}\hat{B} & \dots & a_{1n}\hat{B} \\ a_{21}\hat{B} & a_{22}\hat{B} & \dots & a_{2n}\hat{B} \\ \vdots & & \ddots & \vdots \\ a_{n1}\hat{B} & a_{n2}\hat{B} & \dots & a_{nn}\hat{B} \end{bmatrix} \tag{5.10}$$

which would be a $(n \cdot m) \times (n \cdot m)$ matrix. The action of these operators on states are thus defined as follows.

$$\boxed{(\hat{A} \otimes \hat{B})(|\psi\rangle \otimes |\phi\rangle) = \hat{A}\,|\psi\rangle \otimes \hat{B}\,|\phi\rangle} \tag{5.11}$$

Example
Consider a system of 2 qubits, one at site A and the other at site B (distinguished by their positions). Let's now say that both qubits are initially in the $|0\rangle$ state using the canonical basis. The state of the **total** system is then

$$|\text{state}\rangle_{AB} = |0\rangle_A \otimes |0\rangle_B = \begin{bmatrix}1\\0\end{bmatrix} \otimes \begin{bmatrix}1\\0\end{bmatrix} = \begin{bmatrix}1 & 0 & 0 & 0\end{bmatrix}^T \tag{5.12}$$

If we now perform an operation on the system given by $(Z \otimes Y)(X \otimes X)$, the state of our system would evolve as such.

$$\begin{aligned}(Z \otimes Y)(X \otimes X)(|0\rangle_A \otimes |0\rangle_B) &= (Z \otimes Y)(X|0\rangle_A \otimes X|0\rangle_B)\\ &= (Z \otimes Y)(|1\rangle_A \otimes |1\rangle_B)\\ &= (Z|1\rangle_A \otimes Y|1\rangle_B)\\ &= (-|1\rangle_A) \otimes (-i|0\rangle_B) = |1\rangle_A \otimes i|0\rangle_B\end{aligned} \tag{5.13}$$

Or in the language of matrices,

$$\begin{bmatrix}0 & -i & 0 & 0\\ i & 0 & 0 & 0\\ 0 & 0 & 0 & i\\ 0 & 0 & -i & 0\end{bmatrix}\begin{bmatrix}0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\\ 0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\end{bmatrix}\begin{bmatrix}1\\0\\0\\0\end{bmatrix} = \begin{bmatrix}0\\0\\i\\0\end{bmatrix} \tag{5.14}$$

§5.5 Quantum Circuits

We now introduce the formalism of quantum circuit diagrams. Quantum circuits are drawn in the following steps:

1. Specify the qubit inputs.
2. Connect quantum wires from inputs to outputs.
3. Specify intermediate gates to take inputs to outputs.
4. Include any classical post-processing required.

Example
Below is a quantum circuit for producing the *Greenberger-Horne-Zeilinger* (GHZ) state.

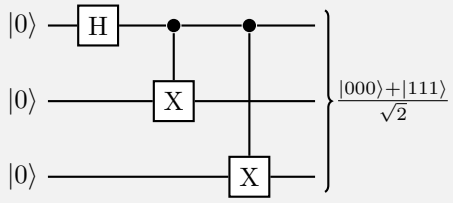


Figure 5.4: Quantum Circuit for GHZ State

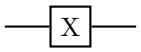
In the circtui above, the H gates are *Hadamard gates* and the gates which span 2 quantum

wires are called *controlled-NOT gates* (CNOT gate). All gates with a linking node to another quantum wire makes that gate a *control gate*.

Above, we have already introduced 2 new gates not previously presented. As such, it would seem a good time to list a set of frequently used quantum gates with their circuit symbols and their matrix representations.

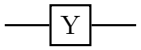
$$\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}$$

Figure 5.5: Hadamard Gate



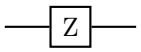
$$\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}$$

Figure 5.6: Pauli-X/NOT Gate



$$\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}$$

Figure 5.7: Pauli-Y Gate

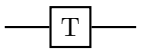


$$\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}$$

Figure 5.8: Pauli-Z Gate

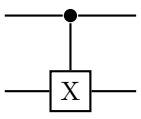
$$\begin{bmatrix}1 & 0\\ 0 & i\end{bmatrix}$$

Figure 5.9: Phase Gate



$$\begin{bmatrix}1 & 0\\ 0 & e^{i\pi/4}\end{bmatrix}$$

Figure 5.10: $\pi/8$ Gate



$$\begin{bmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\end{bmatrix}$$

Figure 5.11: CNOT Gate

Exercise

Given a system of 2 qubits, construct quantum circuits with input $|0\rangle \otimes |0\rangle$ such that they produce the following output states.

1. $|\Phi^+\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$
2. $|\Phi^-\rangle = (|00\rangle - |11\rangle)/\sqrt{2}$
3. $|\Psi^+\rangle = (|01\rangle + |10\rangle)/\sqrt{2}$
4. $|\Psi^-\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$

These are the famous *Bell states*, and are very widely used in quantum information.

§5.6 Spooky Action at a Distance

Consider the state

$$\left|\Phi^+\right\rangle = \frac{|0\rangle_A \otimes |0\rangle_B + |1\rangle_A \otimes |1\rangle_B}{\sqrt{2}} = \frac{|00\rangle_{AB} + |11\rangle_{AB}}{\sqrt{2}} \tag{5.15}$$

The form of this state is very unique because if you notice, having measured and determined the qubit state in A, the state in B is automatically known. In fact, after preparation of the state $|\Phi^+\rangle$, it seems there will always be this binding correlation between particles A and B no matter the distance between them. This phenomena is what physicist termed *quantum entanglement*.

Note: This seems to imply but does **not** actually allow for superluminal information transfer as it would violate Einstein's theory of special relativity.

Entanglement is an integral part of many quantum protocols and algorithms, but is also the biggest challenge impeding the construction of scalable quantum computers today.

§5.7 Beam Me Up, Scotty!

We are now ready to look at our first quantum protocol. This protocol aids in the sending of quantum information, and is made especially useful because of the *no-cloning theorem*.

Theorem 5.7.1. *The no-cloning theorem states that it is impossible to create an identical copy of some arbitrary* ***unknown*** *quantum state* $|\psi\rangle$.

This protocol we are about to learn is called *quantum teleportation*. *Quantum Teleportation* is the process of transmitting quantum information between 2 individuals (Alice and Bob) who

agree on a prior scheme. This is done by means of sending classical bits and utilizing quantum entangle.

The Protocol

1. Alice has a single qubit quantum state which she wants to send over to Bob. Alice and Bob also share a 2-qubit entangled state, which means Alice has 2 qubits and Bob, 1.
2. Alice then performs a measurement in the Bell basis on her 2 qubits which grants her 2 classical bits.
3. Alice then sends her 2 classical bits over a classical channel to Bob.
4. Bob receives the 2 classical bits, and performs the necessary unitary on his qubit according to a previously agreed upon rule, obtaining Alice's original qubit. The state has been effectively teleported.

§5.7.1 Q-Teleportation Analysis

Let's say Alice starts of with an arbitrary single qubit state that she wants to send to Bob, $|\psi\rangle = \alpha |0\rangle_A + \beta |1\rangle_A$. The subscript is used to denote that this is Alice's state. Also assume that Alice and Bob initially share the entangled Bell state, $|\Phi^+\rangle = \frac{|00\rangle_{AB}+|11\rangle_{AB}}{\sqrt{2}}$. The total state of the system is now,

$$\begin{aligned}
\left|\Phi^+\right\rangle_{AB} \otimes |\psi\rangle_A &= \left(\frac{|00\rangle_{AB} + |11\rangle_{AB}}{\sqrt{2}}\right) \otimes (\alpha |0\rangle_A + \beta |1\rangle_A) \\
&= \frac{(\alpha |000\rangle + \alpha |110\rangle + \beta |001\rangle + \beta |111\rangle)_{ABA}}{\sqrt{2}} \\
&= \frac{(\alpha |000\rangle + \alpha |101\rangle + \beta |010\rangle + \beta |111\rangle)_{AAB}}{\sqrt{2}}
\end{aligned}$$

Using the following Bell basis identities,

$$\begin{aligned}
|00\rangle &= \frac{1}{\sqrt{2}}(\left|\Phi^+\right\rangle + \left|\Phi^-\right\rangle) \\
|01\rangle &= \frac{1}{\sqrt{2}}(\left|\Psi^+\right\rangle + \left|\Psi^-\right\rangle) \\
|10\rangle &= \frac{1}{\sqrt{2}}(\left|\Psi^+\right\rangle - \left|\Psi^-\right\rangle) \\
|11\rangle &= \frac{1}{\sqrt{2}}(\left|\Phi^+\right\rangle - \left|\Phi^-\right\rangle)
\end{aligned}$$

$$\Rightarrow \left|\Phi^+\right\rangle_{AB} |\psi\rangle_A = \frac{\alpha(|\Phi^+\rangle + |\Phi^-\rangle) |0\rangle + \alpha(|\Psi^+\rangle - |\Psi^-\rangle) |1\rangle + \beta(|\Psi^+\rangle + |\Psi^-\rangle) |0\rangle + \beta(|\Phi^+\rangle - |\Phi^-\rangle) |1\rangle}{2}$$

$$\Rightarrow \left|\Phi^+\right\rangle_{AB} |\psi\rangle_A = \frac{|\Phi^+\rangle (\alpha |0\rangle + \beta |1\rangle) + |\Phi^-\rangle (\alpha |0\rangle - \beta |1\rangle) + |\Psi^+\rangle (\beta |0\rangle + \alpha |1\rangle) + |\Psi^-\rangle (\beta |0\rangle - \alpha |1\rangle)}{2}$$

The simple rewriting in the Bell basis of Alice's state shows us that Alice's 2 qubits are now entangled, while the entanglement between Alice's and Bob's qubits is broken! Notice how Bob's state now resembles the state that was originally intended for teleportation.

We now have to look into building a circuit that extracts information from Bell states just as measurements in the canonical basis would. The idea behind this is that we would like to first transform the Bell states into separable states, and then into the canonical basis for measurement. It turns out that this can be done by applying the following sequence of gates: *A CNOT gate from the* 1^{st} *to the* 2^{nd} *qubit, then a Hadamard to the* 1^{st} *qubit.*

$$\begin{aligned}
\left|\Phi^+\right\rangle &= \frac{|00\rangle + |11\rangle}{\sqrt{2}} \xrightarrow{\text{CNOT}} \frac{|00\rangle + |10\rangle}{\sqrt{2}} = |+\rangle\,|0\rangle \xrightarrow{H\otimes\mathbb{I}} |00\rangle \\
\left|\Psi^+\right\rangle &= \frac{|01\rangle + |10\rangle}{\sqrt{2}} \xrightarrow{\text{CNOT}} \frac{|01\rangle + |11\rangle}{\sqrt{2}} = |+\rangle\,|1\rangle \xrightarrow{H\otimes\mathbb{I}} |01\rangle \\
\left|\Phi^-\right\rangle &= \frac{|00\rangle - |11\rangle}{\sqrt{2}} \xrightarrow{\text{CNOT}} \frac{|00\rangle - |10\rangle}{\sqrt{2}} = |-\rangle\,|0\rangle \xrightarrow{H\otimes\mathbb{I}} |10\rangle \\
\left|\Psi^-\right\rangle &= \frac{|01\rangle - |10\rangle}{\sqrt{2}} \xrightarrow{\text{CNOT}} \frac{|01\rangle - |11\rangle}{\sqrt{2}} = |-\rangle\,|1\rangle \xrightarrow{H\otimes\mathbb{I}} |11\rangle
\end{aligned}$$

Hence we see that by passing Alice's 2 qubits through the above circuit consisting of a CNOT and a Hadamard gate, we get states in computational basis that will allow us to correct Bob's state! The final step in the protocol for Bob to retrieve Alice's initial quantum state is to apply the respective *recovery operators* as follows

$$\begin{aligned}
00 &\to \mathbb{I} \\
01 &\to \sigma_x \\
10 &\to \sigma_z \\
11 &\to \sigma_x\sigma_z
\end{aligned}$$

Amazingly, Alice has sent her single qubit quantum state to Bob by the transfer of 2 classical bits of information. We can also write this in quantum circuit notation as follows (figure 5.12).

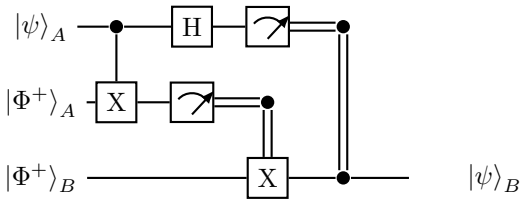


Figure 5.12: Quantum Teleportation Circuit

In the circuit above,

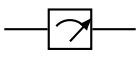


Figure 5.13: Measurement Apparatus

is the symbol for canonical basis measurement.

Note: Single lines are used to indicate quantum wires whereas double lines indicate classical wires.

§5.8 Deutsch–Jozsa's Algorithm

We will now look at a quantum algorithm proposed by David Deutsch and Richard Jozsa in 1992. This simple algorithm was one of the first Q-algorithms promising exponential speed-up from any deterministic classical algorithm. First, we state Deutsch–Jozsa's problem.

Deutsch–Jozsa's problem:
Given an *oracle* function f on n bits, we want to determine if f is either

1. Constant: $f(x) = 0$ (or 1) for all values of x.
2. Balanced: $f(x) = \begin{cases} 0, & \text{half of the } x \text{ inputs} \\ 1, & \text{other half of the } x \text{ inputs} \end{cases}$

In computer science, this is known as a *promise problem*. Classically, we would have to look up exactly $2^n/2+1$, or $\mathcal{O}(2^n)$ function outputs in the most unlucky scenario to confirm the function is **not** constant. The classical circuit would look as such.

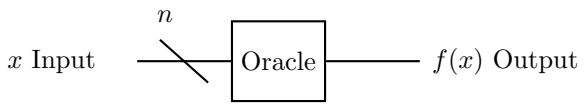


Figure 5.14: Classical Deutsch–Jozsa Circuit

The quantum analog of the classical circuit would be as follows. Note that we have to make the quantum circuit *reversible*[1].

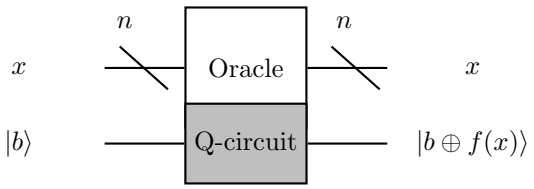


Figure 5.15: Quantum Deutsch–Jozsa Circuit

The x input represents an n-bit binary string (e.g. $x = 0010110...01$). Note that in the quantum circuit above, the qubits which are known in advance are called *ancilla bits*. In this handbook, we will be presenting the algorithm for an n qubit circuit but will only perform an analysis for the 2 qubit case.

[1]Reversible computing is a model of computation where the computational process is reversible (*isentropic*).

