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The Non-Relativistic  
**QUANTUM MECHANICS**

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# Preface

Quantum mechanics is believed to be a abstruse subject of physics. The foremost reason for that is abstractness that it bore. This book (which are my personal notes of quantum mechanics) is not unique than most of contents written on quantum mechanics. However, it is a slightly different approach to quantum mechanics. There are many works that had been done in quantum mechanics, we can not compile the all. But we only mention major developments, which include the ideas of interpretations, wave function, operators, Schrodinger equation, Linear algebra, angular momentum and spins, pictures in quantum mechanics (Heisenberg and Schrodinger), energy levels and systems. There are three short appendices. This book is mostly self-contained and contain no exercises. The material gets advance by every chapter.

We, however, do not report on perturbation theory, which is a very important development in quantum mechanics and field theory. What we not cover are- investigation of Hydrogen atom, effects of angular momentum. We do include the Hamiltonian correction.

I believe that this subject is so whole and so important for what comes next in physics. Without quantum mechanics, one could not think of string theory, which is a major work in progress in physics. An amateur physicist is likely to question quantum mechanics, but that is natural. The idea is to take abstractness mathematically and enjoy it.

- Aayush Verma



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# Background

This brief chapter introduces the reader to a few mathematical concepts. However, the reader might skip it if already aware of these. Quantum mechanics deals with a lot of differentials and partial differential. One should know how to solve them. Solving the partial differential equation (PDE) concerns finding the wave functions, eigenvalues, and more in quantum mechanics. A first-order PDE looks like

$$\frac{\partial x}{\partial y} = z. \quad (0.0.1)$$

One of the nicest PDEs is the three-dimensional Schrodinger equations, which we will discuss in chapter 1. We also encounter Fourier transformations and the Fourier series in this book. It is technical to define them. Simple is that they decompose the functions to work in the space and time desired. For instance, a piano can have different music from the same key in different frequencies. We will encounter it when we desire to change from position space to momentum space.

A four vector  $a^\mu$  is a vector in four-dimensional space-time, where  $\mu = (0, 1, 2, 3)$ . This vectors are used when we discuss relativity and geometry. Note that  $(0 = t)$  and  $(1 = x, 2 = y, 3 = z)$ , where  $t$  is time dimension and  $x, y, z$  are spatial dimensions.

We will also use most linear algebra. A particular chapter is dedicated to it, chapter 4.

Readers must be acquainted with methods to solve integral equations as well.

It would be a bonus if computing is done through many parts with software like *Mathematica* and *Matlab*.





*“This whole book is but a draught nay, but the draught of a draught.”* - Herman  
Melville

**Part 1**  
**A Picture Of Quantum Mechanics**  
**And Linear Algebra**



# Chapter 1

## A Brief Sketch of Quantum Mechanics

*”If we think we understand quantum mechanics, we don’t understand quantum mechanics.” - Richard Feynman*

This chapter will be dedicated to introducing this theory, with more minor mathematics but more intuition. Any physical theory must have two properties- first, it should give us results and some more information about this universe, and second, it should be testable. However, in the case of Quantum Theory, some of the predictions are just predictions, and they can never be tested experimentally. Mainly due to intelligence insufficiency. Quantum mechanics is a theory of low scale and high energy.

### 1.1 Particle and Wave

The universe is fundamentally made up of particles and anti-particles. However, we will be mainly discussing particles, and these particles function the whole universe. It can be fermions or bosons. To be clear, Fermions are particles that have half-integer spin, as an example  $\pm\frac{1}{2}$ . Moreover, the Bosons which have

whole number spin. We will discuss Spins later. Fermions comprise of Leptons and Quarks, both leptons and quarks are of 6 kinds. Leptons are like the electron, the muon. See Appendix 3.

There are six quarks- up, down, charm, strange, top, bottom. These quarks, when added form particles like proton and neutron.

Bosons are, usually, carriers of fundamental forces, Photons carry Electromagnetic force, W and Z bosons for Weak Force, Gluon for Strong interaction and hypothetical particle Graviton <sup>1</sup> for Gravitational force. Coming to wave, waves in my sense is a disturbance. Electromagnetic waves are the propagating waves with the velocity equal the speed of light. It was believed that light is a wave, albeit Newton proposed his theory of corpuscles. Physicists believed that waves and particles are different theories. They believed a wave is just a wave, and a particle is just a particle with different treatments. But this tradition was broken with the Einstein Paper on the Photoelectric Effect <sup>2</sup> which proved that light was the stream of many particles, at that time it was called “quanta”. As like this, in 1924, de Broglie proposed his hypothesis that every matter is dual to a wave-theory with  $\lambda = \frac{h}{p}$ . This was shown in the Double Slit Experiment, first done by Thomas Young in 1801, which proved that light and matter can show both particle and wave properties. This opened a gate to a new theory that became Quantum Theory. Quoting a remark of Albert Einstein on the theory: “*his double nature of radiation (and of material corpuscles) ... has been interpreted by quantum-mechanics in an ingenious and amazingly successful fashion. This interpretation ... appears to me as only a temporary way out...*”.

This shows the disagreement of Einstein over quantum theory, we will discuss later the paper Einstein (and his colleagues) wrote condemning the wave-functions. It is now a strong fact that wave and matter are just different forms of the same component, and we can jump to our next section, which is wave function.

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<sup>1</sup>Graviton is just a hypothetical particle and not yet experimentally found, to unify the force this particle was introduced.

<sup>2</sup>Über einen die Erzeugung und Verwandlung des Lichtes betreffenden heuristischen Gesichtspunkt, A. Einstein, Annalen der Physik Volume 322, Issue 6

## 1.2 Wave Function

$\psi$  (psi) is the term we use to determine the wave function, now for the new reader, it can be a little confusing as it does not provide enough description about it initially, but as we go we will understand these mechanics itself. For now let us call  $\psi$  a function of our wave with parameters  $x, t$ .  $\psi(x, t)$  is complex, but we will see later that this can be chosen real<sup>3</sup> in some conditions. To understand this concept, let us say that we have a particle  $P$ , now what classical mechanics teaches us that position of a particle can be defined as  $x(t)$ , momentum with  $mv$ , the force with  $m d^2/dt^2$ , velocity by  $dx/dt$ .

But in Quantum Mechanics we deal with these things with a little different approach. As in classical mechanics we look for  $m, x$  and  $p$ , in quantum mechanics we have to hunt  $\psi(x, t)$ , and we get it by solving the most first and popular equation i.e Schrödinger Equation.

$$\boxed{i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi} \quad (1.2.1)$$

Where  $i^2$  is  $-1$  and  $\hbar$  is a reduced Planck's constant:

$$\hbar = \frac{h}{2\pi} \quad (1.2.2)$$

Here  $h = 6.626 \times 10^{-34} Js$  and  $\hbar = 1.054 \times 10^{-32} Js$ .

Now, what exactly this Schrödinger Equation is? It is a complete analogy of Newton's Second Law of motion. Schrödinger Equation tells us that how  $\psi(x, t)$  evolves. And You will use how to use it in the later section and how to prove it. These wave function can be both of position space and momentum space,  $\psi(x, t)$  and  $\phi(k, t)$  respectively.<sup>4</sup> But before taking a look at them we have a lot of unfinished sections to complete.

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<sup>3</sup>By real here, we mean we can choose the energy eigenstates to be real

<sup>4</sup>Time parameter can be eliminated for the sake of simplicity

## 1.3 Interpretations

Interpretations are a cool feature of Quantum Mechanics, but what is it?

Quantum Interpretations are just different views, different views of the field. Every person can choose their interpretation or can make one. Nevertheless, as someone reading quantum mechanics must know about interpretations of the subjects. There are many interpretations, and we are mentioning some here.

**Copenhagen Interpretation** - This interpretation is far popular and mostly picked among physicists. This explains to us that a  $\psi$  is not any single object, albeit it is a superposition of many eigenstates and eigenvalues. When we observe our wave function, then it collapses to a single result and an arbitrary solution is given. So it is meaningless to ask about, "Where was our particle before the observation?"

This interpretation is not so easy to catch, but indeed this interpretation is one of the fascinating things about Quantum Mechanics. Also the most debated one. We mostly do not talk about interpretations when we talk about the abstract nature of quantum mechanics, but it was one of the major philosophies behind quantum mechanics in the early years.

Now, there must be some probability to find the particle around some coordinate in space, yes there is a Statistical Interpretation of the very quantum system.  $|\psi(x,t)|^2$  tells us about the probability of the particle at position  $x$  and time  $t$ . Well, a more rigor equation for this same purpose is:

$$\int_a^b |\psi(x,t)|^2 dx \quad (1.3.1)$$

Equation 1.3.1 is for nothing but just finding the wave-function statistics distribution between  $a$  and  $b$  at time  $t$ . And when the particle is observed, the whole wave function gets collapsed to one arbitrary point.

Let's assume that Fig. 1 is our wave function, a typical one, there can be many wave functions according to states. As we can see that wave function localize at points 1.5, 7.5 and 13.5, at least roughly. So we can say that particles are more likely to be found at anti-nodes rather than 4.6 and 11. But this figure visualizes



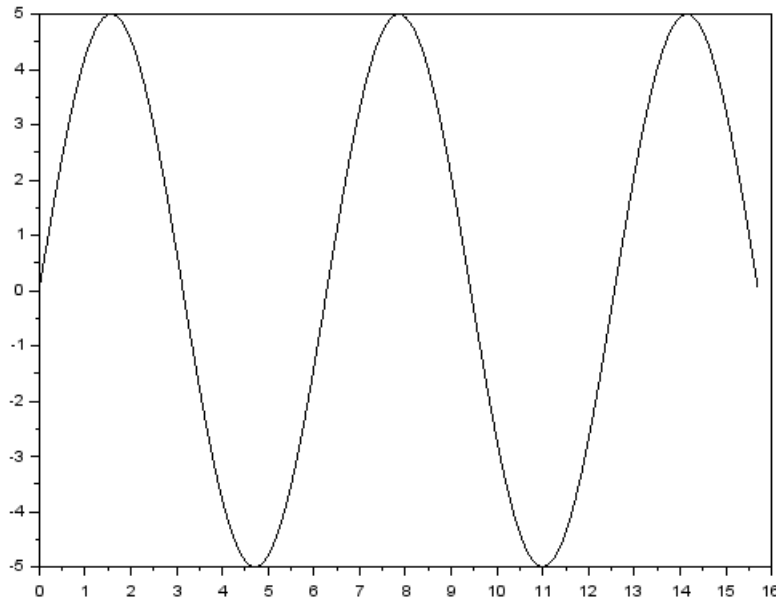


Figure 1.1: Fig. 1, A typical wave function  $\psi(x,t)$

the wave function before the observation. Now the Eq. 1.3.1 will guide us through this complex  $\psi$ , y-axis (horizontal) is  $|\psi(x,t)|^2$  and x-axis is just the  $x$ . The integral will tell us the area under the graph. For example, the probability of finding the particle between 1 and 4 will be given by Eq. 1.3.1, now that will be the probability of finding the particle between 1 and 4. After the observation, it will be more like Fig. 2, where the whole function localizes to a point, in this case, it is 1.5. Hence the particle has found at position 1.5. This tells us that the whole wave function is just crunched into a single line and that is a fascinating thing about this. Copenhagen's interpretation is a spooky thing, as called by a great physicist, but it is reasonable if we believe in this quantum abstractness. The critiques of this interpretation are powerful and believed to be true, and in fact, there are many paradoxes of this interpretation. One famous is Einstein advocated EPR.

Jordan once said, "Observations not only disturb what is to be measured, they produce it", well technically, this interpretation take a stand to the theory of inde-

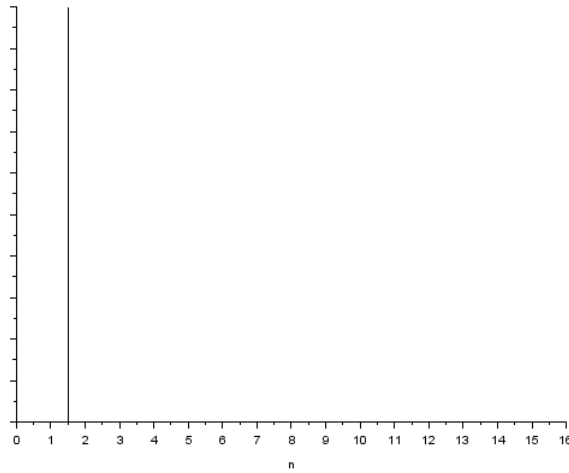


Figure 1.2: Fig. 2, Wave function  $\psi(x, t)$  after collapse

terministic result. Hence, it is not logical to ask about the pre-conditions of the particle before the measurement. There was a great debate on this book, yet it is going on.  $\psi$  is not the complete story, there are hidden variables also, discussed in brief in the later section.

Now what happens for the second observation to this system, will it produce the same result?

Well, maybe or not, Quantum Mechanics is known for this total loss of determinism. We can get the same result or different results. And this is the fact which Einstein criticized the most.