The Deutsch–Jozsa Algorithm

1. We begin with $n+1$ qubit registers, the top n of which start in state $|0\rangle$ while the last is in state $|1\rangle$.
2. We apply Hadamard gates to every qubit in the circuit.
3. The oracle is now applied to all qubits as in figure 5.15.
4. We again apply Hadamard gates, but now only to the top n registers.
5. We measure the top n registers in the canonical basis.

The 2 qubit circuit diagram for this is illustrated below.

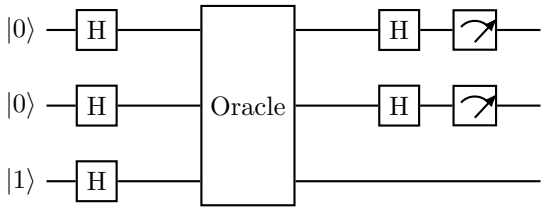


Figure 5.16: 2 Qubit Deutsch–Jozsa Algorithm

§5.8.1 2-Qubit Algorithm Analysis

As seen from the protocol above, we initially start off with the state $|001\rangle$. After passing it through the Hadamard gates, the state evolves as follows.

$$\begin{aligned} H^{\otimes 3}|001\rangle &= \frac{1}{\sqrt{2^3}}(|0\rangle+|1\rangle)\otimes(|0\rangle+|1\rangle)\otimes(|0\rangle-|1\rangle) \\ &= \frac{1}{\sqrt{2^3}}\sum_{x=0}^{2^2-1}|x\rangle\otimes(|0\rangle-|1\rangle) \end{aligned} \tag{5.16}$$

Above, we adopted the shorthand notation where $H\otimes H\otimes H$ is written as $H^{\otimes 3}$. Again, remember that x represents a 2-bit binary string. After this, we apply the oracle which yields

$$\begin{aligned} U_{\text{Oracle}}\left(\frac{1}{\sqrt{2^3}}\sum_{x=0}^{2^2-1}|x\rangle\otimes(|0\rangle-|1\rangle)\right) &= \frac{1}{\sqrt{2^3}}\sum_{x=0}^{2^2-1}|x\rangle\otimes(|f(x)\rangle-|1\oplus f(x)\rangle) \\ &= \frac{1}{\sqrt{2^3}}\sum_{x=0}^{2^2-1}(-1)^{f(x)}|x\rangle\otimes(|0\rangle-|1\rangle) \end{aligned} \tag{5.17}$$

$\oplus$ represents bitwise addition (addition modulo 2). Once again, we apply Hadamards to the first 2 qubits, giving

$$\begin{aligned} &H^{\otimes 2}\otimes\mathbb{I}\left(\frac{1}{\sqrt{2^3}}\sum_{x=0}^{2^2-1}(-1)^{f(x)}|x\rangle\otimes(|0\rangle-|1\rangle)\right) \\ &= \frac{1}{\sqrt{2^5}}\sum_{x=0}^{2^2-1}(-1)^{f(x)}\left(\sum_{y=0}^{2^2-1}(-1)^{x\cdot y}|y\rangle\right)\otimes(|0\rangle-|1\rangle) \end{aligned} \tag{5.18}$$

Above, the dot product between $x \cdot y$ is performed over a *finite field*. More explicitly, $x \cdot y = x_0y_0 \oplus x_1y_1 \oplus ... \oplus x_ny_n$. Lastly, we perform a measurement on the 2 top qubits in the canonical basis. To see what the measurements could yield, we check the probability of obtaining $|00\rangle$. Looking at the final state before measurement (dropping the last auxiliary qubit),

$$\frac{1}{2^2}\sum_{x=0}^{2^2-1}(-1)^{f(x)}\Big(\sum_{y=0}^{2^2-1}(-1)^{x\cdot y}\,|y\rangle\Big) \tag{5.19}$$

we see that only 1 term in the sum over y would be $|00\rangle$ with coefficient $\frac{1}{2^2}\sum_{x=0}^{2^2-1}(-1)^{f(x)}$. Hence the probability of measuring $(0,0)$ from the top 2 qubits is

$$\mathbb{P}(00) = \left|\frac{1}{2^2}\sum_{x=0}^{2^2-1}(-1)^{f(x)}\right|^2 \tag{5.20}$$

From this, we see that if the function f is constant, we get

$$\mathbb{P}(00) = \left|\frac{1}{2^2}\big((-1)^0+(-1)^0+(-1)^0+(-1)^0\big)\right|^2 = \left|\frac{1}{2^2}\big((-1)^1+(-1)^1+(-1)^1+(-1)^1\big)\right|^2 = 1 \tag{5.21}$$

Whereas if the function f is balanced, we get

$$\mathbb{P}(00) = \left|\frac{1}{2^2}\big((-1)^0+(-1)^0+(-1)^1+(-1)^1\big)\right|^2 = 0 \tag{5.22}$$

So amazingly, we see that the Deutsch–Jozsa algorithm definitively produces $|00\rangle$ for constant functions and $|11\rangle$ for balanced functions! This means that with just **one** query, we have solved the Deutsch–Jozsa problem (vs $2^{n-1}+1$ queries classically)! This shows the power of quantum computers.

§ **SUMMARY** §

In this chapter,

- We very briefly looked at some classical models of computation and basic complexity theory.
- We learned what a qubit is and how any 2-level quantum system can be used as implementations of qubits.
- We learned about tensor products as a method to describe many-body quantum systems with exponentially expanding Hilbert spaces.
- We looked at the formalism of quantum circuit diagrams and how single unitary operators can act as quantum gates.
- We finally attained a mathematically rigorous understanding of entanglement that was introduced in chapter 1.
- We saw how entanglement could be utilized in the Q-teleportation protocol to effectively send a quantum state from Alice to Bob. The Q-teleportation protocol was provided in words and a circuit diagram.
- We learned the Deutsch–Jozsa algorithm, which solves the Deutsch–Jozsa problem exponentially faster than any deterministic classical algorithm.

Exercises

1. For all the Pauli matrices σ_j, prove that since they are involutory, they satisfy
$$e^{i\theta\sigma_j} = \mathbb{I}\cos(\theta) + i\sigma_j \sin(\theta) \tag{5.23}$$

2. The *anti-commutator* of 2 operators $\hat{A}$ and $\hat{B}$ is defined as $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$. Prove that
$$\{\sigma_i, \sigma_j\} = 2\delta_{ij}\mathbb{I} \tag{5.24}$$

3. Construct a 4×4 unitary matrix S that swaps the tensor product of 2 qubit states $S|\psi\rangle|\phi\rangle = |\phi\rangle|\psi\rangle$. (Hint: It can be constructed with purely real entries.)

4. Find the recovery operators for the Q-teleportation protocol if Alice and Bob initially shared either $|\Phi^-\rangle, |\Psi^+\rangle$ or $|\Psi^-\rangle$ instead.

5. Following the analysis of the 2-qubit Deutsch-Jozsa algorithm, do the same analysis but extended to the n-qubit case. Be sure to take note of the normalization factors.

Chapter 6

Bell vs EPR

We come to the closing chapter of our journey through the quantum world. Here, I will present the erroneous claims of Einstein, Podolsky, and Rosen (EPR), along with the proof of falsity given by John Stewart Bell. The mathematical statement put forth by Bell (referred to as Bell's theorem) is likely the most profound fact about quantum mechanics. Even though Bell's theorem would not really be considered a 'abstracted' topic from quantum physics, the implications of it seem an appropriate closer that will leave you rightfully baffled by the mysteries of our universe.

§6.1 More on Spin Measurement

Before we discuss what is known as the *EPR paradox*, we have to familiarize ourselves with arbitrary directional spin measurement. As earlier discussed, the spin vector space is embedded in the space of 3D continuous rotations. This means that any axis in 3D space can be an axis for spin measurement. Using polar coordinates, consider some unit vector $\vec{r} = \{\sin\theta\cos\phi, \sin\theta\cos\phi, \cos\theta\}^T$. An illustration of the spin along $\vec{r}$ in the "Lie group/algebra visualization" is shown below.

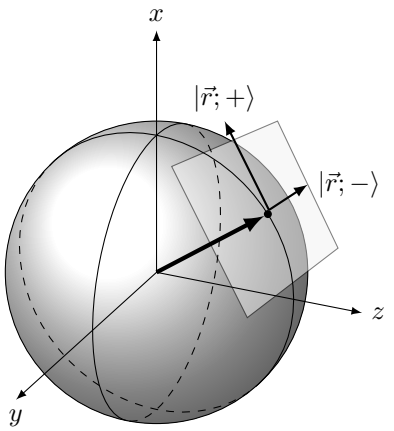


Figure 6.1: Spin Along an Arbitrary Axis

It can be shown that the spin operator along this axis is given by

$$\vec{r}\cdot\hat{\vec{S}} = \hat{S}_x\sin\theta\cos\phi + \hat{S}_y\sin\theta\sin\phi + \hat{S}_z\cos\theta = \frac{\hbar}{2}\vec{r}\cdot\hat{\vec{\sigma}} \tag{6.1}$$

with eigenstates

$$\begin{aligned} |\vec{r};+\rangle &= \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle \\ |\vec{r};-\rangle &= \sin\frac{\theta}{2}|0\rangle - e^{i\phi}\cos\frac{\theta}{2}|1\rangle \end{aligned} \tag{6.2}$$

It is a good exercise for you check that the states and operators presented with arbitrary $\{\theta,\phi\}$ correspond to the Pauli matrices and their eigenstates for $\sigma_x : \{\pi/2, 0\}$, $\sigma_y : \{\pi/2, \pi/2\}$ and $\sigma_z : \{0, 0\}$. From here, consider spin measurements along the arbitrary axis $\vec{r}$. Given some quantum state, we would be able to extract probabilistic information about the result of such a measurement via projective methods. This can be illustrated by considering the following.

Probability Retrieval:

Generally speaking, given some basis $\{|\vec{r};+\rangle, |\vec{r};-\rangle\}$ and an arbitrary quantum state $|\Psi\rangle$, we can compute the probability of attaining the eigenvalue $+1$ as follows.

$$\mathbb{P}(+1) = |\langle\vec{r};+|\Psi\rangle|^2 \tag{6.3}$$

And similarly for the eigenvalue -1. For instance, let's say we want to make a measurement in the canonical basis $\{|0\rangle, |1\rangle\}$ on the state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$. Then we see that the associated probabilities for getting the ±1 eigenvalues are as follows.

$$\begin{aligned} \mathbb{P}(+1) &= |\langle 0|\psi\rangle|^2 \\ &= |\langle 0|(\alpha|0\rangle + \beta|1\rangle)|^2 \\ &= |\alpha|^2 \end{aligned} \tag{6.4}$$

$$\begin{aligned} \mathbb{P}(-1) &= |\langle 1|\psi\rangle|^2 \\ &= |\langle 1|(\alpha|0\rangle + \beta|1\rangle)|^2 \\ &= |\beta|^2 \end{aligned} \tag{6.5}$$

§6.2 Just An Illusion?

In 1935, Albert Einstein, Boris Podolsky and Nathan Rosen (EPR) claimed that the wave function was an incomplete description of our physical reality, implying that the Copenhagen interpretation of quantum mechanics is unsatisfactory. Instead, they proposed the existence of *hidden variables* which govern the quantum phenomena we observe in a deterministic fashion. This followed from their belief of *local realism* (The idea that objects are only affected by their **immediate** surroundings), which was key in classical field theories like general relativity. This greatly contradicted the notion of entanglement, as entanglement seems to allow for **instantaneous action at a distance**.

It was in 1964 that Bell came up with a rigorous proof that EPR's predictions could not be true, which was firmly validated by the experimental works of Alain Aspect [3] in 1981. The rebuttal is as follows.

Elucidation of Bell's Theorem

First consider an entangled state like $|\Psi^+\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$. This is also known as the *singlet state* due to its total spin angular momentum. EPR would say that this so-called entangled state are just pairs of particles with definite spins. The point being that quantum mechanical measurements are reproducible by using a large ensemble of these definite spin pairs with the following distribution:

- In 50% of pairs, particle 1 has spin along $+\hat{z}$ and particle 2 has spin along $-\hat{z}$, and
- the other 50% of pairs have particle 1 along $-\hat{z}$ and particle 2 along $+\hat{z}$.

This would resolve the perfect non-local correlation between the spins of the two particles where $P(+\hat{z}, -\hat{z}) = 1/2$. What if we now tried to measure this state along 3 different axes, $\vec{a}, \vec{b}$ and $\vec{c}$ with equal angular spacing θ between them? A visualization of this is given below (6.2).

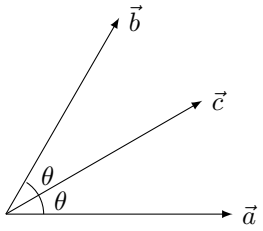


Figure 6.2: Evenly Spaced Axes

Let's see what we would get if we followed EPR's proposition. Given some population of N particle pairs with a deterministic distribution of states as displayed in the table below. We will label the deterministic state of the particles within each pair with a triple $(\pm a, \pm b, \pm c)$, where the parity indicates the corresponding eigenvalue $\pm\hbar/2$ along the measurement axis $\vec{a}$, $\vec{b}$ or $\vec{c}$.

State Population	Particle 1	Particle 2
N_1	(a, b, c)	(-a,-b,-c)
N_2	(a, b,-c)	(-a,-b, c)
N_3	(a,-b, c)	(-a, b,-c)
N_4	(a,-b,-c)	(-a, b, c)
N_5	(-a, b, c)	(a,-b,-c)
N_6	(-a, b,-c)	(a,-b, c)
N_7	(-a,-b, c)	(a, b,-c)
N_8	(-a,-b,-c)	(a, b, c)

Table 6.1: The populations of particle pairs in each unique state. The populations **must** satisfy the relation $\sum_{j=1}^{8} N_j = N$.

From table 6.1, we can derive the following probabilities:

$$\mathbb{P}(a;b) = \frac{N_3 + N_4}{N}, \quad \mathbb{P}(a;c) = \frac{N_2 + N_4}{N}, \quad \mathbb{P}(c;b) = \frac{N_3 + N_7}{N} \tag{6.6}$$

And one can easily see that

$$\begin{aligned} &\frac{N_2 + N_4}{N} + \frac{N_3 + N_7}{N} \geq \frac{N_3 + N_4}{N} \\ \Rightarrow \quad &\boxed{\mathbb{P}(a;c) + \mathbb{P}(c;b) \geq \mathbb{P}(a;b)} \end{aligned} \tag{6.7}$$

Equation 6.7 above is known as *Bell's inequality*. Now we look at the same probabilities but derived from the (experimentally verified) mathematical structure of quantum mechanics. Let's be clear that the point of this proof is to show that we do not need these statistical ensembles for probability to arise. As such, we can simply consider a single pair of spin-$\frac{1}{2}$ particles. To give weight to this proof, we will further assert that this 'spin-pair' is in an entangled state similar to the state $|\Psi^+\rangle$. For convenience, we utilize the *rotational invariance* of this state to say that it is the same for any arbitrary direction $\vec{r}$. As such, we can consider the entangled state along $\vec{r}$ as

$$|\Psi\rangle_{\vec{r}} = \frac{|\vec{r};+\rangle\,|\vec{r};-\rangle + |\vec{r};-\rangle\,|\vec{r};+\rangle}{\sqrt{2}} \tag{6.8}$$

The respective probabilities used in the Bell's inequality under the quantum formalism are then given as follows:

$$\begin{aligned} \mathbb{P}(a;b) &= \left|\langle\vec{a};+|\left\langle\vec{b};+\middle|\Psi\right\rangle_{\vec{a}}\right|^2 \\ &= \frac{1}{2}\sin^2\theta \end{aligned} \tag{6.9}$$

$$\begin{aligned} \mathbb{P}(a;c) &= |\langle\vec{a};+|\,\langle\vec{c};+|\Psi\rangle_{\vec{a}}|^2 \\ &= \frac{1}{2}\sin^2\frac{\theta}{2} \end{aligned} \tag{6.10}$$

$$\begin{aligned} \mathbb{P}(c;b) &= \left|\langle\vec{c};+|\left\langle\vec{b};+\middle|\Psi\right\rangle_{\vec{c}}\right|^2 \\ &= \frac{1}{2}\sin^2\frac{\theta}{2} \end{aligned} \tag{6.11}$$

where we have utilized the probability retrieval method discussed earlier to attain these results. Substituting this into Bell's inequality, we get

$$\begin{aligned} &\frac{1}{2}\sin^2\frac{\theta}{2} + \frac{1}{2}\sin^2\frac{\theta}{2} \overset{?}{\geq} \frac{1}{2}\sin^2\theta \\ \Rightarrow \quad &\boxed{\sin^2\frac{\theta}{2} \overset{?}{\geq} \frac{1}{2}\sin^2\theta} \end{aligned} \tag{6.12}$$

I left the question mark above the inequality because we are still unsure if the inequality holds. To check this, we consider the small angle approximation. For $\theta << 1$, it follows that $\sin(\theta) \approx \theta$. This means that $\sin^2\frac{\theta}{2} \approx \left(\frac{\theta}{2}\right)^2 = \frac{\theta^2}{4}$ and $\frac{1}{2}\sin^2\theta \approx \frac{1}{2}\theta^2$. It is obvious that $\frac{\theta^2}{2} > \frac{\theta^2}{4}$, so we see that the probabilities derived from quantum mechanics causes the inequality to fail! The implication being that Einstein's, Podolsky's, and Rosen's interpretation of quantum mechanics is **wrong**. There are **no** hidden variables. Our universe at such scales is **intrinsically** probabilistic. This is why quantum mechanics is such a useful tool, this is why we need quantum mechanics.

§ **SUMMARY** §

In this chapter,

- We looked at Einstein's, Podolsky's, and Rosen's interpretation of quantum mechanics, which suggests the existence of random variables to resolve local realism.
- We learned how to measure spin along an arbitrary axis in 3D space using polar coordinates.
- We worked through performing spin measurements along 3 different axes with the assumption that EPR were right, only to come to the inevitable conclusion that this disagrees with quantum mechanics.

Exercises

1. Prove that $\{|\vec{r};+\rangle, |\vec{r};-\rangle\}$ are indeed the eigenstates of $\vec{r}\cdot\hat{\vec{S}}$ by deriving them.
2. Take the unit vector $\{1/\sqrt{2}, 0, 1/\sqrt{2}\}^T$ in 3D space.
   (a) What is the spin operator along this direction?
   (b) Find the action of this operator on the states $\{|0\rangle, |1\rangle\}$ and $\{|+\rangle, |-\rangle\}$.
   (c) Using the sphere visualization, find a geometric picture of the action of this operator on the states listed above.
3. Using the techniques that Bell employed for his analysis, re-evaluate the EPR proposition with spin measurements in 2 directions instead of 3. Is this enough to reject the EPR hypothesis?
4. Can you think of alternative interpretations to quantum mechanics apart from the Copenhagen one? Let your imagination run wild and explore these ideas!

Going Beyond

Having read this rapid introduction to quantum science and its emergent technologies, I would like to point you to several invaluable academic resources that will lead you deeper into the rabbit hole. For a more exhaustive coverage of introductory quantum mechanics, I would recommend 2 texts depending on your preference and capacity.

- David J. Griffiths' *'Introduction to Quantum Mechanics'* [4] gives a rather gentle and succinct treatment of quantum mechanics, suitable for the level of an undergraduate.
- Ramamurti Shankar's *'Principles of Quantum Mechanics'* [5] is a much more thorough text on quantum mechanics with extensive mathematical rigour. This text definitely finds its place in an advanced undergraduate or graduate course.

Additionally, *MIT open courseware* has an entire bank of free, high quality educational content that is easily accessible. I highly encourage the use and support of this resource. As for quantum computing, *'Quantum Computation and Quantum Information'* by Nielsen and Chuang [6] gives a wonderfully comprehensive, self-contained text of this field. The *University of California, Berkeley* and *California Institute of Technology* also have well written collections of quantum computing notes ([8], [9]) online which one may find useful. I have personally utilized and

benefited greatly from the use of the resources mentioned above, from which much of these notes are inspired.

Of course, *Google scholar* [11] and *arXiv* [12] are your best friends when it comes to scouting for scientific literature. Being able to sieve through the endless pool of manuscripts for what interests you is definitely a skill on its own, and a valuable one I might add. Be sure to include the appropriate keywords in your searches and use the citations to navigate around other relevant articles. In our day and age, we hold the key to boundless knowledge in the palms of our hands. It is our responsibility to make the best of it as engines of discovery which in turn, will lead to the betterment of humanity.

Appendices

Appendix A

Early Beginnings of QM

§A.1 Catastrophic Beginnings

In 1900, scientists and researches were studying the theory of *Black-Body Radiation*. Black-body radiation is thermal electromagnetic radiation which is emitted by a body in thermal equilibrium with its environment at some temperature, T. It was found that black-body radiation has a characteristic and continuous frequency spectrum (where frequency is denoted by ν). The energy density over an infinitesimal frequency interval $d\nu$ was initially modelled by the *Rayleigh-Jeans Formula*,

$$\rho(\nu, T) = \frac{8\pi k_B T \nu^2}{c^3} d\nu \tag{A.1}$$

However, due to the inverse relationship between wavelengths (λ) and frequencies (ν) of radiation, this equation diverges for small values of λ (in the UV range) and does **not** give a completely accurate picture of the spectrum. This was known as the ***Ultraviolet Catastrophe***.

As a result, Max Planck proposed an exponential term raised to a dimensionless function linear in ν. In doing so, Planck postulated the equation,

$$\boxed{\rho(\nu, T) = \frac{8\pi h \nu^3}{c^3 (e^{\frac{h\nu}{k_B T}} - 1)} d\nu} \tag{A.2}$$

Where the *Planck's Constant* has the value $h = 6.62 \times 10^{-34} Js$. This was eventually discovered to be a *constant of nature*.

Following this, Einstein proposed that light came in discrete packets (*photons*) in 1905. He presented the famous photon energy and momentum equations,

$$E = h\nu,\ p = \frac{h}{\lambda} \tag{A.3}$$

Then in 1920, Louis de Broglie suggested that in fact **all** matter has wave properties. At that time, nobody knew what these waves were and simply called them '*matter waves*'. 1924 was the year Erwin Schrödinger presented his **famous** and **fundemental** equation, *the Schrödinger's Equation*,

$$\boxed{i\hbar\frac{\partial}{\partial t}\Psi = \hat{H}\Psi} \tag{A.4}$$

which revolutionized the study of quantum mechanics...

§A.2 Experimental Persuasions

Physics is a largely experimental science, so it is important that we explore several experiments that proved the existence of quantum phenomena. 2 of the most prominent experimental results are the **photoelectric effect** and **Compton scattering photon energies**.

§A.2.1 The Photoelectric Effect

Performed by Hertz in 1887, the experiment consisted of a metal plate irradiated with photons in an evacuated chamber with a collector metal plate on the opposite end. As a result, an electric current was detected through the wire connecting the 2 metals plates outside the evacuated chamber. This indicated the release of electrons from the irradiated plate, dubbed as **Photoelectrons**.

Unique Properties of Photoelectrons

While performing this experiment, there were several experimental findings which were unexpected in a classical theory of electromagnetic radiation. These are concisely listed below.

1. The energy of photoelectrons are **independent** of the light intensity.
2. There is a minimum *Threshold Frequency* (ν_0), such that only energies associated to frequencies above ν_0 ($E \geq \phi(\nu_0)$) produce a photoelectric current.
3. The magnitude of the photoelectric current (rate of electrons released) is proportional to the light intensity.

The quantized photon energy equation proposed by Einstein in 1905 modelled this result perfectly for which the photoelectron energy is given by,

$$\boxed{E_\gamma = h\nu_\gamma = \frac{1}{2}mv^2 + \phi} \tag{A.5}$$

Where E_γ represents incident photon energy and this result was verfied by Millikan in 1915.

§A.2.2 Compton Scattering

Performed by Arthur Holly Compton in 1923, the experiment consisted of X-ray photons scattering off electrons that were virtually 'free' ($E_{\gamma,X-ray} >> \phi$). Compton scattering showed an experimental violation of *Thompson Scattering*, which was the low energy limit of the scattering experiment leading to classically expected results (incident and outgoing EM radiation carried the same energy).

However in Compton scattering, outgoing photons (measured by a detector at an angle θ from the optical axis) had less energy than the incident photos. This is attributed to the kinetic energy gained by emitted photoelectrons. This phenomena is nicely described by the relationship between the wavelengths of scattered and incident photons (note that $E \propto \frac{1}{\lambda}$),

$$\boxed{\lambda_{scattered} = \lambda_{incident} + (1 - \cos(\theta))\lambda_{Compton}} \tag{A.6}$$

$$\lambda_{Compton} = \frac{h}{cm_{electron}} \tag{A.7}$$

Interestingly, the intensity measured by the detector produced a bi-modal distribution peaked at $\lambda_{incdent}$ and $\lambda_{scattered}$. This result, along with the results of the *Electron Diffraction Experiment* motivated de Broglie to propose in 1924, that **all** particles have wave attributes. This postulate was known as *Wave-Particle Duality* (Note that these 'waves' are **not** the conventional notion of waves like in classical mechanics).

Appendix B

Elitzur-Vaidman Probabilistic Improvements

Earlier, we saw that Mach-Zehnder interferometry enables us to detect working Elitzur Vaidman bombs with a $1/4$ *probability of success. However in practice, a* $1/4$ *probability of success isn't very good, especially when we are dealing with bombs! This chapter in the appendix talks about how we can modify the set-up to increase the probability of detection without detonation. First, consider a new kind of beam splitter that receives, reflects and transmits photons horizontally.*

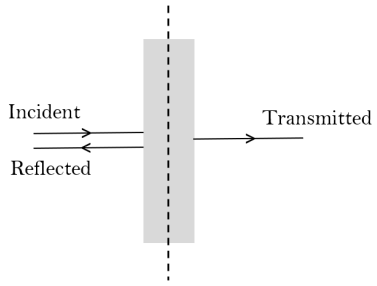


Figure B.1: Horizontal Beam Splitter

For this regime, we will take any beam on the left side of the beam splitter to be $|L\rangle$ and any beam on the right to be $|R\rangle$.

$$|L\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |R\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{B.1}$$

As for our beam splitter matrix, we model it as such.

$$U_{BS} = \begin{bmatrix} \cos\left(\frac{\pi}{2N}\right) & i\sin\left(\frac{\pi}{2N}\right) \\ i\sin\left(\frac{\pi}{2N}\right) & \cos\left(\frac{\pi}{2N}\right) \end{bmatrix}, \quad N \in \mathbb{Z} \tag{B.2}$$

The reason we model our beam splitter in this way is to simplify computation for iterative left multiplication of the matrix. Consider a set-up where we place this horizontal beam splitter

between 2 mirrors and send in a photon from the left. After passing through the beam splitter twice, the resulting action of the beam splitter is given by

$$\begin{aligned} U_{BS}U_{BS} &= \begin{bmatrix} \cos\left(\frac{\pi}{2N}\right) & i\sin\left(\frac{\pi}{2N}\right) \\ i\sin\left(\frac{\pi}{2N}\right) & \cos\left(\frac{\pi}{2N}\right) \end{bmatrix} \begin{bmatrix} \cos\left(\frac{\pi}{2N}\right) & i\sin\left(\frac{\pi}{2N}\right) \\ i\sin\left(\frac{\pi}{2N}\right) & \cos\left(\frac{\pi}{2N}\right) \end{bmatrix} \\ &= \begin{bmatrix} \cos\left(\frac{\pi}{2N}+\frac{\pi}{2N}\right) & i\sin\left(\frac{\pi}{2N}+\frac{\pi}{2N}\right) \\ i\sin\left(\frac{\pi}{2N}+\frac{\pi}{2N}\right) & \cos\left(\frac{\pi}{2N}+\frac{\pi}{2N}\right) \end{bmatrix} \end{aligned}$$

Following this iteratively, after k passes through the beam splitter, we get

$$\boxed{U_{BS}^{k} = \begin{bmatrix} \cos\left(\frac{k\pi}{2N}\right) & i\sin\left(\frac{k\pi}{2N}\right) \\ i\sin\left(\frac{k\pi}{2N}\right) & \cos\left(\frac{k\pi}{2N}\right) \end{bmatrix}} \tag{B.3}$$

$$\begin{aligned} &\Rightarrow U_{BS}^{k}\left|L\right\rangle = \begin{bmatrix} \cos\left(\frac{k\pi}{2N}\right) & i\sin\left(\frac{k\pi}{2N}\right) \\ i\sin\left(\frac{k\pi}{2N}\right) & \cos\left(\frac{k\pi}{2N}\right) \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} \cos\left(\frac{k\pi}{2N}\right) \\ i\sin\left(\frac{k\pi}{2N}\right) \end{bmatrix} \\ &\Rightarrow \mathbb{P}(\text{left}) = \cos^2(\frac{k\pi}{2N}), \quad \mathbb{P}(\text{right}) = \sin^2(\frac{k\pi}{2N}) \end{aligned} \tag{B.4}$$

Now let us reinsert our Elitzur-Vaidman bomb into the experiment on the right-hand side of the beam splitter. We know that after 1 pass, the probability of the photon being on the left is $\cos^2(\frac{\pi}{2N})$. With the bomb in place, the increment stacks different as now with every additional pass, the probability is raised to an additional power.

$$\Rightarrow \mathbb{P}_{N\text{passes}}(\text{left}) = \left(\cos\left(\frac{\pi}{2N}\right)\right)^{2N} \approx 1 - \frac{\pi^2}{4N} \tag{B.5}$$

$$\Rightarrow \boxed{\mathbb{P}(\text{detonation}) = 1 - \left(\cos\left(\frac{\pi}{2N}\right)\right)^{2N} \approx \frac{\pi^2}{4N}} \tag{B.6}$$

This result tells us that we can make the probability of detonation arbitrarily small by having the photon 'bounce back and forth' between the mirrors! Of course to make the bomb detection 100% accurate, one would have to wait an infinitely long amount of time as $N \to \infty$.