Many authors have already written about those things, but we are going to propose a thought experiment, indeed a thought experiment in Quantum Mechanics. Imagine a house in which 1 people live, now there are many rooms, let's say 5 and we go inside the house, we are on the hall floor. Now in which room we are likely to find the person, in his bedroom, but he can be anywhere else!

Unless and Until we do not see that person in a room, we can just assume that the person is in here or there. But when we find him/her, then we can finally believe. Let's say that person is found in the lab room. So the whole probability of thoughts in your mind collapses to the one single result of the lab room. Now

take the house as the wave function, the person as the particle and rooms as their positions. Just make the complete analogy stating that we come again after 1 hour, then the story repeats. We will not tell us that both the house and wave function is the same, but we are just making an analogy, we hope it helps.

### **Many Worlds Interpretation**

- Everett's thesis introduction reads:

*"Since the universal validity of the state function description is asserted, one can regard the state functions themselves as the fundamental entities, and one can even consider the state function of the entire universe. In this sense, this theory can be called the theory of the "universal wave function," since all of physics is presumed to follow from this function alone"*

Before introducing the term to us, we would like to show we the conversation of two physicists.

Ray Streater writes to Everett:

*"The idea of the wave-function of the universe is meaningless; we do not even know what variables it is supposed to be a function of. We find the laws of nature by reproducible experiments. The theory needs a cut, between the observer and the system, and the details of the apparatus should not appear in the theory of the system"*

Hugh Everett writes in response:

*"If we try to limit the applicability so as to exclude the measuring apparatus, or in general systems of macroscopic size, we are faced with the difficulty of sharply defining the region of validity. For what  $n$  might a group of  $n$  particles be construed as forming a measuring device so that the quantum description fails? And to draw the line at human or animal observers, i.e., to assume that all mechanical apparatus obey the usual laws, but that they are not valid for living observers, does violence to the so-called principle of psycho-physical parallelism"*

Coming to the point of Many Worlds Interpretation introduced by Everett, this regards the whole universe as a wave function and there is no wave function collapse. This is a whole opposing interpretation of Copenhagen Interpretation. Albeit it is popular but less believed. The main idea is that there are infinite number of universes each with their correspondence wave functions. When we observe the wave function, we generally see the result in one universe. This is done by Quantum De-coherence (discussed more in later sections). This is a little crazy, but the whole idea just transpose the thing that we have discussed. Although we are not going too deep here at this interpretation.

**De Broglie–Bohm theory** - The last interpretation which we will talk, which also treats wave function collapse as an illogical fact. Known as pilot-wave theory, this theory emphasizes that particle have a configured space even when they are unobserved. And the velocity of the particle is given by the guiding equation:

$$\frac{dQ(t)}{dt} = \frac{\hbar}{m} \text{Im} \left( \frac{\nabla \psi}{\psi} \right) \quad (1.3.2)$$

$$\frac{dQ_k(t)}{dt} = \frac{\hbar}{m} \text{Im} \left( \frac{\nabla \psi}{\psi} (Q_1, Q_2, Q_3 \dots Q_4, t) \right) \quad (1.3.3)$$

The configuration  $Q$  guides eq. (1.3.2) and Eq. 1.3.3 hold for many particles systems. Well, these equations more look like the current density

$$J(x, t) = \frac{\hbar}{m} \text{Im} \left( \frac{\partial \psi^*}{\partial x} \right) \quad (1.3.4)$$

Here,  $\text{Im}$  is the imaginary part and  $\psi^*$  is said to be conjugated. We will discuss Current Density and Probability Density more in later.

## 1.4 Normalization

As we have discussed that the probability current is,

$$\int_{-\infty}^{+\infty} |\psi(x, t)|^2 dx \quad (1.4.1)$$

But there must be some value for this function, and it is 1,

$$\int_{-\infty}^{+\infty} |\psi(x,t)|^2 dx = 1 \quad (1.4.2)$$

What does that mean?, it means that the probability of finding the particle between the region is 1, well it must be 1, because your particle is just at one place at a time, logically.

Not every function is normalized when it is given to we, but we can normalize it by putting a constant at the begging,

$$A^2 \int_{-\infty}^{+\infty} |\psi(x,t)|^2 dx = 1 \quad (1.4.3)$$

Well, A doesn't do anything to our solution, because if  $\psi(x,t)$  is a solution then  $A\psi(x,t)$  is also a solution, that is called linearity. Now, if  $\psi(x,t)$  is a normalized wave function at t, then what is the grantee of it being normalized during whole time. Let's check,

$$\frac{d}{dt} \int_{-\infty}^{+\infty} |\psi(x,t)|^2 dx \quad (1.4.4)$$

By Leibniz rule,

$$\int_{-\infty}^{+\infty} \frac{\partial}{\partial t} |\psi(x,t)|^2 dx \quad (1.4.5)$$

$$\frac{\partial}{\partial t} |\psi(x,t)|^2 = \frac{\partial}{\partial t} (\psi^* \psi) \quad (1.4.6)$$

Which then equals, by product rule,

$$\psi^* \frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t} \psi \quad (1.4.7)$$

By Schrödinger Equation,

$$\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2} - \frac{i}{\hbar} V \psi \quad (1.4.8)$$

$$\frac{\partial \psi^*}{\partial t} = -\frac{i\hbar}{2m} \frac{\partial^2 \psi^*}{\partial x^2} + \frac{i}{\hbar} V \psi^* \quad (1.4.9)$$

Then,

$$\frac{\partial}{\partial t} |\psi(x,t)|^2 = \frac{i\hbar}{2m} (\psi^* \frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi^*}{\partial x^2} \psi) \quad (1.4.10)$$

Which then equals to,

$$\frac{\partial}{\partial x} \left[ \frac{i\hbar}{2m} (\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x} \psi) \right] \quad (1.4.11)$$

Now explicitly,

$$\frac{d}{dt} \int_{-\infty}^{+\infty} |\psi(x,t)|^2 dx = \frac{i\hbar}{2m} (\psi^* \frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi^*}{\partial x^2} \psi) \quad (1.4.12)$$

evaluated at  $-\infty, +\infty$ , now wave function must go to zero as  $x$  goes to  $\pm\infty$ , otherwise the wave function would not be any normalizable, then it is clear than the integral is zero,

$$\frac{d}{dt} \int_{-\infty}^{+\infty} |\psi(x,t)|^2 dx = 0 \quad (1.4.13)$$

hence the integral is independent of time, so if any wave function is normalizable at any particular time, then it is normalized at every time.

What if a wave function is not normalized?

If a wave function cannot be normalized, then it does not represent any particle, although it can be used in quantum mechanics. But in most calculations, a wave function must be normalizable.

## 1.5 Operators and Commutators

Now this part will be more mathematically than any part above. The motivation to read is the Schrödinger Equation, because that equation is intuitively get when derived with operators.

Operator is that mathematical object which acts on a function to given an eigenvalue. They are denoted by a hat in top. This definition is deeply influenced by Quantum Mechanics. And the eigenvalues will be discussed later in Chapter 4. More mathematically, an operator is a mapping between functions in its domain and functions in its range, and our domain and range are both in Hilbert Space<sup>5</sup>.

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<sup>5</sup>Hilbert Space is a physics space where wave functions live

So we can say in my definition that "Operators are nothing more than imposer and giver of a value".

Some examples of the operator in Quantum Mechanics is  $x$ ,  $p$  and  $H$ . We will come to that when we will derive Schrödinger Equation in next chapter and a little bit here. Let us play with operator  $X$  and  $P$  acting on  $\psi$ , where  $P$  is equal to  $\frac{\hbar}{i} \frac{\partial}{\partial x}$

$$\hat{P}\psi(x,t) = \frac{\hbar}{i} \frac{\partial \psi(x,t)}{\partial x} \quad (1.5.1)$$

By idea,

$$\hat{P}\psi(x,t) = p\psi(x,t) \quad (1.5.2)$$

Here,  $p$  is the eigenvalue and  $\hat{P}$  is a momentum operator.

Now these operators can be differential equations as well,<sup>6</sup> they might or might not commute with each other. We call these commutators. It is defined by,

$$[A, B] = AB - BA, \quad (1.5.3)$$

here  $A$  and  $B$  are operators. We will exploit these commutators in every chapters ahead.

$$[x, p] = i\hbar. \quad (1.5.4)$$

---

<sup>6</sup>Because differential operators acts with their right according to their parameters.

**Some useful commutator rules if  $A$ ,  $B$  and  $C$  are operators and  $n$  is constant,**

$$\begin{aligned} [A, B] &= -[B, A] \\ [A, B \pm C] &= [A, B] \pm [A, C] \\ n[A, B] &= [nA, B] = [A, nB] \end{aligned} \tag{1.5.5}$$



## Chapter 2

# Mach-Zehnder Interferometer

Interferometer is a tool for optics, but it is always kind of a game that Quantum Mechanics enjoys, but with an add of loss of determinism and matrix play. So a rough kind of interferometer is depicted in Fig 2.1 .

### 2.1 The Interferometer

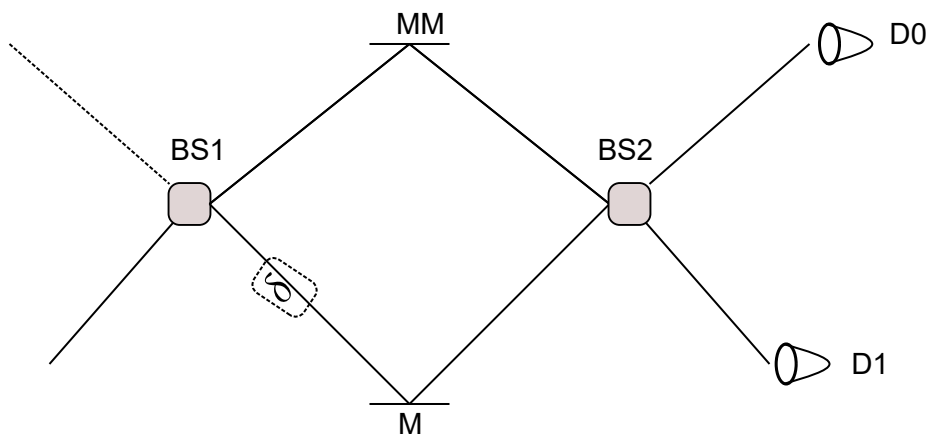


Figure 2.1: Mach-Zehnder Interferometer

Here is depicted is a couple of beam splitters (BS1 and BS2) and two mirrors (one up and another at down), and at last two detectors (D0 and D1). This is a rough kind of design. And two ways to push the particle. Before we start experimenting without doing experiments, we need to adopt the Quantum Interpretations. The  $\delta$  is a phase-shifter.

We of course start with probability amplitude whose norms are point of concern. We can construct a matrix of probability of particle coming either upper or lower beam.

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} \quad (2.1.1)$$

Where  $\alpha$  is always the probability of entering the particle from upper beam and  $\beta$  of the opposite. We can make a complete analogy of Normalization and hence state particle, here as photon must be anywhere, so

$$|\alpha|^2 + |\beta|^2 = 1 \quad (2.1.2)$$

Hence, two possibilities,

1. Photon from upper beam  $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$  2. Photon from lower beam  $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$  we can check the Eq 1.2 criteria, that means they are well-normalized. You can also create a superimposed one,  $\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$

*Short hand Exercise Express Eq 1.2 into a superposition of two possibilities that we have mentioned above.*

Let us get to the phase-shifter in the Fig 2.2, that phase-shifter (assuming that the reader know what a phase is) is, so once a particle (wave amplitude)  $\alpha$  hits the

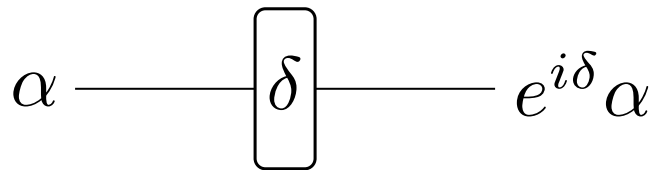


Figure 2.2: Phase

phase, it becomes

$$\alpha \rightarrow e^{i\delta}\alpha \quad (2.1.3)$$

where  $\delta$  in this sense is merely just a phase contributing to  $\alpha$ . So when reflection reflects a particle with  $\pi$  the phase become  $e^{i\pi}$  which is -1 and the overall amplitude  $-\alpha$  which is pretty best agreement with the later discussion on reflection and scattering.

Let's now move on the experiment. So a particle in the form of  $\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$  hits the BS1 (Beam Splitter), now a beam splitter can split the particle either to upper path to lower path. If photon comes to BS1 using upper beam or lower beam we use  $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$   $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$  respectively to represent it.

We now make four-channel a, b, c and d. Channels a and b for the upper branch and channels c and d for the lower branch. Where for the upper branch, a can be seen as reflection, and b can be seen as transmission (coefficient). Same with c and d for the lower branch.