Appendix C

Wave Mechanics

In this chapter of appendices, we present a more indepth coverage of the interpretation and mathematical formalism of quantum matter waves. We will see the differences and similarities between classical waves and matter waves. We will explore interesting properties of these waves and after which, the cumulation of these insights will lead to the conclusion of how these matter waves are to be interpreted.

§C.1 Galilean Transformation of Classical Waves

In classical mechanics, a Galilean transformation is a linear operation used to map coordinates of one inertial reference frame to those in another. These reference frames must differ **only** by constant relative motion. In the study of Galilean transformations, it is useful to look at quantities known as *Galilean invariants* (not to be confused with *Galilean invariance*). These are quantities that remain unchanged despite having moved from one reference frame to another.

In classical wave mechanics, the phase ($\phi = kx - \omega t$) of a wave is a Galilean invariant. Allow us to differentiate between the coordinates of the 2 inertial reference frames by adding a prime superscript. Consider the case where there are 2 observers in 2 different reference frames. The unprimed observer is moving with velocity v and the primed observer is moving with velocity v', both with respect to some stationary observer. Since ϕ is an invariant quantity,

$$\begin{aligned}
&\Rightarrow \phi = \phi' \\
&\Rightarrow kx - \omega t = k'x' - \omega' t' \\
&\Rightarrow \frac{2\pi}{\lambda}(x - vt) = \frac{2\pi}{\lambda'}(x' - (v' - v)t') \\
&\Rightarrow \frac{2\pi}{\lambda}x - \frac{2\pi}{\lambda}vt = \frac{2\pi}{\lambda'}x' - \frac{2\pi}{\lambda'}(v' - v)t' \\
&\Rightarrow \boxed{\lambda = \lambda'}
\end{aligned} \tag{C.1}$$

Thus, this also makes the wavelength, λ of a classical wave to be a Galilean invariant!

§C.2 Matter Waves

A wave can be well described by it's wave vector (k) and frequency ($\frac{\omega}{2\pi}$). This leads us to look for these variables in our attempt to gain a description of matter waves. From the postulates of Einstein and Planck, we know that these quantities arise in the relations

$$p = \hbar k,\ E = \hbar\omega \tag{C.2}$$

Allow us to first look at a quantity that shows up in classical wave mechanics known as the *Phase Velocity*. The phase velocity is defined by the ratio of the angular frequency of the wave and its wave vector. Thus for a matter wave, we see that

$$v_{phase} = \frac{\omega}{k} = \frac{\hbar\omega}{\hbar k} = \frac{E}{p} = \frac{\frac{1}{2}mv^2}{mv} = \frac{1}{2}v$$

This reveals the fact that the phase velocity (also known as the carrier-wave velocity) of a matter wave is twice the velocity of a matter particle with the same energy and momentum. We will soon see that *wavepackets* are what resolves this difference in velocities.

§C.3 Group Velocity

Let us know look at another quantity known as the *Group Velocity*. The group velocity of a wave is defined by the first derivative of its dispersion relation with respect to the wave vector. Hence, for a matter wave, this works out to be

$$v_{group} = \frac{d\omega}{dk} = \frac{dE}{dp} = \frac{d}{dp}(\frac{p^2}{2m}) = \frac{p}{m} = v$$

We see here that the group velocity of a matter wave exactly corresponds to the particle velocity! Therefore it is now useful to define group velocities in this new context of matter waves.

Definition C.3.1. Group Velocity: *The group velocity is defined as the velocity of a wavepacket, which is constructed by a superposition of its constituent (purely sinusoidal) waves denoted by their individual wave vectors, k.*

Definition C.3.2. Wavepacket: *A wavepacket is defined by the integral over k, of all constituent sinusoidal waves.*

$$\Psi_{wavepacket}(x,t) = \int_0^\infty dk\Phi(k)e^{i(kx-\omega(k)t)} \tag{C.3}$$

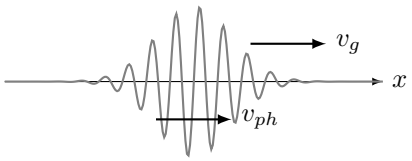


Figure C.1: Wavepacket with Group Velocity v_g and Phase Velocity v_{ph}

The amplitude ($\Phi(k)$) attached to the constituent waves of the wavepacket narrowly peaks at a particular value $k = k_0$, which allows for the construction of the wavepacket in the manner as presented above. As such, matter particles appear to be some kind of wavepacket composed of continuous carrier waves. It is only natural that we now ask how these wavepackets move since they have an associated group velocity.

§C.4 Principle of Stationary Phase

To retrieve a finite value of the group velocity of a wavepacket, we need to evaluate the derivative of ω at some particular value of k. The question is now, how do we find this value of k that accurately gives us an idea of how this wavepacket is travelling? To build intuition to solving this, we must first understand that integrals over high frequency sinusoidal waves tend to vanish due to the oscillatory nature of the function parity. Hence for our wavepacket integral **not** to vanish from the sinusoidal carrier waves, we require that these sinusoidal waves are *'slowly varying'* near the region where our amplitude $\Phi(k)$ peaks. To ensure this, we employ the *Principle of Stationary Phase*.

Principle of Stationary Phase

For a wavepacket that is sharply peaked at $k = k_0$, the integral over k of all constituent sinusoidal waves will only be able to give a significant contribution around $k \sim k_0$. Hence, the phase factor ($\phi(k) = kx - \omega(k)t$) must be stationary at $k = k_0$ to produce a non-vanishing result.

$$\left.\frac{d\phi(k)}{dk}\right|_{k=k_0} = 0 \tag{C.4}$$

Continued analysis of this gives,

$$\begin{aligned} \Rightarrow \quad & x - t \left.\frac{d\omega(k)}{dk}\right|_{k=k_0} = 0 \\ & v_g(k_0) = \left.\frac{d\omega(k)}{dk}\right|_{k=k_0} \\ \Rightarrow \quad & \boxed{x = v_g(k_0)t} \end{aligned} \tag{C.5}$$

This result shows that up to a good approximation within small time intervals, the wavepacket moves linearly in time with a constant velocity v_g.

§C.5 Time-Evolving Wavepackets

For small intervals of time, t, it is convenient to use the *Stationary Phase Approximation* to observe how a wave evolves in time and progresses in space. The stationary phase approximation

is done by taking the *Taylor Expansion* of the angular frequency ($\omega(k)$) around $k = k_0$.

$$\begin{aligned}
\omega(k) \quad &\approx \omega(k_0) + (k - k_0)\left.\frac{d\omega(k)}{dk}\right|_{k=k_0} + O((k-k_0)^2) \qquad \text{(C.6)}\\
\Rightarrow \Psi(x,t) &\approx \int_0^\infty dk\Phi(k)e^{i(kx}e^{-\omega(k_0)t)}e^{ik(\left.\frac{d\omega(k)}{dk}\right|_{k=k_0})t}e^{ik_0(\left.\frac{d\omega(k)}{dk}\right|_{k=k_0})t}\\
&\approx e^{-i\omega(k_0)t}e^{ik_0(\left.\frac{d\omega(k)}{dk}\right|_{k=k_0})t}\int_0^\infty dk\Phi(k)e^{ik(x-t\left.\frac{d\omega(k)}{dk}\right|_{k=k_0})}\\
&\approx e^{-i\omega(k_0)t}e^{ik_0v_g(k_0)t}\int_0^\infty dk\Phi(k)e^{ik(x-v_g(k_0)t)}\\
\Rightarrow \quad &\boxed{|\Psi(x,t)|^2 \approx |\Psi(x-v_g(k_0)t,0)|^2} \qquad \text{(C.7)}
\end{aligned}$$

From this short manipulation, we arrive at a beautiful result that tells us that the wavepacket at some arbitrary (small) time interval (t) after $t = 0$, looks just like the wavepacket at $t = 0$ just displaced in position! Hence for small time intervals, we can use the following steps to propagate a given free particle wavepacket in time.

1. Given $\Psi(x,0)$, we first compute $\Phi(k) = \frac{1}{\sqrt{2\pi}}\int dx\Psi(x,0)e^{-ikx}$.
2. We can now write $\Psi(x,0) = \frac{1}{\sqrt{2\pi}}\int dx\Phi(k)e^{ikx}$.
3. Simply tacking on the time dependence, we get $\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int \Phi(k)dxe^{i(kx-\omega(k)t)}$, where $\omega(k) = \hbar k^2/2m$. Explicitly, the result is expressed as

$$\boxed{\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int dx\Phi(k)e^{i(kx-\frac{\hbar k^2}{2m}t)}} \qquad \text{(C.8)}$$

4. If $\Psi(x,0)$ had already been a plane wave, we can skip steps 1 and 2 and immediately tack on the time dependence in step 3 to give the final solution.

However, the analysis above is only a good model for small time intervals. As t grows to large values, the $O((k-k_0)^2)$ terms in the Taylor expansion become significant and we can no longer ignore them. We will now look at the exact solution of the group velocity by exploring the *Dispersion relation.*

Definition C.5.1. Dispersion Relation: *This is a relation between the angular frequency (ω) of a wave and its wave vector, k.*

For matter waves, we can derive these equations from the quantized momentum and energy equations proposed by Planck and Einstein.

$$\begin{aligned}
& E = \hbar\omega = \frac{p^2}{2m},\ p = \hbar k\\
\Rightarrow\ & \hbar\omega = \frac{(\hbar k)^2}{2m}\\
\Rightarrow\ & \boxed{\omega(k) = \frac{\hbar k^2}{2m}} \qquad \text{(C.9)}
\end{aligned}$$

It is clear now that the angular frequency is a 2^{nd} order polynomial in k, causing 3^{rd} order derivatives (and above) of $\omega(k)$ to vanish. This renders the exact Taylor expansion of $\omega(k)$ around k_0 as,

$$\omega(k) = \omega(k_0) + (k - k_0)\frac{\hbar k_0}{m} + (k - k_0)^2 \frac{\hbar}{2m} \tag{C.10}$$

$$\Rightarrow \boxed{\Psi(x,t) = \int_0^\infty dk \Phi(k) e^{ikx} e^{i(\omega(k_0) + (k-k_0)\frac{\hbar k_0}{m} + (k-k_0)^2 \frac{\hbar}{2m})t}} \tag{C.11}$$

The added $O((k - k_0)^2)$ term causes equation (3.6) to be a poor approximation. Furthermore, the shape of the wavepacket **deforms** as it travels at v_g and time progresses. The exact solution is definitely more difficult to work with than the stationary phase approximation, so it would be good to find bounds on t for which we can safely utilize the approximate solution. By observation of equation (3.9), in order for us to drop the non linear terms we will need to enforce that

$$\frac{(k - k_0)^2}{2} \frac{\hbar}{m} |t| \ll 1 \tag{C.12}$$

$$\begin{aligned} & k - k_0 \equiv \triangle k \\ \Rightarrow \quad & (\triangle k)^2 \frac{\hbar}{m} |t| \ll 1 \\ \Rightarrow \quad & \frac{(\triangle(\hbar k))^2}{\hbar m} |t| = \frac{(\triangle p)^2}{\hbar m} |t| \ll 1 \\ \Rightarrow \quad & \boxed{|t| \ll \frac{\hbar m}{(\triangle p)^2}} \end{aligned} \tag{C.13}$$

From this, we see that the bound on t is related to a quantity known as the *Momentum Uncertainty*, $\triangle p$. By simply eyeballing $\triangle p = \hbar(k - k_0)$, we can see that this momentum uncertainty quantity is somehow related to the 'spread' of the wavepacket around k_0. We will now attempt to build some intuition on uncertainty, but it will only formally be introduced later on in the book.

§C.6 Heisenberg Uncertainty Principle (Qualitative)

First allow us to consider a wave taken at time, $t = 0$. It's wavepacket and corresponding *Fourier Transform* can be written as,

$$\Psi(x, 0) = \frac{1}{\sqrt{2\pi}} \int_0^\infty dk \Phi(k) e^{ikx} \tag{C.14}$$

$$\Phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty dx \Psi(x, 0) e^{-ikx} \tag{C.15}$$

From classical wave mechanics, we know that moving between the frequency and time domain by means of *Fourier Transform* gives rise to an inequality known as the *Time-Bandwidth Product* ($\triangle\omega \triangle t \geq \frac{1}{2}$). Since matter particles also possess wave-like properties, we can make the analytic extension of this into the context of wavepackets.

If we look closer at the Fourier transform of a wavepacket, there is in fact a hidden physical interpretation of this 'k domain'. Recall again the Planck momentum equation, $p = \hbar k$. This

means that we can in fact rewrite the Fourier transform in terms of momentum! By suitable substitutions, we arrive at the equation

$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx \Psi(x,0) e^{-i\frac{px}{\hbar}} \tag{C.16}$$

And just as classical waves have an uncertainty in extracting information about the time and bandwidth simultaneously, so do quantum waves when trying to simultaneously observe the position and momentum of a particle! This is known as the *Heisenberg Uncertainty Principle* for position-momentum, and is derived to be

$$\boxed{\triangle x \triangle p \geq \frac{\hbar}{2}} \tag{C.17}$$

The Heisenberg Uncertainty Principle says that we cannot determine both the position and momentum of a particle simultaneously with absolute precision. In the wavepacket picture, this means that the narrower the wavepacket is in the momentum domain, the wider the wavepacket is in the position domain (and vice versa).

§C.7 Interpretation of Waves and Normalization

We have been working with this mysterious object Ψ (often referred to as the *Wave Function*), which we have termed a quantum or matter wave. When Schrödinger first studied these wave functions, he interpreted Ψ as a particle that had 'disintegrated' and spread itself across space. Regions in space where we found larger values of Ψ meant that more of the disintegrated particle resided there. It was Max Born who proposed that Ψ is in fact some kind of probabilistic distribution of matter particles. The physics community has since adopted Born's interpretation of the wave function, leading to incredibly accurate descriptions of nature. This is known as the *Copenhagen interpretation* of quantum mechanics.

Appendix D

Quintessential 1D Potentials

In this chapter of the appendix, we explore several widely studied 1-dimensional potentials. Something that may have crossed you mind is that working in 1 spatial dimension may seem unrealistically ideal, however great insights can be learned from solving these 1D systems. There are in fact some real physical systems that can be modelled with a 1D Hamiltonian. Below, I present and solve some of commonly taught these 1D quantum systems.

§D.1 Spooky Circles

This system is possibly the simplest quantum system that gives rise to *quantization*. This is more formally known as *first quantization* (where *second quantization* is the quantization of fields covered in *quantum field theory*), and is the transitioning of what would be a continuous spectrum of possible values in classical mechanics to one with a discrete spectra.

Here, we have a particle on a topological 1-dimensional circle. Consider a particle who lives only along a line on the x-axis. The line only goes from $x \in [0, L]$ and dictates that the wave function representing the particle must take on the same values at the line boundaries ($\psi(0) = \psi(L)$). This is effectively a 1-dimensional topological circle. Note that the potential in the physically allowable region is 0. As a result, the time-independent Schrödinger equation for our particle reads,

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x), \quad x \in [0, L] \tag{D.1}$$

As such, we utilize our knowledge of differential equations and the boundary conditions to get a solution.

$$\begin{aligned} & \psi''(x) = -\frac{2mE}{\hbar^2}\psi(x), \\ \Rightarrow \;& \psi(x) = \mathcal{N}e^{ikx}, \quad k \equiv \frac{\sqrt{2mE}}{\hbar} \\ & \psi(0) = \psi(L) \quad \Rightarrow \quad e^{ikL} = e^{ik0} = 1 \\ \Rightarrow \;& \boxed{k_n = \frac{2\pi n}{L}}, \quad n \in \mathbb{Z} \end{aligned} \tag{D.2}$$

From this simple exercise, we see that the wave-vector (and hence momentum) of our wave function here is only allowed to take on integer multiples of $2\pi/L$ and **no longer** a contiuous spectrum!

Imposing the normalization condition (1.5) on $\psi(x)$, we arrive at the following solution.

$$\boxed{\psi(x) = \sqrt{\frac{1}{L}} \cdot e^{ik_n x}} \tag{D.3}$$

Note: there is a subtlety due to the possible parity of the momenta which leads to *degeneracies*.

Definition D.1.1. Degeneracies: *An energy level is called degenerate if there exists 2 or more energy eigenstates that are associated to the same energy.*

§D.2 Quantum Boxes

We already solved the infinite-square well (particle in a box) problem in chapter 4 so we will not be presenting that solution in the appendix. However, we did utilize several theorems while solving this potential without proof. Below is a restatement of those theorems with their proofs included.

§D.2.1 Prove It!

These proofs are non-trivial and should be understood by the reader in order to grasp the significance of these theorems.

Theorem D.2.1. *There are **no** degenerate[1] 1D bound states.*

Proof. Consider a particle of mass m moving in a potential $V(x)$. First assuming that degeneracies do exist, this implies that we can have 2 bound states $\psi_1(x)$ and $\psi_2(x)$ which possess the same energy E. Their time-independent Schrödinger equations are then,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_1(x)}{dx^2} + V(x)\psi_1(x) = E\psi_1(x) \tag{D.4}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_2(x)}{dx^2} + V(x)\psi_2(x) = E\psi_2(x) \tag{D.5}$$

Multiplying (D.4) by $\psi_2(x)$ and (D.5) by $\psi_1(x)$ then taking their difference, we get

$$\begin{aligned}
&-\frac{\hbar^2}{2m}\psi_2(x)\frac{d^2\psi_1(x)}{dx^2}+\frac{\hbar^2}{2m}\psi_1(x)\frac{d^2\psi_2(x)}{dx^2}=0\\
\Rightarrow\ &\psi_2(x)\frac{d^2\psi_1(x)}{dx^2}-\psi_1(x)\frac{d^2\psi_2(x)}{dx^2}=0\\
\Rightarrow\ &\psi_2(x)\frac{d^2\psi_1(x)}{dx^2}-\psi_1(x)\frac{d^2\psi_2(x)}{dx^2}+\frac{d\psi_1(x)}{dx}\frac{d\psi_2(x)}{dx}-\frac{d\psi_2(x)}{dx}\frac{d\psi_1(x)}{dx}=0\\
\Rightarrow\ &\frac{d}{dx}\Big(\psi_2(x)\frac{d\psi_1(x)}{dx}-\psi_1(x)\frac{d\psi_2(x)}{dx}\Big)=\frac{d}{dx}W(\psi_2,\psi_1)=0\\
\Rightarrow\ &W(\psi_2,\psi_1)=\text{constant}
\end{aligned}$$

But we know that for our bound states to be normalizable, $\psi_{1/2}(x)\to 0$ as $|x|\to\infty$.

$$\begin{aligned}
&\Rightarrow W(\psi_2,\psi_1)=0\\
&\Rightarrow \ln\psi_1(x)=\ln\psi_2(x)+C'\\
&\Rightarrow \boxed{\psi_1(x)=C\psi_2(x)}
\end{aligned}\tag{D.6}$$

This proves that the 2 initially assumed different bound states are actually linearly dependent and thus are in fact the same bound state. □

Theorem D.2.2. *For a 1D bound state, the number of nodes[2] increases linearly with the 'quantization index' n following the relation*

$$\text{number of nodes}=(n-1),\quad \text{for } n=1,2,3... \tag{D.7}$$

I will only provide a qualitative argument for this theorem and not a rigorous proof.

Argument of Theorem:

Consider first a particle in an infinite square well of differential width dx. Instead of having $V(x)=0$ for the region $0<x<dx$, $V(x)$ is governed by a smooth potential well that satisfies $V(0)=0$ and monotonically increases for increasing $|x|$. Thus as we expand the 'screens' of the infinite well, we reveal more and more of this potential well. We call this a *screened potential*.
Also, we utilize the following facts.

1. The node theorem holds for an infinite square well of any width (both arbitrarily small or large).
2. A non-trivial wave function can never vanish along with its first spatial derivative (we cannot simultaneously have $\psi(x^*)=0$ and $\psi'(x^*)=0$ for some x^*).

The argument is then, as we gradually move apart the infinite screens causing the potential to deviate away from an infinite square well, we cannot have new nodes appearing. If we did, this would mandate that the derivative at the boundary vanish at some point in the expansion. This violates fact 2 since we have the condition for the wave function to vanish at the infinite potential boundary.

Thus, this proves that the node theorem holds for all 1D bound states.

§D.2.2 Boxes Continued

We move on to studying the 1-dimensional *finite square well* potential. This is similar to the infinite square well under the condition that the energy is lower than the potential barrier. The potential is modelled as

$$V(x) = \begin{cases} -V_0 & -a < x < a \\ 0 & |x| > a \end{cases} \tag{D.8}$$

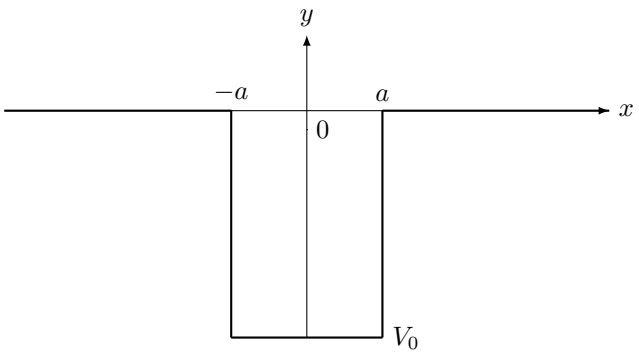


Figure D.1: Finite Square Well

For now, we are interested in bound states and hence will consider the case where $|E| < V_0$, noting that $V_0 > 0$ and $E < 0$. Writing out the time-independent Schrödinger equation for $-a < x < a$,

$$\begin{aligned} -\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) &= E\psi(x) \\ \Rightarrow\ \psi''(x) &= -\frac{2m}{\hbar^2}(E - V(x))\psi(x) \\ \Rightarrow\ \psi''(x) &= -\frac{2m}{\hbar^2}(V_0 - |E|)\psi(x) \end{aligned} \tag{D.9}$$

For simplification of calculation, we define a parameter that has the same units as the wave-vector (we will often do this in our analysis of 1D potentials).

$$\boxed{k^2 = \frac{2m}{\hbar^2}(V_0 - |E|)} \tag{D.10}$$

Then equation (D.9) becomes

$$\psi''(x) = -k^2\psi(x) \tag{D.11}$$

Then by the *symmetry* of the potential and knowing that our *ground state* (lowest energy state) has no nodes, we can check that the solution is given by

$$\boxed{\psi(x) = \mathcal{N}\cos(kx)} \tag{D.12}$$

We see above that we immediately arrived at our solution using 2 facts. The first is by virtue of the node theorem which we have already proven in the particle in a box problem. The second is due to the symmetry of our 1D potential, and in fact this can be generalized to any symmetric potential.

Theorem D.2.3. *Any 1D bound state (energy eigenstate) subject to an even potential can be chosen to be either even or odd.*

Proof. Consider first the time-independent Schr odinger equation with an even potential, that is $V(x) = V(-x)$,

$$\psi''(x) + \frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0$$

Then if we let $x \to -x$ and utilizing the fact that $V(x)$ is even,

$$\begin{aligned} &\psi''(-x) + \frac{2m}{\hbar^2}(E - V(-x))\psi(-x) = 0 \\ \Rightarrow\ &\psi''(-x) + \frac{2m}{\hbar^2}(E - V(x))\psi(-x) = 0 \end{aligned}$$

From this, we can construct even and odd solutions labelled as $\psi_{\text{even}}(x)$ and $\psi_{\text{odd}}(x)$ as such.

$$\psi_{\text{even}}(x) = \frac{1}{2}\big(\psi(x) + \psi(-x)\big), \quad \psi_{\text{odd}}(x) = \frac{1}{2}\big(\psi(x) - \psi(-x)\big) \tag{D.13}$$

This conclusively proves theorem (D.2.3). □

Going back to our finite square well problem, allow us to construct the rest of the solution for $|x| > a$. We employ the same process as before and define another parameter κ.

$$\psi''(x) = \frac{2m|E|}{\hbar^2}\psi(x) \tag{D.14}$$

$$\boxed{\kappa^2 = -\frac{2mE}{\hbar^2}} \tag{D.15}$$

$$\Rightarrow\ \psi''(x) = \kappa^2\psi(x) \tag{D.16}$$

$$\Rightarrow\ \boxed{\psi(x) = \mathcal{A}e^{\kappa x} \ \text{ or } \ \mathcal{B}e^{-\kappa x}} \tag{D.17}$$

The Schrödinger equation mandates that our solution along with its first derivative to be continuous since it is a second order differential equation in x. With these 2 conditions, we attain boundary conditions at $x = \pm a$ so we can stitch our 2 solutions together attaining the following equations.

$$\mathcal{N}\cos(k(-a)) = \mathcal{N}\cos(ka) = \mathcal{A}e^{\kappa(-a)} \tag{D.18}$$

$$\mathcal{N}\cos(ka) = \mathcal{B}e^{-\kappa a} \tag{D.19}$$

In (D.18), we used the fact that cosine functions are even. The order arises from the necessity of the wave function to be normalizable ($\psi \to 0$ as $|x| \to \infty$). We can also see as a consequence of symmetry that $\mathcal{A} = \mathcal{B}$, hence we can set them to be 1 without any loss of generality.

$$\Rightarrow \mathcal{N}\cos(ka) = e^{-\kappa a} \tag{D.20}$$

Utilizing the continuity of the first derivative at $x = a$, we arrive at the following equation.

$$-\mathcal{N}k\sin(ka) = -\kappa e^{-\kappa a} \tag{D.21}$$

Taking the ratio of equations (D.20) and (D.21), we arrive at the following result.

$$k\tan(ka) = \kappa \tag{D.22}$$

At this point, it is convenient for us to define several dimensionless quantities. These can easily be verified to be dimensionless as will be done below their definitions.

$$\eta \equiv ka \tag{D.23}$$
$$\xi \equiv \kappa a \tag{D.24}$$
$$z_0^2 \equiv \eta^2 + \xi^2 = \frac{2mV_0a^2}{\hbar^2} \tag{D.25}$$

The following **proof** will show that all 3 of these parameters are dimensionless.

Proof. We first point out that it is obvious η, ξ and z_0 have the same dimensions. So proving that one of these quantities is dimensionless will imply that so are the others. Allow us to look at z_0.

$$\begin{aligned} z_0^2 = \frac{2mV_0a^2}{\hbar^2} &\sim \frac{mEL^2}{E^2t^2} \\ &\sim \frac{mL^2}{Et^2} \\ &\sim \frac{mL^2}{mL^2} \sim 1 \end{aligned}$$

Hence this shows that z_0^2 is dimensionless, and hence so is z_0 along with η and ξ. □

Using these dimensionless parameters, we incorporate them into (D.22) which gives the following unit-free relation.

$$\boxed{\xi = \eta\tan(\eta)} \tag{D.26}$$

For a better picture, we can plot this relation shown in figure D.2.

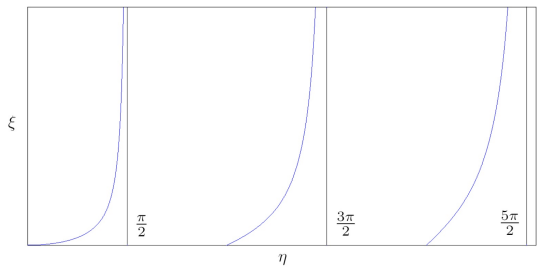


Figure D.2: ξ vs η Plot

z_0 on this plot would then be a circle with a radius that varies monotonically with the value of $V_0 > 0$. The interesting thing we can learn by simply looking at this graph comes from the fact that

$$\boxed{\textbf{number of intersections} = \textbf{number of bound states}} \tag{D.27}$$

Intersections here of course referring to the intersections between the $z_0^2 = \eta^2 + \xi^2$ and $\xi = \eta \tan(\eta)$ graphs. The analogy we can use to understand this comes from thinking about an actual physical well. The deeper this well (larger the *strength of the potential* V_0), the larger the number of levels (occupy-able quantized energy states) that can fit into this well!

A good thing to note about the plot is that the $\eta \tan(\eta)$ curve intersects the η-axis in $n\pi$ intervals, where $n \in \mathbb{N}$. This means for instance, that z_0 would have to minimally be π in order for there to be 2 bound states. The relation between the number of bound states and z_0 is summarized by the following.

$$\boxed{n\pi \leq z_0 < (n+1)\pi \Rightarrow n \text{ bound states}} \tag{D.28}$$

So far, all our computation has been done on the assumption that we are working with even bound states. However, theorem (D.2.3) tells us that we can also have odd bound states and in fact has to be true for the node theorem to be satisfied! By utilizing analytic continuity, we can respectively modify our solutions as follows.

$$\psi(-a < x < a) = \mathcal{N} \sin(kx) \tag{D.29}$$
$$\psi(x < -a) = -e^{\kappa x} \tag{D.30}$$
$$\psi(x > a) = e^{-\kappa x} \tag{D.31}$$

Then enforcing the continuity conditions, we get

$$\mathcal{N} \sin(ka) = e^{-\kappa a} \tag{D.32}$$
$$\mathcal{N} k \cos(ka) = -\kappa e^{-\kappa a} \tag{D.33}$$
$$\Rightarrow \quad k \cot(ka) = -\kappa \tag{D.34}$$
$$\Rightarrow \quad \boxed{\eta \cot(\eta) = -\xi} \tag{D.35}$$

Where we attained (D.35) from taking the ratio of the first 2 equations and multiplying (D.34) through by a. The new plot of (D.35) is given below.