Hence when  $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$  hits the BS1

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \rightarrow \begin{pmatrix} a \\ b \end{pmatrix} \quad (2.1.4)$$

and

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} \rightarrow \begin{pmatrix} c \\ d \end{pmatrix} \quad (2.1.5)$$

Now, as

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \alpha \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (2.1.6)$$

so replacing the Eq 1.6 with Eq 1.4 and Eq 1.5,

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \alpha \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta \begin{pmatrix} 0 \\ 1 \end{pmatrix} \rightarrow \alpha \begin{pmatrix} a \\ b \end{pmatrix} + \beta \begin{pmatrix} c \\ d \end{pmatrix} \quad (2.1.7)$$

which can be written as

$$\begin{pmatrix} \alpha a + \beta c \\ \alpha b + \beta d \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \quad (2.1.8)$$

The matrix  $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$  is the calculation we have to do. There is a defined parameter already set for that matrix. Because of Eq 1.2, we have

$$|a|^2 + |b|^2 = 1 \quad (2.1.9)$$

$$|c|^2 + |d|^2 = 1 \quad (2.1.10)$$

The beam splitter we have to use is balanced so coefficients of probability of reflection and transmission is same, hence we use the norm

$$|a|^2 = |b|^2 = |c|^2 = |d|^2 = \frac{1}{2} \quad (2.1.11)$$

So, the matrix can be constructed as the value of  $\pm \frac{1}{\sqrt{2}}$ . We will try the simplest one which is

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \quad (2.1.12)$$

But this kind of matrix is harmful for normalized wave function as we will see

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \quad (2.1.13)$$

While that works, let us see a different example

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad (2.1.14)$$

But as we see the Eq 1.2 this is not satisfied. So the matrix is not Eq 1.12. But what it can be?

A slight change in d where we swap the sign can yield a better matrix.

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} \quad (2.1.15)$$

It can be checked that it is good for BS1, and has a good agreement with all our previous statements. The - minus there is for reflection that we discussed over,

but only when there is higher refractive index (unfortunately we will not go in details). And then pretty much the content after hitting the beam splitter is

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \quad (2.1.16)$$

which is

$$\frac{1}{\sqrt{2}} \begin{pmatrix} \alpha + \beta \\ \alpha - \beta \end{pmatrix} \quad (2.1.17)$$

we can check that  $\frac{1}{\sqrt{2}}|\alpha + \beta|^2 + \frac{1}{\sqrt{2}}|\alpha - \beta|^2 = |\alpha|^2 + |\beta|^2 = 1$ , that is a quite exercise.

And then, the experiment proceeds it gets reflected toward the next BS2 by the mirror. The same strategy for BS2 can yield a similar matrix.

$$\begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \quad (2.1.18)$$

You can check it also by using the same technique and analysis. So we have now two encounters with  $\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$  that will be,

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \quad (2.1.19)$$

which can be further down to

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \quad (2.1.20)$$

then,

$$\frac{1}{2} \begin{pmatrix} 0 & 2 \\ -2 & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \quad (2.1.21)$$

which eventually leads to our final result that is

$$\begin{pmatrix} \beta \\ -\alpha \end{pmatrix} \quad (2.1.22)$$

So here we have a better-computed result from which we can immediately extract the answer.

$$BS_1 BS_2 \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \beta \\ -\alpha \end{pmatrix} \quad (2.1.23)$$

So when we put  $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$  then the result will be  $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$  that means the probability of finding the photon at D0 is 1 and D1 is 0. So clearly if all things performs well, out photon will be at D0.

$$\text{Input: } \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\text{Output: } \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

### 2.1.1 Some Other Test

We can also perform another test as in Fig 2.3, where we block the lower branch, then the probability changes. So our photon with  $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$  hits the BS1 then

$$\frac{1}{\sqrt{2}} \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \quad (2.1.24)$$

But after that only upper beam proceeds, then the matrix will be  $\begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$  and

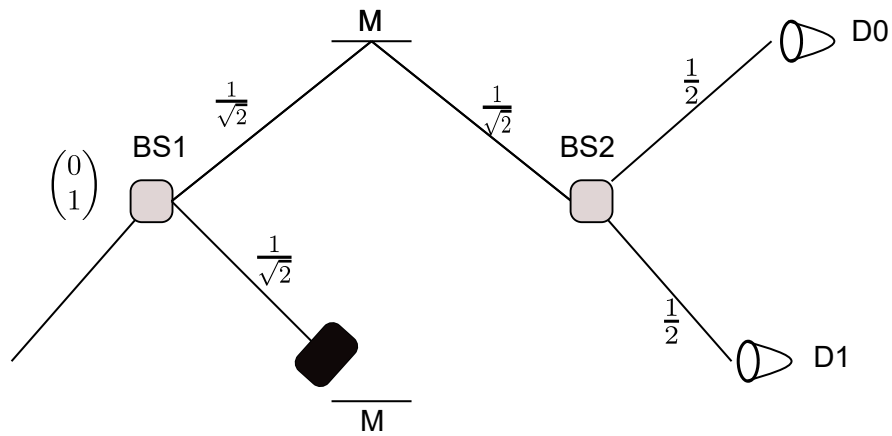


Figure 2.3: Blocking the path, changes the probability of same photon.

then it hits the BS2, then it will be like  $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$  and then last probability will be  $\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$ .

Hence we see that blocking one path will give us an equal probability of finding the photon at either of the detectors. So we see that before not blocking the path, we could not get photon at D1, but here we are with forcing physics to work.





# Chapter 3

## Schrödinger Equation

*"Where did we get that (equation) from? Nowhere. It is not possible to derive it from anything we know. It came out of the mind of Schrödinger."*

- Richard Feynman

### 3.1 The Building of the Equation

Schrödinger Wave Equation was given by Erwin Schrödinger, In January of 1926, Schrödinger published in Annalen der Physik the paper "Quantisierung als Eigenwertproblem" and this is now known that the famous Schrödinger Equation, which is none other than a complex mathematical equation with lots of space-time derivative and Hamiltonian;

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi \quad (3.1.1)$$

$$H\psi = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi \quad (3.1.2)$$

$$H\psi = E\psi \quad (3.1.3)$$

Where,  $H$  is Hamiltonian,  $T$  is kinetic energy and  $V$  is potential energy

$$H = T + V \quad (3.1.4)$$

$$H = \frac{p^2}{2m} + V(x) \quad (3.1.5)$$

Well in Eq (3.1.3) we can observe the operator's operation. These are some common forms of the equation in one-dimension and in 3-dimensions it becomes,

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \psi + V\psi \quad (3.1.6)$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad (3.1.7)$$

## 3.2 Derivation

In this section, we will do the most awaited thing. We will be deriving the equation with the help of the basic kinds of stuff in one-dimensional space and time  $t$ . For the sake of readers, we will not extend the proof, we will try to keep it simple. Before moving on we will take the solution to be,

$$\psi(x,t) = e^{ikx - i\omega t} \quad (3.2.1)$$

Here,  $k$  is wave number and  $\omega$  is the angular frequency. What is a Hamiltonian?, It is nothing other than our total energy system which we can denote by

$$H = \frac{p^2}{2m} + V(x) \quad (3.2.2)$$

Here,  $p$  is momentum,  $m$  is mass and  $V$  is potential of the system. As we have discussed in the section 1.4 that  $p$  is also an operator with value,

$$\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x} \quad (3.2.3)$$

In Eq (3.2.2), there is  $p$  squared, so we can take  $p$  as a momentum operator. Now that  $\hat{H}$  is also an operator, let us act it on wave function  $\psi(x,t)$

$$H\psi = \frac{p^2}{2m}\psi(x,t) + V(x)\psi(x,t) \quad (3.2.4)$$

Now expanding the operator  $p$ -squared

$$\hat{p}^2 = \frac{\hbar}{i} \frac{\partial}{\partial x} \cdot \frac{\hbar}{i} \frac{\partial}{\partial x} \quad (3.2.5)$$

$$\hat{p}^2 = -\hbar^2 \frac{\partial^2}{\partial x^2} \quad (3.2.6)$$

As  $i^2$  is -1, now let us apply the result to the Eq 2.9

$$H\psi = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x)\psi(x,t) \quad (3.2.7)$$

And here our result is, the Hamiltonian action on the wave function, but what the left hand side of Eq (3.1.1). For that,

$$E = \hbar\omega \quad (3.2.8)$$

$$E\psi = \hbar\omega\psi \quad (3.2.9)$$

$$\frac{\partial \psi}{\partial t} = -i\omega\psi \quad (3.2.10)$$

Now in Eq (3.2.9), let us multiply both sides by  $-\frac{i}{\hbar}$ , then it contributes to,

$$-\frac{i}{\hbar}E\psi = -\frac{i}{\hbar}\hbar\omega\psi \quad (3.2.11)$$

$$-\frac{i}{\hbar}E\psi = -i\omega\psi \quad (3.2.12)$$

Using Eq (3.2.10), one can replace  $-i\omega$ ,

$$-\frac{i}{\hbar}E\psi = \frac{\partial \psi}{\partial t} \quad (3.2.13)$$

In more general,

$$E\psi = i\hbar \frac{\partial \psi}{\partial t} \quad (3.2.14)$$

And since  $E\psi = H\psi$

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi. \quad (3.2.15)$$

And that is our result in most simple way, now this is not only the solution, there can be many solutions to the equation. But we will for now just look at time dependent wave equation. In next section, we will talk about the applications of this wave equation and how it is useful.

### 3.3 Applications of the Equation

There are many applications of this equation as it is the most precise and powerful equation in Quantum Mechanics. Not only the Quantum Mechanics, but many fields in physics take help from Schrödinger Equation. Here we will discuss some important application of this equation in non-relativistic quantum mechanics.

#### 3.3.1 Energy Level

The most important application is finding Energy levels of the quantum particle. In fact, the equation was set-up in need of energy eigenstates and eigenvalues. So it is not surprising that if Hamiltonian  $H$  is in the equation as an operator so it must give eigenvalues of Energy. As it is a second-order linear differential equation, it may be sometimes easy and sometimes hard to find the energy levels of particles. But using Eq 2.21 and Eq 2.2, which are almost the same but in different forms, one can find the energy level. We will talk more about this as we will discuss the basic potential cases in non-relativistic quantum mechanics.

#### 3.3.2 Space, Momentum and Time

If we have wave function at position  $x$ , we can find its position in space at  $t = t_0$  using the Schrödinger Equation. And similarly, we can find when that equation

evolves at a particular time.

Note: This does not mean that we can trace the particle, we can just trace nature the wave function which is similar to the below figure. We are more or less just drawing the wave-diagrams.

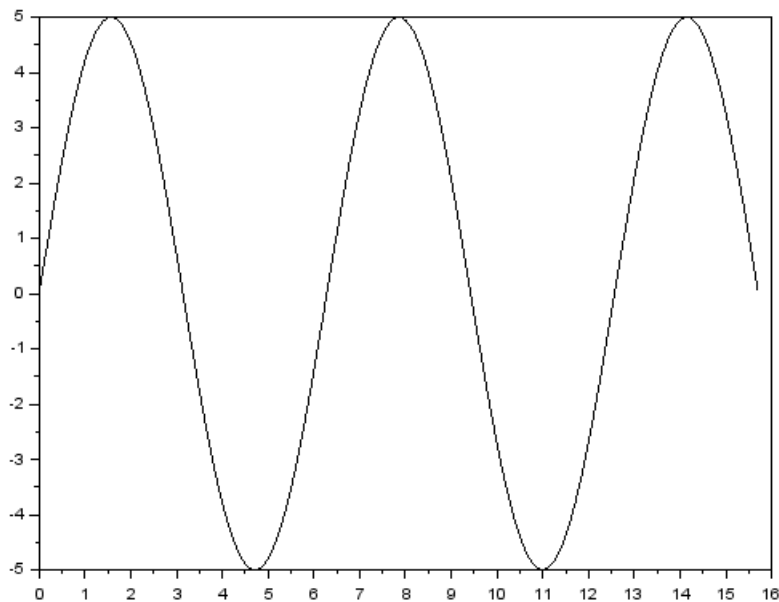


Figure 3.1: Wave diagram.

In the figure (3.1) we can see that at any point the wave function has some value, so as we go along x-axis we see the evolution of wave function which results in quantum mechanics and Schrödinger equation helps to find those space, time and momentum parameters when needed.

### 3.3.3 Measurement and Uncertainty

In classical mechanics, position and all that classical physics are deterministic means we can find them at any time in space. But in Quantum Mechanics, we don't have that certain and precise position and energy results. As we have read Copenhagen is an unbeaten army to perfect result. So Schrödinger Equation deterministically guides us about the wave function and allow the probability in.

### 3.3.4 Quantization

Quantization refers to the transition of view and mathematics from classical formalism to the quantum mechanical. We try to quantize everything now, from gravity to motion. Sometimes we fail and pass. Quantizing gravity is a part of the Fundamental Theory of Physics.