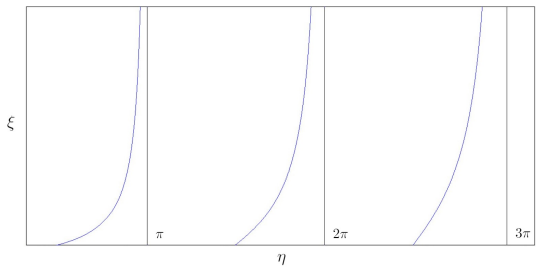


Figure D.3: ξ vs η Plot

For this plot, the $\eta\cot(\eta)$ curve only intersects the η axis in $(2n+1)\pi/2$ intervals where $n \in \mathbb{N}$. This means if we again consider the $z_0^2 = \eta^2 + \xi^2$ curve and (D.27), the first bound state will only appear for $z_0 > \pi/2$ whereas the even solution will **always** have a bound state! The relation between the number of bound states and z_0 is summarized by the following.

$$\boxed{(n - \frac{1}{2})\pi \leq z_0 < (n + \frac{1}{2})\pi \Rightarrow n \text{ bound states}} \tag{D.36}$$

Finally, we write out the full normalized wave function for the odd and even solutions.

$$\psi_{\text{even}}(x) = \begin{cases} e^{\kappa x}, & x < -a \\ \left(\frac{e^{-\kappa a}}{\cos ka}\right)\cos(kx), & -a < x < a \\ e^{-\kappa x}, & x > a \end{cases} \tag{D.37}$$

$$\psi_{\text{odd}}(x) = \begin{cases} -e^{\kappa x}, & x < -a \\ \left(\frac{e^{-\kappa a}}{\sin ka}\right)\sin(kx), & -a < x < a \\ e^{-\kappa x}, & x > a \end{cases} \tag{D.38}$$

Great! We have completed a comprehensive analysis of the finite square well potential! One could now ask, what if the energy of the particle falls below that of the potential? Is this even possible? Well it turns out that this can never be the case.

Theorem D.2.4. *The energy of the particle must **always** exceed the minimum energy of the potential it is subject to.*

Proof. Consider a normalized wave function $\psi(x)$ subject to a potential $V(x)$ with an energy E. Also recall that $E = \langle \hat{H} \rangle_\psi$. Using this fact,

$$\begin{aligned} E &= \big(\psi(x), \hat{H}\psi(x)\big) \\ &= \Big(\psi(x), \big(\frac{\hat{p}^2}{2m} + V(x)\big)\psi(x)\Big) \\ &= \langle \frac{\hat{p}^2}{2m} \rangle_\psi + \langle V(x) \rangle_\psi \end{aligned}$$

Because the kinetic energy term is always positive being a squared quantity,

$$\Rightarrow E \geq \langle V(x) \rangle_\psi \geq V_{\min}(x) \tag{D.39}$$

Thus proving that the particle energy E is always greater than $V_{\min}(x)$. □

§D.3 Infinitely Sharp Wells

Continuing on to the next 1D potential, we now look at the *attractive Dirac delta potential* written as

$$V(x-a) = -\alpha\delta(x-a) = \begin{cases} -\infty, & x = a \\ 0, & \text{otherwise} \end{cases} \tag{D.40}$$

Notice that the delta function here is attractive since it is negative. This is to facilitate the possibility and study of bound states. Potentials that allow for bound states are called attractive potentials. For our analysis, we begin by looking for a quantity with the units of energy from our available parameters. We perform the dimensional analysis as follows. The only parameters in this problem are α, $\hbar$ and m.

$$\begin{aligned} & \alpha \sim \frac{E}{L} \Rightarrow E \sim \frac{\alpha}{L} \\ & E \sim \frac{p^2}{2m} \sim \frac{\hbar^2}{mL^2} \\ \Rightarrow \quad & E \sim \frac{m\alpha^2}{\hbar^2} \\ \Rightarrow \quad & \boxed{\tilde{E} = \frac{m\alpha^2}{\hbar^2}} \end{aligned}$$

$\tilde{E}$ is our newly defined energy parameter. For bound states, we know that the energy of a bound state particle has to be 1) negative 2) proportional to $\tilde{E}$. As such, we define our bound state energy as

$$\boxed{E_b = -C\frac{m\alpha^2}{\hbar^2}}, \quad C \geq 0 \tag{D.41}$$

Now we attempt to solve the eigenvalue problem with the attractive delta potential. For convenience, we set $a = 0$ so that the delta function is centered at the origin. Now looking at time-independent Schrödinger equation for $x \neq 0$ and using the tricks employed for previous potential problems, we arrive at

$$\psi''(x) = -\frac{2mE}{\hbar^2}\psi(x) = \kappa^2\psi(x), \quad E < 0 \tag{D.42}$$

Since a bound state would classically live within the potential, any region where $x \neq 0$ would be classically forbidden and hence *convex toward the axis*. Furthermore, since our wave function has to be normalizable, it must decay as $x \to \infty$. Taking from the results of the finite square well

and considering the limit as its width shrinks while its depth grows indefinitely, we instinctively choose exponentials as our solution.

$$\psi(x>0) = \mathcal{N}e^{-\kappa x}, \quad \psi(x<0) = \mathcal{N}e^{\kappa x} \tag{D.43}$$

Again we know their normalization constants are equal due to the symmetry of the problem. What about at $x = 0$? This makes things a little more challenging, but thankfully for our knowledge of delta functions we know it is defined by its integral!

$$-\frac{\hbar^2}{2m}\psi''(x=0) - \alpha\delta(x)\psi(x=0) = E\psi(x=0) \tag{D.44}$$

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\int_{-\epsilon}^{+\epsilon}\psi''(x)dx - \alpha\int_{-\epsilon}^{+\epsilon}\delta(x)\psi(x)dx = E\int_{-\epsilon}^{+\epsilon}\psi(x)dx \tag{D.45}$$

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\,\psi'(x)|_{-\epsilon}^{+\epsilon} - \alpha\psi(0) = 0$$

$$\Rightarrow \quad \boxed{\psi'(x)|_{-\epsilon}^{+\epsilon} = -\frac{2m\alpha}{\hbar^2}\psi(0)} \tag{D.46}$$

The result in (D.46) is known as the *discontinuity condition* and arises due to the unique nature of the Dirac delta function. In fact, the Dirac delta function is the **only** 1D potential that causes a discontinuity in the derivative of the wave function. From here, we plug in our solutions from (D.43) into (D.46) to get

$$-\kappa\, e^{-\kappa x}\big|_{+\epsilon} - e^{+\kappa x}\big|_{-\epsilon} = -\frac{2m\alpha}{\hbar^2}\mathcal{N}$$

$$\Rightarrow \quad \kappa = \frac{m\alpha}{\hbar^2} = \sqrt{-\frac{2mE}{\hbar^2}}$$

$$\Rightarrow \quad E = -\frac{\kappa^2\hbar^2}{2m} = -\frac{\hbar^2}{2m}\left(\frac{m\alpha}{\hbar^2}\right)^2$$

$$\Rightarrow \quad \boxed{E_b = -\frac{1}{2}\tilde{E}} \tag{D.47}$$

Hence we have found our proportionality constant in (D.41), $C = 1/2$. To complete our solution to the delta function potential, we have to normalize our wave function. For this, we can exploit the symmetry of our bound state once again as such

$$\mathcal{N}^2\int_{-\infty}^{\infty} dx\cdot e^{-2\kappa|x|} = 2\mathcal{N}^2\int_0^{\infty} dx\cdot e^{-2\kappa|x|} = 1$$

$$\Rightarrow \quad 2\mathcal{N}^2\cdot\frac{-1}{2\kappa}e^{-2\kappa x}\Big|_0^{\infty} = \frac{2\mathcal{N}^2}{2\kappa} = 1$$

$$\Rightarrow \quad \mathcal{N} = \sqrt{\kappa}$$

$$\Rightarrow \quad \boxed{\psi(x) = \sqrt{\kappa}\cdot e^{-\kappa|x|}} \tag{D.48}$$

The attractive delta potential only admits **one** bound state because it disallows the first excited odd state and must adhere to the node theorem. Therefore, solution (D.48) is the only allowable solution to this problem.

§D.4 Quantum Springs

We are now going to learn about one of the most important systems in all of physics, the *harmonic oscillator*. Since this is the quantum mechanical version, we shall refer to the system as the quantum harmonic oscillator (QHO). In this book, we will be solving this system using an algebraic approach (operator method). Alternative derivations can be found in other readily available textbooks if one is interested. Again taking cue from classical mechanics, the quantum harmonic oscillator Hamiltonian is given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \tag{D.49}$$

We can rewrite this as,

$$\begin{aligned}\hat{H} &= \frac{1}{2}m\omega^2\left(\hat{x}^2 + \frac{\hat{p}^2}{2m}\right) \\ &= \frac{1}{2}m\omega^2\left(\left(\hat{x} - i\frac{\hat{p}}{m\omega}\right)\left(\hat{x} + i\frac{\hat{p}}{m\omega}\right) + \frac{\hbar}{m\omega}\mathbb{I}\right) \\ &\equiv \frac{1}{2}m\omega^2\hat{V}^\dagger\hat{V} + \frac{1}{2}\hbar\omega\mathbb{I}\end{aligned} \tag{D.50}$$

Where we have split the Hamiltonian using a sum of squares. However, we are working with operators that do not commute ($[\hat{x}, \hat{p}] = i\hbar\mathbb{I}$), hence we get an additional $\frac{1}{2}\hbar\omega\mathbb{I}$ term. We also define the following **unit-free** operators.

$$\boxed{\hat{a} \equiv \sqrt{\frac{m\omega}{2\hbar}}\hat{V}, \quad \hat{a}^\dagger \equiv \sqrt{\frac{m\omega}{2\hbar}}\hat{V}^\dagger} \tag{D.51}$$

$\hat{a}^\dagger$ and $\hat{a}$ are known as the *raising* and *lowering* operators respectively. From these definition, we again update the form of our Hamiltonian as written below.

$$\boxed{\hat{H} = \hbar\omega(\hat{N} + \frac{1}{2})}, \quad \hat{N} \equiv \hat{a^\dagger}\hat{a} \tag{D.52}$$

$\hat{N}$ is known as the *number operator* and notice that it is a Hermitian operator. As a next step, let us look at several commutator identities between the operators we have just defined. In this book, I will simply list them out but I urge you to take the time to derive them on your own. It is a relatively simple exercise but worth the time.

$$\left[\hat{a}, \hat{a}^\dagger\right] = 1, \quad \left[\hat{H}, \hat{a}^\dagger\right] = \hbar\omega\hat{a}^\dagger, \quad \left[\hat{H}, \hat{a}\right] = -\hbar\omega\hat{a} \tag{D.53}$$

It may not be clear yet, but we have already done most of the work for solving the harmonic oscillator system! To see why, we act with the raising operator and Hamiltonian on some energy eigenstate ψ_E with energy E.

$$\begin{aligned} & \hat{H}\psi_E = E\psi_E \\ \Rightarrow\ & \hat{a}^\dagger\hat{H}\psi_E = \Big(\hat{H}\hat{a}^\dagger + (\hat{a}^\dagger\hat{H} - \hat{H}\hat{a}^\dagger)\Big)\psi_E = E(\hat{a}^\dagger\psi_E) \\ \Rightarrow\ & \Big(\hat{H}\hat{a}^\dagger + \left[\hat{a}^\dagger, \hat{H}\right]\Big)\psi_E = \Big(\hat{H}\hat{a}^\dagger - \hbar\omega\hat{a}^\dagger\Big)\psi_E = E(\hat{a}^\dagger\psi_E) \\ \Rightarrow\ & \hat{H}(\hat{a}^\dagger\psi_E) = (E + \hbar\omega)(\hat{a}^\dagger\psi_E) \end{aligned} \tag{D.54}$$

Showing us that when we apply the Hamiltonian to the new 'raised' state $\hat{a}^\dagger\psi_E$, we get an energy that is $\hbar\omega$ higher than the 'unraised' state ψ_E! The algebraic manipulation we performed above using the commutator is known as '*commuting an operator through*', and is a very useful technique. We can do a similar derivation for $\hat{a}$ to get that

$$\hat{H}(\hat{a}\psi_E) = (E - \hbar\omega)(\hat{a}\psi_E) \tag{D.55}$$

This explains why $\hat{a}^\dagger$ and $\hat{a}$ are known as the raising and lowering operators, since they raise and lower the energies of a given state. Be clear that the raising and lowering operators are **not** unitary, so they cannot be realized as a real implementable operation on quantum states. They are simply mathematical tools to aid us in finding the spectrum of the QHO.

To complete the spectrum of our theory, we utilize theorem D.2.4, which says that $E \geq V_{\min} = 0$. This means that the ground state $\psi_0(x)$ must be a state that imposes the following condition:

$$\hat{a}\psi_0(x) = 0 \tag{D.56}$$

Otherwise, the lowering operator has the capacity to lower the energy of our state indefinitely. Writing $\hat{a}$ in terms of $\hat{x}$ and $\hat{p}$, the above condition (equation D.56) expresses itself as a first order differential equation. This we know how to solve.

$$\sqrt{\frac{m\omega}{2\hbar}}\Big(\hat{x} + \frac{i\hat{p}}{m\omega}\Big)\psi_0(x) = \sqrt{\frac{m\omega}{2\hbar}}\Big(\frac{\hbar}{m\omega}\frac{d}{dx} + x\Big)\psi_0(x) = 0 \tag{D.57}$$

Using equation (D.57) and the normalization condition, we get the ground state wave function of a QHO is

$$\psi_0(x) = \Big(\frac{m\omega}{\pi\hbar}\Big)^{1/4}\exp\Big(-\frac{m\omega}{2\hbar}x^2\Big) \tag{D.58}$$

Plugging this into equation (D.52), we get that the ground state energy is simply $E_0 = \hbar\omega/2$. So by the relation in equation (D.54), we get that the spectrum of the QHO takes the elegant form,

$$\boxed{E_n = \hbar\omega(n + \frac{1}{2})} \tag{D.59}$$

Where $n \in \mathbb{N}$ and denotes the energy excitation level of the state. The ladder operators also conveniently allow us to generate any arbitrary QHO eigenstate. We simply apply the appropriate number of raising operators on ψ_0 and normalize as follows:

$$\boxed{\psi_n(x) = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}\psi_0(x)} \tag{D.60}$$

This shows us the power of these operators, and the elegance of this construction. Below (figure D.4) is a visualization of the wave functions for the lowest 3 energy levels $n = 0, 1, 2$.

Exercise

Using equation (D.60), find the $n = 1$ and $n = 2$ energy eigenstates for the quantum harmonic oscillator $(\psi_1(x), \psi_2(x))$.