There are two kinds of Quantization, First Quantization and Second Quantization. In First Quantization it is particles which are thought and treated as wave functions, but the overall system except the **Wave Function** is still dealt classically. It is generally used for single systems. For multi systems, we have Second Quantization, it is kind of canonical quantization (for mostly free interaction system) in which fields are thought of as field operators. It is vastly a tool for Quantum Field Theories.

Of Course not only equations, Simple Harmonic Oscillators (discussed later) is also very helpful in Quantum Field Theories.

# Chapter 4

## Linear Algebra and Spaces

*"Algebra is generous; she often gives more than is asked of her."*  
- Jean le Rond d'Alembert

This chapter will be an introduction to Linear Algebra that is language in which Quantum Mechanics is often written. This one is going to be the longest in this monograph. A short discussion about momentum and position space has been given, but if one want to start the Linear Algebra, the reader may jump to section 4.2.

### 4.1 Momentum and Position Space

Every aspiring physicist has some difficulty at quantizing the momentum and space for its practical and theoretical uses in Quantum Mechanics. Momentum and space are two important views of seeing any phenomena in the quantum world. But these two views are interconnected with each other through Fourier Transformation. Which helps us to understand the view by chaining into one and another and still get the perfect result that we want.

$[x, p]$  as we discussed later is  $i\hbar$ , that means,  $xp - px = i\hbar$ . The convention

while doing this transformation is the basis sum convention, our book is not exception. We start with, a wave function  $\psi(x)$  and write it in terms of basis and momentum space  $\phi(k)$

$$\psi(x) = \sum_j \phi(k) \psi_j(x) \quad (4.1.1)$$

or

$$\psi(x) = \int_{\text{momentum-space}} \phi(k) \psi_j(x) d^3k \quad (4.1.2)$$

where  $\psi_j(x)$  is by calculation using matrix laws

$$\psi_j(x) = \frac{1}{(\sqrt{2\pi})^3} e^{ik \cdot x} \quad (4.1.3)$$

that makes up Eq 4.1.2, which is integration under momentum space or k space.

$$\psi(x) = \int_{k\text{-space}} \frac{1}{(\sqrt{2\pi})^3} e^{ik \cdot x} \phi(k) d^3k \quad (4.1.4)$$

This is what we want. Though the prove is so trivial type, but for now, this should be satisfactory for new ones. This is called Fourier Transformation. It is actually a connection between position space and momentum space.

Eq 4.1.4 can also be written as

$$\phi(k) = \int_{x\text{-space}} \frac{1}{(\sqrt{2\pi})^3} e^{-ik \cdot x} \psi(x) d^3x \quad (4.1.5)$$

these two equations are very insightful mathematics which helps the very application of quantum problems, we will see it later.

## 4.2 A First Look at Linear Algebra

In this section and remainders of the chapter, it is all about Linear Algebra, which is a language which is mostly spoke in Quantum Mechanics and advanced physics. It is perhaps the best algebra, which will entertain we. Not only Quantum Mechanics, but Linear Algebra has it roots in every modern theories and mathematical subject. Though we will only try to implicate the necessary algebra, but for



a good reading, one can check Linear algebra done right by Sheldon Axler and Barton Zwiebach section Notes.

One start with Vector Spaces. You have studied vectors, but linear algebra takes it to a further step by creating a whole new space, and incidentally it is called Vector Space. It can be seen as a collection of vectors, but follows some rules. These rules cum better conditions described for vector space  $\mathcal{V}$  are,

1. If  $u \in \mathcal{V}$  and  $v \in \mathcal{V}$  then  $u + v \in \mathcal{V}$ .
2. There are elements from  $\mathcal{F}$ , such that  $av \in \mathcal{V}$  where  $a \in \mathcal{F}$  and  $v \in \mathcal{V}$
3. Three elements (vectors) from  $\mathcal{V}$ , let us say  $u, v$  and  $w$ , then,  $u + (v + w) = (u + v) + w$
4. There is an additive identity i.e  $0, v \in \mathcal{V}$ , then  $0 + v = v \in \mathcal{V}$
5. The number  $1 \in \mathcal{F}$  satisfies  $1v = v$
6. For each  $v \in \mathcal{V}$  there is a  $u \in \mathcal{V}$ , where  $u$  is inverse of  $v$ , such that  $v + u = 0 \in \mathcal{V}$
7. For number  $a$  and two vectors  $u$  and  $v$ , we have,  $a(v + w) = av + aw$ . And for two numbers  $a$  and  $b$  and a vector  $v$ ,  $(a + b)v = av + bv$

Hence  $\mathcal{V}$  is a vector space satisfying the addition rule of vectors, having an identity vector, having a 0 vector and multiplying any number with vector, just yield the scaled vector from same vector space.

Most of the claims are very self-realizing, such as 0 vector thing and identity thing.

There are very known algebras and mathematical systems which can be thought as Linear Algebra. But first why Linear Algebra?

It may be thought as a language of Quantum Mechanical descriptions. One can't offer anyone to talk unless he uses this mathematical tool of algebra. In fact, few theories requires it's own algebra, Supersymmetry is one of them. However,

one should not think of Linear Algebra as a Quantum tool, but one may think of as a language that we use when discussing this subject.

But there is question which we must ask first before proceeding. Where do wave functions live? This is most important and too subtle right now for us to ask, maybe stubborn as well. The answers lies in the root of this very algebra.

### 4.3 A Simple Kind of Vector Space

*We must emphasize that while the numbers, in  $F$  are sometimes real or complex, we never speak of the vectors themselves as real or complex. A vector multiplied by a complex number is not said to be a complex vector, for example! The vectors in a real vector space are not themselves real, nor are the vectors in a complex vector space complex. A few examples of vector space are:*

1. A Set of Vector

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix} \quad (4.3.1)$$

where  $x_i \in \mathcal{V}_{\mathcal{R}}$ , it is simply a real vector space that spans the matrix.

2. A Set of infinite sequences, so  $x_i \in \mathcal{F}$
3. A Complex Matrix with Complex entries, of  $M \times N$

$$\begin{pmatrix} a_{11} & a_{12} & \dots & a_{1M} \\ \vdots & & & \\ a_{N1} & a_{N2} & \dots & a_{NM} \end{pmatrix} \quad (4.3.2)$$

where  $a_{ij} \in \mathcal{V}_{\mathcal{C}}$  is a complex vector space.

There are so many different vector space and basis in mathematics and physics. Such as sets of polynomials, sets of complex function, or even a superimposed Wave Function can be treated as a vector space.

## 4.4 More About Vectors!

Now for every set there is a sub-set, for every discipline there is a sub-discipline and for every physicist there is prejudice<sup>1</sup>. So, for every vector spaces, there are sub-spaces from which a vector space is constructed.

$$\mathcal{V} = \sum_{i=1}^j \mathcal{U}_i \quad (4.4.1)$$

so it can be easily seen that  $v \in \mathcal{V}$  can be written as  $\sum_i^k u_i$  where  $u_i \in \mathcal{U}$ .

One also do have an option of creating lists of Vectors of finite length as well as dimensional,  $(v_1 \ v_2 \ v_3 \ \dots \ v_n)$ .

**A basis of vectors V, is simply a collector or list of vectors in the vector space, which do need to span the V. They are linearly dependent and can generate all the other elements of the vector space.**

**Note:** Dimension of a vector space can be configured using the length (or entries) of vectors in any basis.

## 4.5 Dirac Notation

Now it is an appropriate time for introducing the arithmetics <sup>2</sup> of Quantum Mechanics, which is Bra-Ket Notation. It was first intoduced by Paul Dirac in 1939.

Usually, we have two things to discuss by breaking the word **Bracket**. "Bra" and "Ket", now we are not going to miss the chance to throw the joke, **We don't**

---

<sup>1</sup>Sorry, but I am not a poet.

<sup>2</sup>Not the genuine one, but it can be said as alphabets, though *sine quo nan*

**know where C is! trust me, we don't.**

$$|\alpha\rangle - \text{ket} \quad (4.5.1)$$

$$\langle\beta| - \text{bra} \quad (4.5.2)$$

$|\alpha\rangle$  is just a vector representing a state, there are many notations which replaces the  $\alpha$ , primarily, it will be a state ket, like  $|\psi\rangle$ ,  $|n\rangle$ , etc. So, as like vector, our ket can be written as,

$$|\alpha\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \vdots \\ \alpha_n \end{pmatrix} \quad (4.5.3)$$

and the definition, we adapt for our bra is, they are simply conjugates of some state, for this matter, let us say  $\beta$ .

$$\langle\beta| = (\beta_1^* \ \beta_2^* \ \beta_3^* \ \dots \ \beta_n^*) \quad (4.5.4)$$

At first it would be not a crime to think of  $\langle\alpha|\alpha\rangle$  and  $\langle\beta|\beta\rangle$ , it will be simply 1<sup>3</sup>. Because,  $\langle\beta|\alpha\rangle$  is nothing but a inner product of two states. In case, one is not exposed to inner product, it is more like general dot product, but with a little twist.

In general,  $\langle\beta_i|\alpha_j\rangle = \delta_{ij}$ , where  $\delta$ , is a Kronecker delta (distribution), one would like to see Appendix B, for more. But in general,

$$\delta_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i=j \end{cases} \quad (4.5.5)$$

Let's back to the bracket, so

$$\langle\beta|\alpha\rangle = (\beta_1^* \ \beta_2^* \ \beta_3^* \ \dots \ \beta_n^*) \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \vdots \\ \alpha_n \end{pmatrix} \quad (4.5.6)$$

---

<sup>3</sup>This tells that both states are not orthogonal states, and overlap between two is maximum.

So, the inner product space would be,

$$\beta_1^* \alpha_1 + \beta_2^* \alpha_2 + \beta_3^* \alpha_3 + \cdots + \beta_n^* \alpha_n = \sum_i \beta_i^* \alpha_i \quad (4.5.7)$$

So, we see that the notation is helpful and conventionally easy for writing out our models, using such algebra. We will wait for later sections to know more.

## 4.6 Inner Product

As we discussed that Inner Product is nothing but a different name for conventional Dirac Notation. In this section, we discuss about more general ideas about inner product and Dirac notations.

Let us get first with bra  $\langle \beta |$ , we say  $\langle \beta |$  is a map  $\beta : \mathcal{V} \rightarrow \mathbb{C}$ . Mapping is a general geometry, where certain functions or sets are reproduced with slight changes using functions.

Then,  $\langle \beta |$  is generally producing complex vectors, hence it is easy to see that  $\langle \alpha | \beta \rangle \in \mathbb{C}$  (only in this case, it may be real also). Now, we must take out time so avoid a confusion that  $(\phi, \psi)$  and  $\langle \phi, \psi \rangle$  is same as  $\langle \phi | \psi \rangle$ . So we will see in various text using either former or latter. We will stick to  $\langle, \rangle$  notation<sup>4</sup>.

Before we move to lay out some rules for Inner Product, let us lay down some dot product rules, they are as follows for vector  $a$  with components  $(a_1, a_2, \dots, a_n)$ .

In general we say the dot product is defined as

$$a \cdot b = a_1 b_1 + a_2 b_2 + \cdots + a_n b_n \quad (4.6.1)$$

and for that matter the vectors should abide that,

1.  $a \cdot b \neq a, b$  for  $a, b > 1$ .

---

<sup>4</sup>For the respect of Mathematicians.

2.  $a \cdot a \geq 0$ , for all vectors  $a$ .
3.  $a \cdot a = 0$ , if only  $a = 0$ .
4.  $a \cdot b = b \cdot a$ .
5.  $a \cdot \alpha(b) = \alpha a \cdot b$ ,  $\alpha \in \mathbb{C}$ .
6.  $a \cdot (b + c) = a \cdot b + a \cdot c$ .

and  $|a| \geq 0$ . For those who don't know  $|a| = \sqrt{a_1^2 + a_2^2 + \dots + a_n^2}$ .

There is a famous Inequality, called Schwarz Inequality, which thus can be proven by above axioms, holds

$$|a \cdot b| \leq |a||b| \quad (4.6.2)$$

proof is easy, and we should attempt it, if we haven't. Now we say  $z$  is vector  $\in \mathbb{C}$

$$|z| = \sum_i^n z_i^* z_i \quad (4.6.3)$$

that suggests that inner product works in a way it is. Now let us again redirect ourselves to pure inner product, we take  $u$  and  $v$  vectors from  $\mathcal{V}$ , inner product is a map over  $\mathcal{F}$  to a number  $\in \mathcal{F}$ . That number is determined by  $\langle u, v \rangle$ . Now, the axioms are same as dot products'.

1.  $\langle u, u \rangle \geq 0$ , for  $u \in \mathcal{V}$ .
2.  $\langle u, u \rangle = 0$ , for  $u = 0$ .
3.  $\langle u, \alpha v \rangle = \alpha \langle u, v \rangle$ ,  $\alpha$  is a number.
4.  $\langle u, v + w \rangle = \langle u, v \rangle + \langle u, w \rangle$ .
5.  $\langle u, v \rangle = \langle v, w \rangle^*$ , reverse implies a conjugate.

The last one is intuitive, and very helpful for our manipulations, whenever needed. So, it is evident that we need Complex Spaces in order to perform Inner Product, otherwise it will step down to regular Dot Product.

**Exercise**

Perhaps, we would like to do a problem with inner product. So

$$\langle \alpha u + \beta v, w \rangle \quad (4.6.4)$$

from axiom 5, the 4.6.4 will be

$$\langle w, \alpha u + \beta v \rangle^* \quad (4.6.5)$$

because we assume  $\alpha$  and  $\beta$  is a number, it can be out of the product from Eq 4.6.4

$$\alpha^* \langle u, w \rangle + \beta^* \langle v, w \rangle \quad (4.6.6)$$

now Eq 4.6.5 may written as

$$(\alpha \langle w, u \rangle + \beta \langle w, v \rangle)^* \quad (4.6.7)$$

that is

$$\alpha^* \langle w, u \rangle^* + \beta^* \langle w, v \rangle^* \quad (4.6.8)$$

this inner product with the help the axiom 5, written as

$$\alpha^* \langle u, w \rangle + \beta^* \langle v, w \rangle \quad (4.6.9)$$

which is evidently equal to Eq 4.6.6. Hence we can practically (we mean Mathematically) see that Inner Product works!

\* \* \*

Now there are many Inner Product configurations we see in various problems, what we just saw was of  $\mathbb{C}^n$  vector spaces, where  $n$  is dimension.

There can be another kind of genuine integral inner product, that is of

$$\mathcal{V} = \{\text{set of } F(x) \in \mathbb{C}, x = [0, A]\} \quad (4.6.10)$$

$f, g \in \mathcal{V}$

$$\langle f|g \rangle = \int_0^A f(x)g(x)dx \quad (4.6.11)$$

this is evident. As we know, how a sign in mathematics changes into other, without any legal (or illegal) objection.

### 4.6.1 Orthogonal

The word orthogonal, can be meant and compared with right angles. But however, not justified. But  $90^\circ$ , is an important ingredient in discussing orthogonal. Now, this orthogonal word is going to help we a lot, during calculations, and would reduce to the simplest expression, if any. "Orthogonality" is the term, perhaps a good and wide term in linear algebra. When simple,  $u$  and  $v$  vectors  $\in \mathcal{V}$  are orthogonal, when

$$\langle u, v \rangle = 0 \quad (4.6.12)$$

that means by orthogonality (i.e because of Eq. (4.6.12))  $u$  and  $v$  are perpendicular to each other.

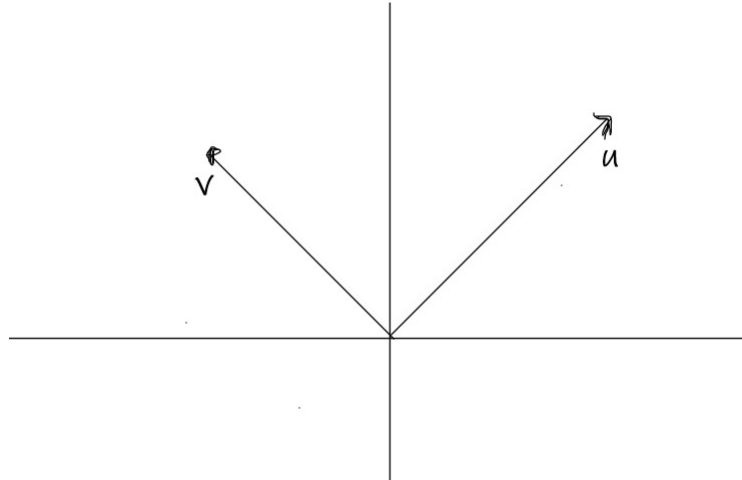


Figure 4.1: Representation of  $u$  and  $v$  vectors, orthogonal.

Orthogonal operators are those operators

$$A^T = A^{-1} \quad (4.6.13)$$

where  $T$  is transpose (studied in next section) and right side is inverse matrix. This follows that  $A$  must leave  $u$  and  $v$  inner product invariant

$$\langle Au, Av \rangle = \langle u, v \rangle \quad (4.6.14)$$

and  $\det A = 1$ . Product of two orthogonal matrix is orthogonal matrix, and hence one can form a orthogonal group.



There is another term called "Orthonormal", not it is distinct. It means that if  $u$  and  $v$  are orthonormal, then they are unit vectors (that automatically deduce the idea of orthogonality)<sup>5</sup>.

Above discussions, implies also sets, or vector spaces. So, two vector spaces or sets are orthogonal, if the inner product is 0. And they are orthonormal, if the set or vector space is orthogonal and every element is unit.

And if we have set of vectors  $\{e_1, e_2, \dots, e_n\}$  and

$$\langle e_m, e_n \rangle = \delta_{mn} \quad (4.6.15)$$

then the set is orthonormal. As we claimed. And  $\delta$  is Eq (4.5.5). And the norm game is also there, for  $a_i \in \mathcal{F}$

$$\left| \sum_i^n a_i e_i \right|^2 = \left\langle \sum_i^n a_i e_i \middle| \sum_i^n a_i e_i \right\rangle \quad (4.6.16)$$

$$= \sum_i^n \langle a_i a_i \rangle \quad (4.6.17)$$

$$= \sum_i^n |a_i|^2 \quad (4.6.18)$$

this means that vectors from an orthonormal basis/list is linearly independent. For more on inevitable inner product and linear algebra, Appendix C.

## 4.7 Linear Maps, Hermitian and Adjoins

We owe to start this section, with **Operators**. So operators, as we discussed in Chapter 3, are mapping between function to its value (more rigid, eigenvalues). They are preferable to be linear in Quantum Mechanics, even in Mathematics. Then  $(A + B)\hat{O} = A\hat{O} + B\hat{O}$  and  $\hat{O}A = A\hat{O}$ . Then in that case, these things commute. However, not all operators commute, because of their non-linear property.

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<sup>5</sup>A mathematician see this same orthogonality with perspective of projection. The idea of **Orthogonality** is very much indeed original. But whatsoever it may lack the meaning for few subjects outside the Linear Algebra.

In case, if the operator is Differential, then one must be better acquainted with mathematical prospect of the problem, such as Green Functions in inhomogenous case. And as per our previous discussion, these commutators, may or may not commute, that depends on their nature.

**Linear Maps**, yet another Linear, but not last. These maps, in subjects are widely use for their purpose of connecting vector spaces, as operators connects domain and range.

A linear map  $\mathcal{L}$ , has a bracket right to it specifying the map from where to where,  $\mathcal{L}(U, V)$ , is a linear map from vector space U to vector space V. Now there is also a concept called "Linear Function", which shares its identity with linear maps. This linear function  $\mathcal{T}$  in calculus many times coincides with linear maps, because of their origin.

For few moments, we must held a job of discussing the abstruse, but somehow simple Linear Map. A linear map, as we have said is nothing but a transformation from one space configuration to another space configuration, like  $\mathcal{L}(U, V)$ .  $\mathcal{L}(U)$ , what would we call it? It is a linear map from a vector space U to itself. And as Operators, if we call them linear, they must follow the same rule of linearity. Same applies to  $\mathcal{T}$ . One may speak, **don't operators also act like linear functions and linear maps?** Yes, indeed they act like that. A linear operator can be said  $\mathcal{T}$ , and vice versa. For example position operator,

$$\hat{x}v = xv \quad (4.7.1)$$

so x just mapped v to another v with eigenvalue x. we can also tell we a favourite of mine, which is somewhat called "Shift" (if not, then we must call), for this we need a list or set of numbers

$$\mathcal{A} = \{x_1, x_2, \dots, x_n\} : x_i \in \mathcal{F} \quad (4.7.2)$$

we have now, two new operators cum maps, Left Shift and Right Shift, L and R respectively. As per their names, it must be clear that they swap the things to left and right.

$$\begin{aligned} L\mathcal{A} &= L\{x_1, x_2, \dots, x_n\} \\ &= \{x_2, x_3, \dots, x_n\} \end{aligned} \quad (4.7.3)$$

So Left shift, just shifts the set to a left position, that means if we apply the left shift, the first element get deleted and replaced by the next element. Same goes for Right shift, but will feel intriguing

$$\begin{aligned} R\mathcal{A} &= R\{x_1, x_2, \dots, x_n\} \\ &= \{x_0, x_1, x_2, \dots, x_n\} \end{aligned} \quad (4.7.4)$$

we have to add a null space, to preserve the linearity. Zero Vectors and Identity Vectors (or operators) also acts as linear functions and maps.

One thing to mention that besides  $\mathcal{L}(V)$  is a vector space, there will be no inverse element property and vectors will not be commutative.

Now we must go into a little details of linear function, what they contains (more precisely, what they spans), or when they said to be injective or surjective (or invertible). We start with range of  $\mathcal{T}$  i.e. Range ( $\mathcal{T}$  )

$$\text{Range}(\mathcal{T}) = \{\mathcal{T}v; v \in \mathcal{V}\} \quad (4.7.5)$$

in fact, it is a sub-space of  $\mathcal{V}$  as per theorems discuss above.

$$\text{null}(\mathcal{T}) = \{v \in \mathcal{V}; \mathcal{T}v = 0\} \quad (4.7.6)$$

This null space is also a subspace of  $\mathcal{V}$ . Basically, vectors which would get killed by  $\mathcal{T}$  falls into the null space. And one can get the dimension of  $\mathcal{V}$  by

$$\dim \mathcal{V} = \dim \text{null}(\mathcal{T}) + \dim \text{range}(\mathcal{T}) \quad (4.7.7)$$

this is the beautiful connection, where dim is dimension (we will discuss about dimensions in spaces). How to know if  $\mathcal{T}$  is injective or not? It would be injective under these condition

$$\Leftrightarrow \text{if } v \neq w, \text{ then } \mathcal{T}(v - w) \neq 0 \quad (4.7.8)$$

$$\Leftrightarrow \text{if } v \neq w, \text{ then } \mathcal{T}(v) \neq \mathcal{T}(w)$$

$$\Leftrightarrow \text{if } v - w, \text{ then } \mathcal{T}(v - w) \neq 0$$

$$\Leftrightarrow \text{null}(\mathcal{T}) = 0$$

and if  $\mathcal{T}$  is surjective, our range is just the vector space itself. And when dimension of the  $\mathcal{T}$  is way less than infinity, they are injective, surjective and invertible<sup>6</sup>, all.  $\mathcal{T}$  also have inverses, basically two, left and right inverse. Left inverse, let say,  $Q$ ,  $Q\mathcal{T} = we$ , this inverse is injective and right inverse,  $Q'$ ,  $\mathcal{T}Q' = we$ , this one is surjective, we is identity.

Is it necessary that all vector spaces (or sub-spaces) get transformed by  $\mathcal{T}$ ? No, a vector space or a sub-space, let us say  $\mathcal{U}$ , then it will be invariant under  $\mathcal{T}$  if

$$\mathcal{T}(u) = \{T(u); u \in \mathcal{U}\} \subseteq \mathcal{U} \quad (4.7.9)$$

Hermitian Operators are very fruitful in Quantum Mechanics because their eigenvalues are real, not complex, that just means they represent some physical system. Hermitian operators have also a complete set of orthonormal eigenfunctions (or eigenvectors). And in fact, they are observable, such as Hamiltonian. Though, we can have much to say about the Hermitian Operators, which we will do (but not in the section of Linear Algebra) but for now, our concern is Adjoints.

Hermitian Adjoints of an operator is defined as for operator  $A$  by  $A^\dagger$ . That means we have complex conjugated the operator and then transposed it (or by doing the latter first), hence collecting our adjoints.

$$\langle u, Av \rangle \quad (4.7.10)$$

The above equation is the inner product, where  $A$  is an operator acting on  $v$ . It is simple. One advantage we get by using Adjoints is that we can manipulate the above equation by using the adjoint acting on the  $u$  vector, yet yielding the same inner product. That means

$$\langle u, Av \rangle = \langle A^\dagger u, v \rangle \quad (4.7.11)$$

To check that if indeed the dagger ( $\dagger$ ) on  $T$  is a transpose of a conjugate, we may do a quick calculation. We replace our  $u$  and  $v$  vectors by a set of orthonormal

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<sup>6</sup> $\mathcal{T}$  is invertible if it is surjective and injective, which is said to be  $\frac{1}{\mathcal{T}} = Q$ .

basis  $e_i$  and  $e_j$  respectively. And

$$\begin{aligned}\langle A^\dagger u, v \rangle &= \langle u, Av \rangle \\ \langle A^\dagger e_i, e_j \rangle &= \langle e_i, Ae_j \rangle\end{aligned}\quad (4.7.12)$$

by now use of contraction

$$\begin{aligned}\langle (A^\dagger)_{mi} e_m, e_j \rangle &= \langle e_i, (A)_{mj} e_m \rangle \\ (A^\dagger)_{mi}^* \delta_{mj} &= A_{kj} \delta_{im} \\ (A^\dagger)_{ji}^* \delta_{jj} &= A_{ij} \delta_{ii}\end{aligned}\quad (4.7.13)$$

we used the delta function here by setting to equals, then reducing the calculation to

$$\begin{aligned}(A^\dagger)_{ji}^* &= A_{ij} \\ A_{ji}^\dagger &= A_{ij}^*\end{aligned}\quad (4.7.14)$$

there would better and intuitive explanation that this, in fact it is true. And,  $A^\dagger$  is linear and we can check it

$$\langle \alpha u, Av \rangle = \langle A^\dagger(\alpha u), v \rangle \quad (4.7.15)$$

but also

$$\begin{aligned}\langle \alpha u, Av \rangle &= \alpha^* \langle u, Av \rangle \\ &= \alpha^* \langle A^\dagger u, v \rangle \\ &= \langle \alpha A^\dagger u, v \rangle\end{aligned}\quad (4.7.16)$$

that means

$$\langle A^\dagger(\alpha u), v \rangle = \langle \alpha A^\dagger u, v \rangle \quad (4.7.17)$$

and this implies that,  $A^\dagger$  is a linear operator. One thing to notice that  $(A^\dagger)^\dagger = A$ .