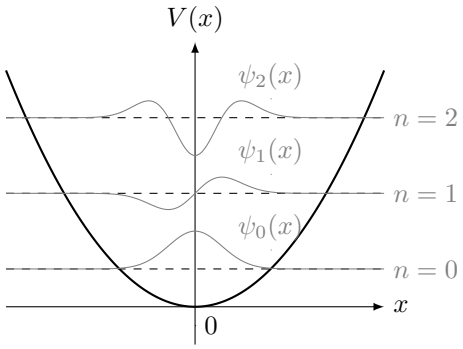


Figure D.4: Wavefunction plot for the lowest 3 energy levels

Some other useful identities pertaining the QHO are listed below.

$$\left[\hat{N}, \hat{H}\right] = 0 \tag{D.61}$$

$$\hat{N}\psi_n(x) = n\psi_n(x) \tag{D.62}$$

$$\hat{a}\psi_n(x) = \sqrt{n}\,\psi_{n-1}(x) \tag{D.63}$$

$$\hat{a}^\dagger\psi_n(x) = \sqrt{n+1}\,\psi_{n+1}(x) \tag{D.64}$$

Why QHOs are so important is because many a time, bound state quantum systems can (to a good approximation) be thought of as a QHO plus some perturbative term. This allows us to employ the techniques developed in perturbation theory (not covered in this book) to very accurately solve much more complex quantum systems where brute force analytic methods would otherwise fail.

Appendix E

Spin

In 1922, 2 physicist performed the Stern-Gerlach experiment in Frankfurt which yielded puzzling results. Stern and Gerlach were atomic physicist concerned with measuring the thermal motion of ions. They did this primarily by sending beams of ions through magnetic fields and then measuring their deflected velocities. While doing so, they observed a weird phenomena while shooting beams of silver atoms through a magnetic field. This was the first experimental observation of quantum mechanical spin.

§E.1 Head Spinning Results

Silver atoms have 47 electrons, of which 46 fill up the $n = 1, 2, 3, 4$ levels, leaving a lone electron in the outermost $5s$ orbital. As such, shooting silver atoms are electrostatically equivalent to shooting singular electrons. The experimental set-up is shown below.

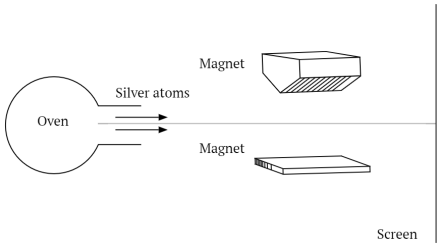


Figure E.1: Stern-Gerlach Experiment

When these silver atoms were shot through the $\vec{B}$ field, Stern and Gerlach observed that the electrons were **not** consistently deflected in the same direction! A consistent deflection direction with varying deflection angles is what would be classically expected with a time-independent $\vec{B}$ field and like-charged particles of varying velocities. With this, Ralph Kronig suggested that this had to do with some kind of electron rotation. Wolfgang Pauli rejected this proposition as he refused to accept the premise that point particles could have a spin angular momentum. But we now know that Kronig was not entirely wrong.

§E.1.1 Magnetic Moments

To understand why Kronig proposed this, we require a little knowledge of *magnetic moments* $\vec{\mu}$. The Magnetic moment of a closed current carrying loop is given by

$$\boxed{\vec{\mu} = I\vec{A}} \tag{E.1}$$

where A is the cross-sectional area of the loop and $|\vec{\mu}|$ has the units of $[\mu] \doteq \frac{\text{Energy}}{\text{Tesla}}$. Now consider a rotating ring, rotating with linear velocity v, having total charge Q, total mass M and linear charge density λ as illustrated below.

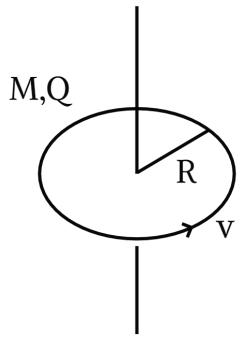


Figure E.2: Rotating Charged Ring

The magnetic moment of this charged ring can be calculated as follows.

$$\begin{aligned} I = \lambda v &= \frac{Qv}{2\pi R} \\ \Rightarrow\ \mu = IA &= \frac{Qv}{2\pi R}(\pi R^2) = \frac{1}{2}QvR \end{aligned}$$

Then since the angular momentum is defined as

$$L = |\vec{r} \times \vec{p}| = RMv \tag{E.2}$$

$$\Rightarrow\ \mu = \frac{1}{2}Q\Big(\frac{MvR}{M}\Big)$$

$$\Rightarrow\ \boxed{\mu = \frac{1}{2}\frac{Q}{M}L} \tag{E.3}$$

This is actually the classical, universal relation for all axially symmetric charged rotating objects. Hence if we follow this result and take electrons as spinning on their own axis, we should arrive at the equation,

$$\mu_e \stackrel{?}{=} \frac{e}{2m_e}S \tag{E.4}$$

where e is the electronic charge, m_e is the mass of the electron and we have swapped out L for S since we are considering the electron as having a spin angular momentum, not an orbital one. However, experimental results show that this is **not** exactly accurate. The actual relation gives

an additional prefactor known as the '***Lande factor***', g. As such, the precise magnetic moment of an electron is

$$\boxed{\mu_e = g\Big(\frac{e\hbar}{2m_e}\Big)\Big(\frac{S}{\hbar}\Big)} \tag{E.5}$$

Notice that we have added factors of $\hbar$ to this equation. Since $\hbar$ has units of angular momentum, this allows for $S/\hbar$ to be unit-free. Additionally, the middle constant term is known as the '***Bohr magneton***' defined as

$$\boxed{\mu_B \equiv \frac{e\hbar}{2m_e} = 9.274 \times 10^{-24}\text{J/T}} \tag{E.6}$$

For electrons, their Lande factor is found to be extremely close to $g_e = 2$, and hence their magnetic moment vector relation is given as

$$\boxed{\vec{\mu} = -2\mu_B \frac{\vec{S}}{\hbar}} \tag{E.7}$$

where the negative sign arises from the negative charge of the electrons. In the experiment, these electrons were passed through a magnetic field and thus it would be good for us to know how this works in theory. The resultant force that a magnetic field applies on an object with a given magnetic moment is

$$\vec{F} = \boldsymbol{\nabla}\Big(\vec{\mu} \cdot \vec{B}\Big) \tag{E.8}$$

This implies that in the Stern-Gerlach experiment, treating the central axis as z, we get a force on our silver atoms

$$\begin{aligned} \vec{F} &\approx \boldsymbol{\nabla}(\mu_z B_z) \\ &= \mu_z \boldsymbol{\nabla}(B_z) = \mu_z \frac{\partial B_z}{\partial z}\hat{z} \end{aligned} \tag{E.9}$$

There is an approximate sign since the B field is not perfectly uniform. Following the classical picture, what we would expect is a *normal distribution* of silver atoms that appear on the screen, since the silver atoms emitted from the oven would have a *Boltzmann distribution* of magnetic moments. But this is **not** the case. Intead, Stern and Gerlach observed a bi-modal distribution!

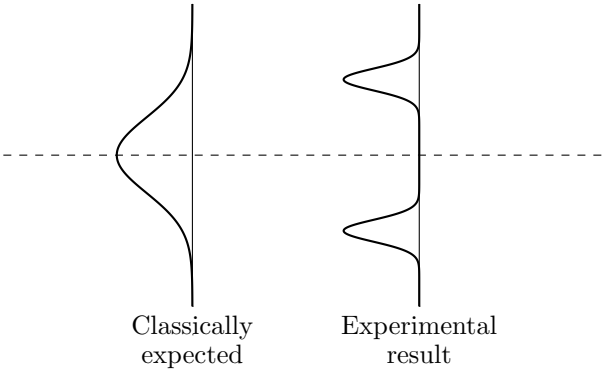


Figure E.3: Stern-Gerlach Distributions

This result was originally termed '*space quantization*', which is slightly misleading as space is **not** actually quantized here. But from this, since μ_B and μ_z are adjustable parameters, we can use (E.7) to get the values of S_z. Stern and Gerlach discovered these to be

$$\boxed{S_z = \pm\frac{\hbar}{2}} \tag{E.10}$$

§E.2 Superposition of Spin States

Allow us now to treat the Stern-Gerlach apparatus oriented along a particular axis as a black box, such that when we send in spin 1-half particles, they emerge as either their '*up*' or '*down*' states.

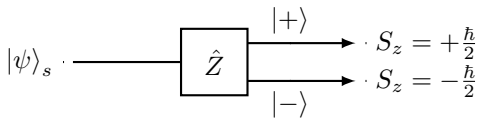


Figure E.4: Spin-Z Black Box

Stern and Gerlach continued to perform experiments by placing these black boxes in a chain, and the results are as follows.

1. The first experiment set up as shown in figure E.5 showed that we can have 2 orthogonal states for the electron. These states are with respect to the $\hat{z}$ orientation and we will label them as $\{|z;+\rangle, |z;-\rangle\}$.

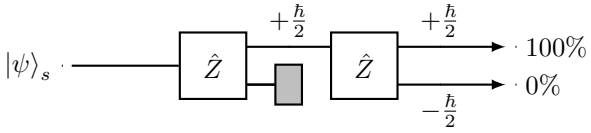


Figure E.5: 2 $\hat{z}$-oriented Black Boxes with Blockage

2. A second experiment set up as shown in figure E.6. These results show that basis states of one orientation of the Stern-Gerlach experiment have overlap with the basis states of another orientation $\Rightarrow \langle x;\pm|z;\pm\rangle \neq 0$.

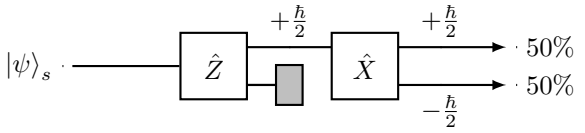


Figure E.6: $\hat{z}/\hat{x}$-oriented Black Boxes with Blockage

3. The last experimental set up shown in figure E.7 shows that any 'memory' of a having passed through previous filters is **not** retained.

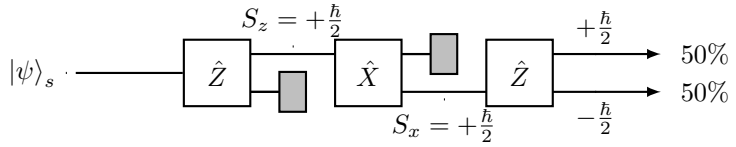


Figure E.7: $\hat{z}/\hat{x}/\hat{z}$-oriented Black Boxes with Blockages

As implied by the first experiment above, it turns out that this system can be modelled as a 2-dimensional complex vector space with an orthonormal basis consisting of these up and down states $\{|+\rangle, |-\rangle\}$. This is perfect for the implementation of a qubit. In this short write-up on spin, I have adopted the physicists' convention of representing the canonical basis with $\{|+\rangle, |-\rangle\}$. Do not confused these as the $\hat{S}_x$ eigenstates which quantum information scientists write them as. However, do bear in mind that these are simply labels, so as long as there is no ambiguity, there is no issue with using whatever label you prefer.

Appendix F

Abstract and Linear Algebra

In this chapter, we will introduce material from modern/abstract and linear algebra that will be useful for the study of quantum mechanics. Although not all of it's applications may be found in this book, they will still be helpful in gaining a clearer picture of the material. As stated in the preface, some prior knowledge of linear algebra is assumed so these notes will not be giving in depth coverage. However, if I feel that something is needed to be emphasized or not taught in a usual linear algebra course, I will expound on it in greater detail. For this section in the appendix, I will drop the usual frames around definitions and theorems.

§F.1 Groups, Rings and Fields

This section will be rather dense with definitions and theorems, but is meant as a build up to the following sections. Note that the proofs for the theorems will not be given in these notes and is left as exercises for the reader.

Definition F.1.1. Set: *A set S is a distinct collections of objects known as elements $a \in S$.*

Definition F.1.2. Subset: *Given 2 sets T and S, we say S is a subset of T if all elements in S are also in T. We denote subsets as $S \subset T$.*

Definition F.1.3. Morphism: *Let S and T be sets. A morphism or map of sets of S into T is written as*

$$\begin{aligned} f &: S \to T \\ f(s) &\mapsto t \end{aligned} \tag{F.1}$$

just as a function which assigns an element $f(s) \in T$ for each $s \in S$.

Definition F.1.4. Group: *A group is a set G equipped with a binary operation '$\cdot$' satisfying the following axioms for $a, b, c \in G$.*

1. *Associativity:* $(a \cdot b) \cdot c = a \cdot (b \cdot c)$
2. *Identity:* $\exists e \in G$ *s.t.* $e \cdot a = a \cdot e = a$
3. $\forall a \in G$, $\exists a^{-1} \in G$ *s.t.* $a^{-1} \cdot a = a \cdot a^{-1} = e$

Examples

- Integers $\mathbb{Z}$ under usual addition.

- The n^{th} roots of unity $\mu_n = \{ \exp\left(\frac{2\pi i j}{n}\right) \mid j \in \mathbb{Z}\}$.
- The set of $n \times n$ invertible matrices, $GL_n = \{M \in \mathbb{R}^{n\times n} \mid \det(M) \neq 0\}$

Theorem F.1.1. *For a group G, the following properties hold.*

1. *The identity element is **unique**.*
2. *For any $a \in G$, if $x, y \in G$ are such that $xa = ya$ or $ax = ay$, then $x = y$. This is known as **cancellation**.*
3. *The inverses of any element of G is also **unique**.*

Definition F.1.5. Abelian Group: *A group G is called Abelian if for each $a, b \in G$, we have $a \cdot b = b \cdot a$ (group elements commute under the binary operation).*

Definition F.1.6. Subgroup: *A subgroup K in a group G is a subset $K \subset G$ such that,*

1. *K is closed under multiplication in G*
2. *K is a group under induced multiplication from G*

We denote a subgroup by $K < G$.

Definition F.1.7. Group Homomorphism: *Given 2 groups $(G, \cdot)$ and $(G', *)$, a group homomorphism is a morphism ϕ,*

$$\phi : G \to G' \tag{F.2}$$

that satisfies the following for any $a, b \in G$.

$$f(a \cdot b) = f(a) * f(b) \tag{F.3}$$

In the above definition, we have used the notation of $(G, \cdot)$ where in the given tuple, the left most entry represents the group and the rightmost entry represents the associated binary operation.

Definition F.1.8. Rings: *A ring is a set R equipped with 2 binary operations "+" and "$\cdot$" which satisfies the following.*

1. *$(R, +)$ is an Abelian group.*
2. *The ring contains **unity** $\mathbb{I}$ with $\mathbb{I} \cdot a = a \cdot \mathbb{I} = a$ for $a \in R$.*
3. *"$\cdot$" satisfies **associativity**, $(a \cdot b) \cdot c = a \cdot (b \cdot c)$.*
4. *"$\cdot$" and "+" satisfy **distributivity**, $(a + b) \cdot c = a \cdot b + a \cdot c$*

Examples

1. $\mathbb{Z}$, $\mathbb{Q}$, $\mathbb{R}$ and $\mathbb{C}$ under usual addition and multiplication.
2. $n \times n$ matrices with entries in a given set, $M_n(\mathbb{Z})$, $M_n(\mathbb{Q})$, $M_n(\mathbb{R})$ and $M_n(\mathbb{C})$.
3. The set of integers modulo n $\mathbb{Z}/_n\mathbb{Z}$, under usual addition and multiplication given by $\overline{a} \cdot \overline{b} = \overline{a \cdot b}$. $(\overline{a}, \overline{b} \in \mathbb{Z}/_n\mathbb{Z})$

Theorem F.1.2. *A ring R satisfies the following properties for any 2 elements $a, b \in R$.*

1. $0 \cdot a = a \cdot 0 = 0$
2. $a \cdot (-b) = (-a) \cdot b = -(a \cdot b)$
3. $(-a) \cdot (-b) = a \cdot b$

$(-a)$ and $(-b)$ above are the additive inverses of a and b.