Our discussion (though very partial) on Hermitian Operator can be fulfilled by mentioning that a Hermitian operator is nothing but those operators which satisfy the Hermiticity Condition

$$A = A^\dagger \quad (4.7.18)$$

which means operators are self-adjoint. And that is why they play such important role in Quantum Mechanics. For Hermitian Operator following holds true.

$$\langle u, Av \rangle = \langle Au, v \rangle \quad (4.7.19)$$

There is much to be discussed however less the pages we have. However, we can look for much in the textbooks. But there is one last thing we would like to discuss that what  $A_{ij}$  (it is simple and illustrating), and few other important features about this adjoints, remember we called  $\langle u, v \rangle$  is nothing but another way of saying  $\langle u|v \rangle$ .

$$\begin{aligned} \langle u|Av \rangle &= \langle u|A|v \rangle \\ &= \langle v|A|u \rangle^* \end{aligned} \quad (4.7.20)$$

$$\begin{aligned} \langle u|v \rangle &= \langle v|u \rangle^* \\ \langle u|A^\dagger|v \rangle &= \langle v|A|u \rangle^* \end{aligned} \quad (4.7.21)$$

and now a good property which we have already discussed, as we have defined  $u$  and  $v$  using orthonormal basis

$$\begin{aligned} \langle e_i|Ae_j \rangle &= \langle e_i|A_{mj}e_m \rangle \\ &= A_{ij} \end{aligned} \quad (4.7.22)$$

and again we used the delta function.

## 4.8 Eigenvector, Eigenfunction, and Eigenvalue

The Eigen-Algebra, is the most profound example of application of Linear Algebra in Quantum Mechanics. We will try to discuss in minimal words, the Eigenvalues, Eigenfunction, Eigenstates and Eigenvector. And Eigen means "Its own" extracted from German.

We will first jump into the discussion of Eigenvalue Equations. Because maximum data is expected to fit into a matrix when we do Physics. It is true in Mathematics also. This encoding of values in Matrix, partially explored in Chapter 2, is very precious for determining the results. A Eigenvalue Equation

$$A|\psi\rangle = \lambda|\psi\rangle \quad (4.8.1)$$

$\lambda$  is said to be the eigenvalue,  $|\psi\rangle$  is the object upon which we act the operator or whatever, and this  $|\psi\rangle$  is called Eigenfunction. (In case, it is a vector, it is called Eigenvector.)

A is the operator or the mathematical (or physical) object which we act upon the function, on which we want to know the value of that particular operator. That, however is not true in every sense, but for a beginning we must should adopt it. It must not be hard, as we have done this kind of things in our Chapter 3 (Schrödinger Equation).

Eq (4.8.1) shows that  $|\psi\rangle$  is unchanged. Indeed it is true. So the condition is that, A must be a linear operator which leaves eigenfunction unchanged, but however scales it with value of  $\lambda$ . There can not be any good figure than Fig 4.2<sup>7</sup>.

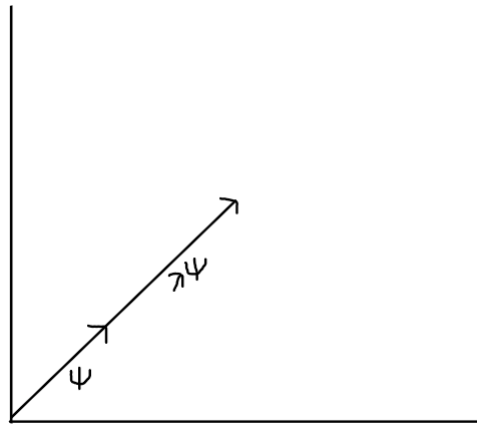


Figure 4.2: Demonstration of Eigenvalue, which in a naive way is scaling the function or vector.

So,  $\lambda$  is the key to our result. Let us see an example, in Chapter 3, we solved Schrödinger Equation, in Eq (3.1.3) we say,

$$H|\psi\rangle = E|\psi\rangle \quad (4.8.2)$$

we now used the ket. If we see our eigenvalue equation, we see that Eq (4.8.2) is a that kind of equation. H is our Hamiltonian Operator with its corresponding eigenvalue Energy (E). So Energy is the value of state which we are seeking. And

<sup>7</sup>First arrow is the mark when  $|\psi\rangle$  is not touched but scales when multiplied by a factor of  $\lambda$ .

we get it after we drag the wave function to be acted by our Hamiltonian. So it is pretty clear, we will be needing particular operators of kinds to get some particular eigenvalue.

So, how do we find the eigenvalue? We solve it by looking for **Matrix Eigenvalue Equation**. As it suggests, it is clear that there is matrix in this game.

We will do an exercise, first a simple and another degenerate exercise (which has multiple roots). We solve for

$$A\phi = \lambda\phi \quad (4.8.3)$$

our equation is a homogeneous linear equation. Without doubt it can be said

$$(A - \lambda\mathbf{1})\phi = 0 \quad (4.8.4)$$

the solution seems to be  $\phi = 0$ , but that is not what we want. But matrices tells us that if  $\det(A - \lambda\mathbf{1}) = 0$ , then there are non-zero solutions for  $\phi$ . So for what values of  $\lambda$  they (determinant) vanish?

$$\begin{vmatrix} a_{11} - \lambda & a_{12} \\ a_{21} & a_{22} - \lambda \end{vmatrix} = 0 \quad (4.8.5)$$

where  $a_{uv}$  are elements of A. So by Eq (4.8.5 or 4.8.6) we can find the eigenvalues and eventually eigenfunctions (or eigenvectors). By expanding this determinant into an algebraic expression (or secular determinant), we get,<sup>8</sup>

$$(a_{11} - \lambda)(a_{22} - \lambda) - a_{12}a_{21} = 0. \quad (4.8.6)$$

For simple A, where A is known, for our case,

$$A = \begin{pmatrix} 1 & 1 \\ 2 & 0 \end{pmatrix} \quad (4.8.7)$$

the secular equation now tells us

$$\det(A - \lambda\mathbf{1}) = \begin{vmatrix} 1 - \lambda & 1 \\ 2 & -\lambda \end{vmatrix} = \lambda^2 - \lambda - 2 = 0 \quad (4.8.8)$$

---

<sup>8</sup>This is just for  $2 \times 2$  matrix. Same applies for  $n \times n$  matrix.



which easily goes and says,  $\lambda_1 = 1$  and  $\lambda_2 = -2$ . Now we have computed the eigenvalues, we can now compute the eigenvectors as well. To our equation 4.8.4, we can get the  $\phi$ . Our  $\phi$  will be in this case a 2 component matrix. And for two eigenvalues we will get two components respectively. For  $\lambda_1$

$$(A - \lambda_1 \mathbf{1})\phi = \begin{pmatrix} 0 & 1 \\ 2 & -1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0 \quad (4.8.9)$$

for this, we know

$$\begin{aligned} -\alpha + \beta &= 0 \\ \alpha - \beta &= 0 \end{aligned} \quad (4.8.10)$$

they are linearly dependent equation and that is  $\alpha = \beta$ , so

$$\phi_1 = N \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad (4.8.11)$$

N is the constant, and the adjacent matrix is nothing but from our  $\alpha = \beta$ . For  $\lambda_2$ , we write,

$$(A - \lambda_2 \mathbf{1})\phi = \begin{pmatrix} 3 & 1 \\ 2 & 2 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0 \quad (4.8.12)$$

and for this we will have.

$$\begin{aligned} 3\alpha + \beta &= 0 \\ 2\alpha + 2\beta &= 0 \end{aligned} \quad (4.8.13)$$

which suggests that  $\beta = -\alpha$ ,

$$\phi_2 = N \begin{pmatrix} -1 \\ 1 \end{pmatrix} \quad (4.8.14)$$

and we have computed our eigenvectors! We can check it.

$$A\phi = \begin{pmatrix} 1 & 1 \\ 2 & 0 \end{pmatrix} N \begin{pmatrix} -1 \\ 1 \end{pmatrix} = -2N \begin{pmatrix} -1 \\ 1 \end{pmatrix} = \lambda\phi \quad (4.8.15)$$

we can check the other one. So this is a way we find the matrix eigenvalues. It is a must in Quantum Mechanics. This was a classic example of  $2 \times 2$  matrix.

For  $n \times n$  matrix, we will have to just do the same thing, subtracting from traces, and evaluating the determinant setting equal to zero.

Now, we have a claim. The eigenvalues of Hermitian operators are real. We can prove it in few lines. For Hermitian operator  $A$ ,

$$\begin{aligned}\langle u, Av \rangle &= \langle A^\dagger u, v \rangle \\ &= \langle Au, v \rangle \\ &= \langle \lambda u, v \rangle \\ &= \lambda^* \langle u, v \rangle\end{aligned}\tag{4.8.16}$$

but we also have

$$\begin{aligned}\langle u, Av \rangle &= \langle u, \lambda v \rangle \\ &= \lambda \langle u, v \rangle\end{aligned}\tag{4.8.17}$$

that means

$$\lambda^* = \lambda\tag{4.8.18}$$

hence, our eigenvalue is real. Yet, another thing we can conclude from above calculation. For two different eigenvalues of same Hermitian operator, eigenvectors are orthogonal. As we have said

$$\begin{aligned}\langle u, Av \rangle &= \langle u, \lambda_1 v \rangle \\ &= \lambda_1 \langle u, v \rangle\end{aligned}\tag{4.8.19}$$

and

$$\begin{aligned}\langle u, Av \rangle &= \langle Au, v \rangle \\ &= \lambda_2 \langle u, v \rangle\end{aligned}\tag{4.8.20}$$

we used label 1 for eigenvalue of  $v$  and 2 for eigenvalue for  $u$ . Now as we see both of the results are of the same inner product

$$\begin{aligned}\lambda_1 \langle u, v \rangle &= \lambda_2 \langle u, v \rangle \\ \lambda_1 \langle u, v \rangle - \lambda_2 \langle u, v \rangle &= 0 \\ \lambda_1 - \lambda_2 \langle u, v \rangle &= 0\end{aligned}\tag{4.8.21}$$

and as per our condition,  $\lambda_1 \neq \lambda_2$ , then the inner product between  $u$  and  $v$  is zero.

$$\langle u, v \rangle = 0.\tag{4.8.22}$$

We can discuss a lot about these Eigen-Algebra, however we must now drop this, here. Though, we will having regular discussion on this topic in future chapters.

## 4.9 Unitary Operator

An Unitary Operator<sup>9</sup> is that linear operator which preserve the inner product. This is somewhat identical to identity, but properly applicable in inner products. Let us get a little back to unitary element. An unitary element is  $U$  if it satisfies this condition

$$U^\dagger U = I \quad (4.9.1)$$

where  $I$  is identity operator, and as well as the commutator  $[U^\dagger, U]$  must vanish.  $U^\dagger$  is adjoint of  $U$ . Now this unitary operator which gives us the linear map to nowhere, but preserves the state, is somewhat in sense trivial. That simply means

$$\langle Uu, Uv \rangle = \langle u, v \rangle \quad (4.9.2)$$

$u$  and  $v$  are as usual our vectors. It is something, which a field theorist would say in discrete terms as "Symmetry". Unitary operator implies a more general idea of 'Unitarity'. Consider the following time evolution operator<sup>10</sup>

$$e^{-iHt/\hbar} \quad (4.9.3)$$

we can say

$$\langle \phi | e^{-iHt/\hbar} \psi \rangle = \langle e^{-iHt/\hbar} \phi | \psi \rangle \quad (4.9.4)$$

where  $\phi$  is basis vectors meant to evolve backwards in time. Since  $H$  is hermitian and  $H = H^\dagger$ , using the conjugation, we can also do

$$\langle \phi | e^{-iHt/\hbar} \psi \rangle = \langle \phi e^{-iHt/\hbar} | \psi \rangle \quad (4.9.5)$$

which implies that the time evolution is unitary and  $H$  is hermitian.  $H$  can only have real values. When Unitarity is combined with Born rule, it is phrased that sum of probabilities is always one. Note that if unitary operator (or matrix) is real,

<sup>9</sup>It is a bounded operator and a surjective one.

<sup>10</sup>We will discuss it widely later.

then it is just orthogonal operator (or matrix). And  $\det U = 1$ . Unitarity also has a very strong place in quantum field theory and discussions of philosophy related to it.

We also have an anti-unitary operator defined as

$$\langle Uu, Uv \rangle = \overline{\langle u, v \rangle} \quad (4.9.6)$$

where the horizontal bar represents complex conjugate. From here, we can see that it is always that

$$|\langle Uu, Uv \rangle| = |\langle u, v \rangle| \quad (4.9.7)$$

and for every  $u$  and  $v$  in our Hilbert space. That above equation comes from **Wigner's** Theorem. It categorizes such invariance into unitary and anti-unitary transformation.

## 4.10 Hilbert Space

Now, we have successfully landed to our precious discussion of a very pure (and impure at the same time) space, **Hilbert Space** ( $\mathcal{H}$ ). If we discussed infinite dimensional spaces, and left the Hilbert Spaces, we did a crime<sup>11</sup>

So, Hilbert Space is a vector space which makes us accessible to define the angles and distances, they arise as infinite dimensional spaces. It can be quite confusing that what infinite dimensional means. But first, let us divert our attention to understand it in quantum mechanics perspective and get ourselves averred to a mathematical perspective.

A Hilbert Space comes with a complete metric, just like any other vector space it has inner product, in fact every finite (almost all the basic) vector spaces are nothing but Hilbert space. Hilbert Space has a feature to treat functions as vectors in inner product, for which it is famous among physicists and mathematicians. To be a Hilbert Space, a vector space must be having normalized vectors. So for  $f(x)$  functions<sup>12</sup>

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<sup>11</sup>The punishment of this crime is however inevitable to all mathematicians (and physicists too), either they perform the crime or not.

<sup>12</sup>Which can be treated as vectors here

$$\int_a^b |f(x)|^2 dx < \infty \quad (4.10.1)$$

hence, integrable functions which have property (4.10.1) being normalized are living in Hilbert Space. From here, we can assert that wave functions live in Hilbert space. Non-normalized wave functions don't live in Hilbert Space.

We have one unfinished business, which is diagonalization. Unfortunately, we do not cover it in book. Diagonalization would be word which we first think when solving a problem. Reader is referred to a standard book on linear algebra.

## 4.11 Conclusions from Linear Algebra

This is where we must conclude the Linear Algebra. We experienced how linear algebra is largely influencing the greater parts of quantum mechanics. Linear algebra mainly deals with vector space. However, that is not entirely true as one shall see in studies beyond quantum mechanics. Furthermore, linear algebra take care of many mathematical grammars of quantum mechanics.

**Summary** - We studied in section 4.2 that how vector spaces are introduced in linear algebra. Then, afterward, we took an example of vector spaces that are frequently seen everywhere. In 4.5, we introduced the Dirac notation ( $\langle | \rangle$ ) in forms of  $\langle a |$  and  $| b \rangle$ . In 4.6, we discussed how inner products are relevant in wave functionality of quantum mechanics. In 4.7, we talk extensively of how linear maps (which has a more mathematical consequence in field theory) are perfect example from topological geometry. We also discuss the adjoints and hermitian operators. Hermitian operators are real eigenvalue bearing operators that, in fact, act like observables. In section 4.8, which is main part, we discuss the eigenphysics.



## Part 2

### **The Quantum Stuff and Application to Models**





# Chapter 5

## Quantum Things

In this chapter, we got to discuss the application of the linear algebras and start out with practical models. However, to make it mostly intuitive would be my aim. But quantum is a bit mathematical, and we have to treat it with care-hands.

### 5.1 Plancherel Theorem

At the beginning of the last chapter, we discussed the Fourier Transformation. (Speaking of which, Fourier Operators which perform the transformations are also unitary.) So as we said, momentum space and position space are nothing but two observables<sup>1</sup> to the same problem in different configurations. Parseval theorem is yet another theorem related to the relation of position and momentum and connected with our discussion of Unitarity.

Dates back to 1799, a formulated series about Fourier transformation by Marc-Antoine Parseval, Parseval Theorem is also known as Rayleigh's Theorem<sup>2</sup>. But Parseval Theorem is often seen not as we are doing, hence we say the following formulated theorem as Plancherel theorem, or Plancherel-Parsvel Identity (and

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<sup>1</sup>Observables in Quantum Mechanics are Hermitian Operators.

<sup>2</sup>After Lord Rayleigh.

Parseval Theorem too). As we had stated

$$\begin{aligned}\psi(x) &= \int_{k\text{-space}} \frac{1}{(\sqrt{2\pi})^3} e^{ik \cdot x} \phi(k) d^3k \\ \phi(k) &= \int_{x\text{-space}} \frac{1}{(\sqrt{2\pi})^3} e^{-ik \cdot x} \psi(x) d^3x\end{aligned}\quad (5.1.1)$$

in one dimension, we just get the power of constant to one and integrate over  $dx$  and  $dk^3$ . And we claimed  $\psi(x)$  and  $\phi(k)$  contains the same information. We can see in Eq (5.1.1) that we can put the values of  $\phi$  and  $\psi$  respectively in the integrals, and for convenience, we would like to put the  $dk$  or  $dx$  in the first place and begin the calculations in only one dimension.

$$\begin{aligned}\psi(x) &= \frac{1}{(\sqrt{2\pi})} \int dk e^{ik \cdot x} \phi(k) \\ &= \frac{1}{2\pi} \int dk e^{ik \cdot x} \int dx' e^{-ik \cdot x'} \psi(x') \\ &= \int dx' \psi(x') \frac{1}{2\pi} \int dk e^{ik \cdot (x-x')}\end{aligned}\quad (5.1.2)$$

This is not any ordinary integral. It is a special integral of kind

$$\int dx' f(x') \delta(x-x') = f(x) \quad (5.1.3)$$

and easily noticable the  $\delta(x-x')$  in the above equation is

$$\delta(x-x') = \frac{1}{2\pi} \int dk e^{ik \cdot (x-x')} \quad (5.1.4)$$

and record this delta function which we are about to do in the following question.

If the momentum space and position space are connected, their probability amplitude must be the same. Let us check.

$$\begin{aligned}\int dx |\psi|^2 &= \int dx \psi^*(x) \psi(x) \\ &= \frac{1}{2\pi} \int dx \int dk \phi^*(k) e^{-ik \cdot x} \int dk' \phi(k') e^{ik' \cdot x} \\ &= \int dk \phi^*(k) \int dk' \phi(k') \frac{1}{2\pi} \int dx e^{i(k'-k)x}\end{aligned}\quad (5.1.5)$$

---

<sup>3</sup>We will be dropping the  $x$ -space and  $k$ -space indication under the integral sign, from here. And if the limits are not given, believe it from  $-\infty$  to  $\infty$ .

You can sparkly recognize the similar delta function, now with  $k$  vectors and we do the integral over  $k$  we get  $\phi(k)$  over the right side.

$$\int dk \phi^*(k) \int dk' \phi(k') \delta(k' - k) = \int dk \phi^*(k) \int dk \phi(k) \quad (5.1.6)$$

which is,

$$\int dk \phi^*(k) \phi(k) \quad (5.1.7)$$

hence

$$\int dx' \psi^*(x) \psi(x) = \int dk' \phi^*(k) \phi(k) \quad (5.1.8)$$

This is the Plancherel Theorem. And hence indicate similarity between two spaces (or two observables, if talking is done in operators) in Quantum Mechanics. And it is easy to construct a 3d Plancherel Theorem, which we must take as an exercise.

We can also write the position operator in momentum space by changing the basis, hence

$$x \rightarrow \frac{\hbar}{i} \frac{d}{dp} \quad (5.1.9)$$

how we will mostly restrict ourselves to the momentum space.

## 5.2 Current Conservation

Current and Current Density is one of the those topics which a physicist must take care of in Electrodynamics. We write current density as a function of  $x$  (point in space)<sup>4</sup>

$$j(x) = \rho \dot{x} \quad (5.2.1)$$

which describes the density of the current at  $x$ , and  $\rho$  is the probability density. Here for of course, our probability density is.

$$\rho(x, t) = \psi^*(x, t) \psi(x, t). \quad (5.2.2)$$

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<sup>4</sup>In the equation, we use the the dot at  $x$  to define the velocity, as differentiation of position with time.

And here we introduce some constant  $A$ , such as

$$A(t) = \int \rho(x,t) dx \quad (5.2.3)$$

and at  $t = 0$ , this is what it should be

$$A(t = 0) = 1. \quad (5.2.4)$$

Now we ought to check whether,

$$\frac{dA}{dt} = 0 \quad (5.2.5)$$

and to check that, we have,

$$\frac{dA}{dt} = \frac{d}{dt} \int \rho(x,t) dx \quad (5.2.6)$$

following Leibniz rule, we change them to partial derivatives and perform the multiple rules of differentiation,

$$\begin{aligned} \frac{dA}{dt} &= \int \frac{\partial}{\partial t} \rho(x,t) dx \\ &= \int \frac{\partial}{\partial t} (\Psi^*(x,t) \Psi(x,t)) dx \\ &= \int \left( \frac{\partial}{\partial t} \Psi^*(x,t) \right) \Psi(x,t) + \Psi^*(x,t) \left( \frac{\partial}{\partial t} \Psi(x,t) \right) dx \end{aligned} \quad (5.2.7)$$

So we now have to find the derivatives, which in fact we did while doing normalization, but yet again.

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \Psi^*(x,t) &= \hat{H} \Psi^*(x,t) \\ \frac{\partial}{\partial t} \Psi^*(x,t) &= \frac{i}{\hbar} \hat{H} \Psi^*(x,t) \end{aligned} \quad (5.2.8)$$

and similarly for  $\Psi(x,t)$

$$\frac{\partial}{\partial t} \Psi(x,t) = \frac{-i}{\hbar} \hat{H} \Psi(x,t) \quad (5.2.9)$$

putting it in Eq. 5.2.7 and we get

$$\frac{\partial}{\partial t} A = \int \frac{i}{\hbar} [(\hat{H}\psi^*)\psi - \psi^*(\hat{H}\psi)] dx \quad (5.2.10)$$

so now,

$$\frac{\partial}{\partial t} \rho = \frac{i}{\hbar} [(\hat{H}\psi^*)\psi - \psi^*(\hat{H}\psi)] \quad (5.2.11)$$

expanding the Hamiltonian,

$$\begin{aligned} \frac{\partial}{\partial t} \rho &= \frac{i}{\hbar} \left[ \frac{-\hbar^2}{2m} \frac{\partial^2 \psi^*}{\partial x^2} \psi + V(x,t)\psi + \psi^* \frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} - V(x,t) \right] \\ &= \frac{-i\hbar}{2m} \left( \frac{\partial^2 \psi^*}{\partial x^2} \psi - \frac{\partial^2 \psi}{\partial x^2} \psi^* \right) \\ &= \frac{-i\hbar}{2m} \frac{\partial}{\partial x} \left( \frac{\partial \psi^*}{\partial x} \psi - \frac{\partial \psi}{\partial x} \psi^* \right) \end{aligned} \quad (5.2.12)$$

arranging a bit by swapping the sign will let us have.

$$\frac{\partial}{\partial t} \rho = \frac{-\partial}{\partial x} \left[ \frac{\hbar}{2im} \left( \psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right) \right] \quad (5.2.13)$$

These things are going to vanish by applying the boundary condition. Now, the above equation has two terms related i.e. conjugate of each other, and for that we have an identity,

$$Z - Z^* = 2i \operatorname{Im}(z) \quad (5.2.14)$$

applying that

$$\frac{\partial}{\partial t} \rho = \frac{-\partial}{\partial x} \left[ \frac{\hbar}{2im} \left( 2i \operatorname{Im} \left( \psi^* \frac{\partial \psi}{\partial x} \right) \right) \right] \quad (5.2.15)$$

and here we have successfully discovered the current density which is

$$J(x,t) = \frac{\hbar}{2m} \operatorname{Im} \left( \psi^* \frac{\partial \psi}{\partial x} \right) \quad (5.2.16)$$

so, here we get our continuity equation and conservation of current.

$$\begin{aligned} \frac{\partial}{\partial t} \rho &= \frac{-\partial}{\partial x} J(x,t) \\ \frac{\partial}{\partial t} \rho + \frac{\partial}{\partial x} J(x,t) &= 0. \end{aligned} \quad (5.2.17)$$

### 5.3 Expectation Values

In section 4.5, we talked about Dirac notation, and here we will be using it for one mathematical construct. In Quantum Mechanics, we give probability a much esteem position, and hence we talk mostly about expectations. Like, what is the momentum in the given state, or perhaps Hamiltonian?

$$H|\psi\rangle \tag{5.3.1}$$

Eq. 5.3.1 is the acting of  $H$  on wave function<sup>5</sup>. But what if we insert  $\langle\psi|$  from left?

$$\langle\psi|H|\psi\rangle \tag{5.3.2}$$

This is called the expectation value of  $H$  in  $\psi$  state. But the general question is how is it that and why do we need it? It is actually simple, for different values of  $H$ , we will get different probabilities of finding them, so we just multiply the possibilities of the system with the eigenfunction set we have. It might seem complicated, but it is simple. It simply means finding the expectation value (in a more naive way, finding the average) of an operator in the given state.