Definition F.1.9. R-module: *Given a ring R, a left R-module M is defined as an additive Abelian group $(M, +)$, with the operation*

$$\bullet : R \times M \to M \tag{F.4}$$

such that for any $r, r' \in R$ and $v, u \in M$, the operation satisfies

1. $s \bullet (v + u) = s \bullet v + s \bullet u$
2. $(s + s') \bullet v = s \bullet v + s' \bullet v$
3. $(rs) \bullet v = r \bullet (s \bullet v)$
4. $\mathbb{I}_R \bullet v = v$

A right R-module is defined in a similar way with the operation defined on $M \times R$ instead.

R-modules are generalizations of the notion of vector spaces which we will formally come to in a bit.

Definition F.1.10. Commutative Rings: *A ring R is called commutative if for all $a, b \in R$, we have $a \cdot b = b \cdot a$.*

Definition F.1.11. Units: *An element is called a unit $u \in R$ if it has both left and right inverses, $u^{-1} \cdot u = u \cdot u^{-1} = \mathbb{I}$.*

Definition F.1.12. Field: *A field $\mathbb{F}$ is commutative ring in which all non-zero elements are units.*

Examples

1. $\mathbb{Q}, \mathbb{R}$ and $\mathbb{C}$ are fields.
2. $\mathbb{Z}$ is **not** a field
3. $\mathbb{Z}/_p\mathbb{Z}$ is a field **only** if p is a prime integer.

Definition F.1.13. Ring Homomorphism: *Given 2 rings R and R', a ring homomorphism is a morphism ϕ,*

$$\phi : R \to R' \tag{F.5}$$

that satisfies the following for any $a, b \in R$.

1. $f(ab) = f(a)f(b)$
2. $f(a + b) = f(a) + f(b)$
3. $f(\mathbb{I}_R) = \mathbb{I}_{R'}$

Definition F.1.14. Associative $\mathbb{F}$-Algebra: *Given a field $\mathbb{F}$, an associative $\mathbb{F}$-algebra (or just $\mathbb{F}$-algebra) is an $\mathbb{F}$-module with an $\mathbb{F}$-bilinear map $A \times A \to A$ that satisfies associativity*

$$x(yz) = (xy)z \tag{F.6}$$

for all $x, y, z \in A$.

Examples

1. The *polynomial ring* over $\mathbb{Q}$, written as $\mathbb{Q}[x] = \{\sum_j c_j x^j \mid \forall c_j \in \mathbb{Q}\}$ is a $\mathbb{Q}$-algebra.
2. $M_n(\mathbb{F})$ is an $\mathbb{F}$-algebra for $\mathbb{F} \in \{\mathbb{Q}, \mathbb{R}, \mathbb{C}\}$
3. The *ring of Quaternions* $\mathbb{H}$, is an $\mathbb{R}$-algebra.

§F.2 Vector Spaces, Hilbert Spaces and Lie Algebras

Again, the material covered in this section does not constitute a comprehensive course on vector spaces, Hilbert spaces and Lie algebras. Content is presented on a need to know basis, relevant for understanding this book.

Definition F.2.1. $\mathbb{F}$-Vector Space: *An $\mathbb{F}$-vector space is an additive, Abelian group V with an operation $\bullet : \mathbb{F} \times V \to V$ called multiplication which satisfies*

1. $c \bullet (\vec{v} + \vec{u}) = c \bullet \vec{v} + c \bullet \vec{u}$
2. $(c + d) \bullet \vec{v} = c \bullet \vec{v} + d \bullet \vec{v}$

3. $\mathbb{I} \bullet \vec{v} = \vec{v}$

for $c, d \in \mathbb{F}$ *and* $\vec{v}, \vec{u} \in V$*.*

Examples

1. The set of n-dimensional number arrays $V = \{(v_1, v_2, ..., v_n) \mid v_j \in \mathbb{F}\}$.
2. The set of polynomial functions over a field $\mathbb{F}$ written as $\mathbb{F}[x]$.
3. The set of 2×2 Hermitian matrices $V = \{M \in \mathbb{C}^{2\times 2} \mid M^\dagger = M\}$ over $\mathbb{C}$.

Definition F.2.2. Subspace: *A subset* W *of an* $\mathbb{F}$*-vector space* V *is a subspace if* W *satisfies*

1. *closure under vector addition*
2. *closure under multiplication with elements of the field* $\mathbb{F}$*.*

Definition F.2.3. Linear Combination: *Given an* $\mathbb{F}$*-vector space* V*, a linear combination of a set of vectors* $\{\vec{v}_1, \vec{v}_2, ..., \vec{v}_n\} \subset V$ *with* $\mathbb{F}$*-coefficients* $\{c_1, c_2, ..., c_n\} \subset \mathbb{F}$ *is defined as*

$$\sum_{j=1}^{n} c_j \vec{v}_j = c_1\vec{v}_1 + c_2\vec{v}_2 + ... + c_n\vec{v}_n \tag{F.7}$$

Definition F.2.4. Span: *Given a list of vectors* $S = (v_1, v_2, ..., v_n)$ *from an* $\mathbb{F}$*-vector space* V*, the span of* S *is defined as the set of all linear combinations of the vectors in* S*.*

$$\text{span}(S) = \{\sum_{j=1}^{n} c_j \vec{v}_j \mid c_j \in \mathbb{F}\} \tag{F.8}$$

Definition F.2.5. Linear Independence: *Given an* $\mathbb{F}$*-vector space* V*, a list of vectors* $\{\vec{v}_1, \vec{v}_2, ..., \vec{v}_n\} \subset V$ *is linearly independent iff*

$$\sum_{j=1}^{n} c_j \vec{v}_j = 0 \iff c_j = 0 \ \ \forall j \tag{F.9}$$

Definition F.2.6. Basis: *The basis of an* $\mathbb{F}$*-vector space* V*, is a linearly independent list of vectors that spans* V*.*

§F.2.1 Linear Operators and $\mathscr{L}(V)$

Operators play a huge role in quantum mechanics so it is essential that we look a little deeper into what exactly they are and their properties.

Definition F.2.7. Linear Operators: *Given an* $\mathbb{F}$*-vector space* V*, a linear operator is a vector space map,* $T : V \to V$ *(linear endomorphism) which satisfies*

1. $T(\vec{v} + \vec{u}) = T(\vec{v}) + T(\vec{u})$
2. $T(a\vec{v}) = aT(\vec{v})$

for $\vec{v}, \vec{u} \in V$ *and* $a \in \mathbb{F}$*.*

Examples

1. Given the vector space $V = \mathbb{F}[x]$, differentiation $\frac{d}{dx}$ is a linear operator on V.
2. Given the vector space $V = \mathbb{F}[x, y, z]$, the Laplacian $\boldsymbol{\nabla}^2$ is a linear operator on V.
3. Given the vector space $V = \mathbb{R}^n$, any $n \times n$ real matrix is a linear operator on V.

§ **Structure of $\mathscr{L}(V)$**

$\mathscr{L}(V)$ is the set of linear operators on some $\mathbb{F}$-vector space V. Given 2 operators $S, T \in \mathscr{L}(V)$ and some element $a \in \mathbb{F}$, the operators satisfy the following properties.

1. $(S+T)\vec{v} = S\vec{v} + T\vec{v}$
2. $(aS)\vec{v} = a(S\vec{v})$

Additionally, we can check that $(S+T)$ and (aS) are also both linear operators. We can also check that $\mathscr{L}(V)$ is in fact an $\mathbb{F}$-vector space and the proof is left as an exercise for the reader. Now, we equip our vector space $\mathscr{L}(V)$ with an additional binary operation "$*$" defined by

$$(S * T)\vec{v} \equiv S(T(\vec{v})) \tag{F.10}$$

which grants additional structure to our vector space. We term this operation as *operator multiplication*. Note that "$*$" is *associative* and $\mathscr{L}(V)$ has a *operator multiplicative identity*, but it **may not** be *commutative* nor necessitate having *inverses*.

§F.2.2 Kernel and Range

As a little overview, I would like to point out that for the following structures being introduced,

- the *kernel* is associated to a property known as *injectivity*.
- the *range* is associated to a property known as *surjectivity*.

Keep this in mind as we present their definitions.

Definition F.2.8. Kernel: *Given a linear map (not necessarily an operator) T acting on an $\mathbb{F}$-vector space V, the kernel (or nullspace) of T denoted as null(T), is defined as*

$$\text{null}(T) = \{\vec{v} \in V \mid T(\vec{v}) = \vec{0}\} \tag{F.11}$$

Definition F.2.9. Injectivity: *An operator T acting on the vector space V is injective if for 2 vectors $\vec{v}, \vec{u} \in V$,*

$$T(\vec{v}) = T(\vec{u}) \Rightarrow \vec{v} = \vec{u} \tag{F.12}$$

Theorem F.2.1. *An operator T is injective $\iff$ null$(T) = \{\vec{0}\}$.*

The theorem above is very useful for proving if operators are injective or not (simply look at the kernel of the operator).

Definition F.2.10. Range: *Given a linear map (not necessarily an operator) T acting on an $\mathbb{F}$-vector space V, the range of T denoted as range(T) is defined as*

$$\text{range}(T) = \{T(\vec{v}) \mid \vec{v} \in V\} \tag{F.13}$$

Theorem F.2.2. *For an operator T acting a vector space V, range(T) is a subspace of V.*

Definition F.2.11. Surjectivity: *An operator T acting on a vector space V is surjective if range$(T) = V$ (the range of T generates the entire vector space).*

Definition F.2.12. Bijectivity: *An operator T acting on a vector space V is bijective iff it is both injective and surjective.*

Theorem F.2.3. Rank-Nullity Theorem: *For a linear map T acting on the vector space V,*

$$\dim(\text{null}(T)) + \dim(\text{range}(T)) = \dim(V) \tag{F.14}$$

§ **Inverses of Linear Operators**

Let's now ask the question, when do operators have inverses? Firstly, since operator multiplication is **not** a commuative operation on $\mathscr{L}(V)$, an operator T can have 2 kinds of inverses.

- A *left inverse*: $S \in \mathscr{L}(V)$ s.t. $S * T = \mathbb{I}$.
- A *right inverse*: $S' \in \mathscr{L}(V)$ s.t. $T * S' = \mathbb{I}$.

Well, it is actually proven that S and S' are in fact the same operator!
Theorem F.2.4. *Given some operator $T \in \mathscr{L}(V)$, if both S and S' exists such that $S * T = T * S' = \mathbb{I}$, then we have $S = S'$.*
Theorem F.2.5. *For a given operator $T \in \mathscr{L}(V)$, the existence of a T inverse operator implies that T is injective and vice versa.*
Theorem F.2.6. *Given a **finite** dimensional $\mathbb{F}$-vector space and an operator T that acts on it, T is injective iff T is surjective.*

§ **Eigenvalues and Eigenvectors**

In linear algebra, specific vectors associated to linear operator carry a special property. This property allows these vectors to remain unchanged (up to a scale factor) when acted on by their associated operator. These vectors are what are known as *Eigenvectors*.
Definition F.2.13. Eigenvector: *If T is a linear operator mapping a **non-zero** vector $v \in \mathbb{V}$ over field $\mathbb{F}$ onto itself, such that*

$$T(v) = \lambda v \tag{F.15}$$

*then v is known as the **Eigenvector** of T with an **Eigenvalue** λ.*

§F.2.3 Hilbert Spaces and Lie Algebras

Definition F.2.14. Hilbert Space: *A Hilbert space $\mathcal{H}$, is a $\mathbb{C}$-vector space with a defined inner product operation on 2 $\mathcal{H}$-elements as given by*

$$\langle\ ,\ \rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{C} \tag{F.16}$$

Definition F.2.15. Orthogonality: *Given a Hilbert space $\mathcal{H}$, 2 elements $\psi, \phi \in \mathcal{H}$ are called orthogonal iff*

$$\langle \psi, \phi \rangle = \langle \phi, \psi \rangle = 0 \tag{F.17}$$

Definition F.2.16. Lie Algebra: *A Lie algebra $\mathcal{L}$, is a **finite** dimensional $\mathbb{C}$-vector space equipped with a binary operation $[\ ,\ ] : \mathcal{L} \times \mathcal{L} \to \mathcal{L}$ called the **bracket**. The bracket satisfies the following properties.*

1. *Bilinearity*
2. *Antisymmetry:* $[x, y] = -[y, x]$
3. *Jacobi Identity:* $[x, [y, z]] + [z, [x, y]] + [y, [z, x]] = 0$

for $x, y, z \in \mathcal{L}$.
Definition F.2.17. Lie Subalgebra: *A subspace $\mathcal{L}' \subset \mathcal{L}$ (with $\mathcal{L}$ being a Lie algebra) is a Lie subalgebra if $[\mathcal{L}', \mathcal{L}'] \subset \mathcal{L}'$. In this case, $\mathcal{L}'$ inherits the bracket operation from $\mathcal{L}$ and is therefore also a Lie algebra.*

Bibliography

[1] Cerf, N. J., Adami, C. (1996). *Quantum mechanics of measurement.* arXiv preprint quant-ph/9605002.

[2] Moldoveanu, F. (2016). *Unitary realization of wave function collapse.* International Journal of Quantum Information, 14(04), 1640015.

[3] Aspect, A., Grangier, P., Roger, G. (1982). *Experimental Realization of Einstein-Podolsky-Rosen-BohmGedankenexperiment: A New Violation of Bells Inequalities.* Physical Review Letters, 49(2), 91-94. doi:10.1103/physrevlett.49.91

[4] Griffiths, D. J., Schroeter, D. F. (2018). *Introduction to quantum mechanics.* Cambridge University Press.

[5] Shankar, R. (1995). *Principles of Quantum Mechanics.* doi:10.1007/978-1-4615-7673-0

[6] Nielsen, M. A., Chuang, I. (2002). *Quantum computation and quantum information.* Cambridge University Press.

[7] Fraleigh, J. B. (2003). *A first course in abstract algebra.* Pearson Education India.

[8] Vazirani: Quantum Computation.
`https://people.eecs.berkeley.edu/ vazirani/quantum.html`

[9] Preskill: Quantum Computation.
`http://theory.caltech.edu/people/preskill/ph229/`

[10] MIT: MIT OCW.
`https://ocw.mit.edu/courses/physics/`

[11] Google: Google Scholar.
`https://scholar.google.com.sg/`

[12] Cornell University Library: arXiv.
`https://arxiv.org/`