If we check the expanded form of Eq. (5.3.2), then the summation over the overall probabilities becomes the integral and hence,

$$\langle H \rangle = \int_{-\infty}^{\infty} \psi^*(x,t) H \psi(x,t) \tag{5.3.3}$$

or using the hermiticity or adjoint conclusion,

$$\langle H \rangle = \int_{-\infty}^{\infty} H \psi^*(x,t) \psi(x,t). \tag{5.3.4}$$

There can be a quick exercise to demonstrate that the expectation value of momentum in momentum space and position space is the same in a given state.

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<sup>5</sup>We don't need to put a hat on  $H$ . And we will ignore the  $(x,t)$  as well, but we can keep it in mind. However, it will be there where it is needed.

## 5.4 Evolution of Expectation Values

Now, a quick mathematical question would be what is the value of

$$\frac{d}{dt} \langle A \rangle \quad (5.4.1)$$

this may seem to be an unproductive calculation. However, we should do this, at least to gain some insights. The question is how the expectation value of  $A$  is dependent on time.

We begin by,

$$\begin{aligned} \frac{d}{dt} \langle A \rangle &= \frac{d}{dt} \int dx \psi^*(x,t) A \psi(x,t) \\ &= \int dx \left( \frac{\partial}{\partial t} \psi^*(x,t) A \psi(x,t) + \psi^*(x,t) A \frac{\partial}{\partial t} \psi(x,t) \right) \end{aligned} \quad (5.4.2)$$

Once again, we will put the value of those differential equations and get the step further.

$$\begin{aligned} \frac{d}{dt} \langle A \rangle &= \int dx \left( \frac{i}{\hbar} H \psi^*(x,t) A \psi(x,t) - \frac{i}{\hbar} A \psi^*(x,t) H \psi(x,t) \right) \\ i\hbar \frac{d}{dt} \langle A \rangle &= \int dx ( \psi^*(x,t) A H \psi(x,t) - \psi^*(x,t) H A \psi(x,t) ) \end{aligned} \quad (5.4.3)$$

Using Hermiticity,

$$\begin{aligned} i\hbar \frac{d}{dt} \langle A \rangle &= \int dx ( H \psi(x,t) A \psi^*(x,t) - \psi^*(x,t) H A \psi(x,t) ) \\ &= \int dx \psi^*(x,t) [A, H] \psi(x,t) \end{aligned} \quad (5.4.4)$$

this is nothing but,

$$i\hbar \frac{d}{dt} \langle A \rangle = \langle [A, H] \rangle \quad (5.4.5)$$

This insightful calculation tells a operator (observable) evolve, and have a deep connection with a Hamiltonian Operator. Eq. (5.4.5) also known as Ehrenfest Theorem.

## 5.5 Uncertainty in Quantum

One thing that is most important and famous is "Uncertainty", every organic person may have encountered a term if the person got into science, **Uncertainty Principle**. In this section, we would encounter such a thing in a mathematical manner.

Besides uncertainty in life, what could it possibly mean to have uncertainty? You may have read about uncertainty, like measuring the distance between some cosmological object and Earth and finding out that it is  $x \pm 150$  light-years. However, in quantum mechanics, we have a mathematical yet physical uncertainty.

Uncertainty defined in Quantum Mechanics is sort of insufficient experimental data and theoretical guesses. This has a concrete theoretical meaning. Let us say we have a hermitian operator, call it  $A$ . In a  $\psi$  state, the expectation value of  $A$  is

$$\langle A \rangle = \langle \psi | A | \psi \rangle \quad (5.5.1)$$

and we define uncertainty of  $A$  in  $\psi$  (normalized) as

$$\Delta A(\psi) = |(A - \langle A \rangle \mathbb{1})\psi| \quad (5.5.2)$$

Here the  $\Delta A$  is uncertainty and  $\mathbb{1}$  is identity operator. That is how it is defined. If the uncertainty is zero,

$$\Delta A(\psi) = |(A - \langle A \rangle \mathbb{1})\psi| = 0 \quad (5.5.3)$$

that follows

$$\begin{aligned} |(A - \langle A \rangle \mathbb{1})\psi| &= 0 \\ A\psi &= \langle A \rangle \psi \end{aligned} \quad (5.5.4)$$



if we get that, then  $\langle A \rangle$  is the eigenvalue, means the solution. Without uncertainty, one can have a fine solution which the expectation value. If we decide or get some uncertainty is your operators, it become a loss to determinism. We can do some pretty good algebraic calculation for fun and insights, like the following.

$$\begin{aligned} [\Delta A(\psi)]^2 &= |(A - \langle A \rangle \mathbb{1})\psi|^2 \\ &= \langle (A - \langle A \rangle \mathbb{1})\psi | (A - \langle A \rangle \mathbb{1})\psi \rangle \\ &= \langle \psi | (A^2 - A \langle A \rangle - \langle A \rangle A + \langle A \rangle^2 \mathbb{1}) \psi \rangle \end{aligned} \quad (5.5.5)$$

Doing the expectation value, We mean putting the expectation value to the whole problem, gives<sup>6</sup>

$$\langle A^2 \rangle - 2 \langle A \rangle^2 + \langle A \rangle^2 \quad (5.5.6)$$

which gives our the very first result, the following,

$$\boxed{[\Delta A(\psi)]^2 = \langle A^2 \rangle - \langle A \rangle^2}. \quad (5.5.7)$$

## 5.6 Uncertainty Principle

For two hermitian operators, let us say A and B, we define uncertainty for that A and B as

$$(\Delta A(\psi))^2 (\Delta B(\psi))^2 \geq \left( \langle \psi | \frac{1}{2i} [A, B] | \psi \rangle \right)^2 \quad (5.6.1)$$

$$\Delta A(\psi) \Delta B(\psi) \geq \left| \left( \langle \psi | \frac{1}{2i} [A, B] | \psi \rangle \right) \right| \quad (5.6.2)$$

Where ”|...|“ is the absolute value. We will see how we can derive that equation. But first, let us check whether the  $\frac{1}{2i} [A, B]$  is hermitian or not. They are if A

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<sup>6</sup>Do it for some time if we still don't get the result.

and  $B$  are hermitian. To check that, we put the dagger on it<sup>7</sup>

$$\begin{aligned} \left(\frac{1}{i}[A, B]\right)^\dagger &= \left(\frac{1}{-i}(AB - BA)^\dagger\right) \\ &= \left(-\frac{1}{i}((AB)^\dagger) - ((BA)^\dagger)\right) \end{aligned} \quad (5.6.3)$$

What is  $(AB)^\dagger$ ? Let us do a quick calculation.

$$\langle u|AB|v\rangle = \langle (AB)^\dagger u|v\rangle \quad (5.6.4)$$

We define  $B|v\rangle \rightarrow w$

$$\begin{aligned} \langle u|A|w\rangle &= \langle A^\dagger u|w\rangle \\ &= \langle A^\dagger u|Bv\rangle \\ &= \langle B^\dagger A^\dagger u|v\rangle \end{aligned} \quad (5.6.5)$$

$$(AB)^\dagger = B^\dagger A^\dagger \quad (5.6.6)$$

Putting the value back to our question in Eq (5.6.2). We see

$$\left(-\frac{1}{i}((AB)^\dagger) - ((BA)^\dagger)\right) = \left(-\frac{1}{i}(B^\dagger A^\dagger - A^\dagger B^\dagger)\right) \quad (5.6.7)$$

Using hermiticity, we get

$$\left(-\frac{1}{i}(B^\dagger A^\dagger - A^\dagger B^\dagger)\right) = \left(\frac{1}{i}[A, B]\right) \quad (5.6.8)$$

Hence, the commutator is hermitian.

---

<sup>7</sup>We can leave out two as it is a real number and have no practical results.

Let us get back to our discussion of uncertainty. You must have heard about Heisenberg Principle, relating the uncertainty of two operators, namely position and momentum. You can use the Eq (5.6.1) to calculate the uncertainty relation. It is quite easy.

In Eq (5.6.2), we just put the  $[x, p]$  which is  $i\hbar$ ,

$$\Delta\hat{x}(\psi) \hat{p}(\psi) \geq \left| \left( \langle \psi | \frac{1}{2i} i\hbar | \psi \rangle \right) \right| \quad (5.6.9)$$

$$\Delta\hat{x}(\psi) \hat{p}(\psi) \geq \frac{\hbar}{2}$$

We can easily drag out the constants from the inner product. So this was the uncertainty between the two operators. There is a wide philosophical meaning behind it. We will discuss it next.

## 5.7 A Little Diversion

This section will be a bit of philosophy, or we should rather say we were doing quantum as physics and now will do as philosophy. But this privilege has been given to us for only this section.

Uncertainty is one of the famous physics words; as discussed earlier, two operators could have uncertainty if we measure both. There can be uncertainty in just one operator, just like we have in astrophysics. However, this uncertainty is not applied to the macroscopic world. You may, however, encounter the calculations doing astrophysics. Before we proceed, here it is. Quantum mechanics were of two types. One being the Wave Mechanics by de-Broglie and Schrodinger and the other one is the Matrix mechanics by Heisenberg.

Werner Heisenberg is credited for his work on the uncertainty principle. Indeed there is a significant influence of his ideas in this particular principle, as Pauli has in exclusion principle<sup>8</sup>.

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<sup>8</sup>Not to mention his destructing powers, which were terrible for many experiments. Indeed a

Heisenberg, having created matrix mechanics<sup>9</sup>, now was developing a theory. After this, we (they) realized that electrons are not easy to understand just by using simple orbital theories. Then, a lot of studies went into prints to explain the electron quantum mechanically. So, we see an influence by Heisenberg in Uncertainty or Quantum Mechanics on the whole.

## 5.8 Uncertainty Proof

This section will be about the proof of uncertainty equation 5.6.1. The proof is non-typical and mathematical. We define:

$$\begin{aligned} |a\rangle &= (A - \langle A \rangle \mathbb{1}) |\psi\rangle \\ |b\rangle &= (B - \langle B \rangle \mathbb{1}) |\psi\rangle \end{aligned} \quad (5.8.1)$$

From 5.5.5 we have

$$\begin{aligned} \langle A \rangle^2 &= \langle a|a\rangle \\ \langle B \rangle^2 &= \langle b|b\rangle. \end{aligned} \quad (5.8.2)$$

Here we would like to point ourselves to **Schwarz Inequality**. This inequality can be found in many corners of physics and mathematics. It, here, can be written as:

$$\langle a|a\rangle \langle b|b\rangle \geq |\langle a|b\rangle|^2 \quad (5.8.3)$$

It is easy to see that this Schwarz inequality resembles the closest of 5.6.1.

$$(\Delta A)^2 (\Delta B)^2 \geq \text{Re}(\langle a|b\rangle)^2 + \text{Im}(\langle a|b\rangle)^2 \quad (5.8.4)$$

It should not a hard look on the last equation as it resembles the Schwarz Inequality. As we have,

$$\begin{aligned} \langle a|b\rangle &= \langle \psi|(A - \langle A \rangle)(B - \langle B \rangle)|\psi\rangle \\ &= \langle \psi|AB|\psi\rangle - \langle A \rangle \langle B \rangle \end{aligned} \quad (5.8.5)$$

---

Super-TheoristMan.

<sup>9</sup>It was introduced to replace the old quantum theory.

and

$$\begin{aligned}\langle b|a\rangle &= \langle \psi|(B - \langle B \rangle)(A - \langle A \rangle)|\psi\rangle \\ &= \langle \psi|BA|\psi\rangle - \langle B \rangle \langle A \rangle\end{aligned}\quad (5.8.6)$$

If we calculate the imaginary part in our calculation, then

$$\text{Im}g \langle a|b\rangle = \frac{1}{2i}(\langle a|b\rangle - \langle b|a\rangle) \quad (5.8.7)$$

$$\begin{aligned}\langle a|b\rangle - \langle b|a\rangle &= \langle \psi|AB|\psi\rangle - \langle \psi|BA|\psi\rangle \\ &= \langle \psi|AB - BA|\psi\rangle \\ &= \langle \psi|[A, B]|\psi\rangle\end{aligned}\quad (5.8.8)$$

$$\text{Im}g \langle a|b\rangle = \frac{1}{2i} \langle \psi|[A, B]|\psi\rangle \quad (5.8.9)$$

Meanwhile, we can compute the real part of the equation as

$$\begin{aligned}\text{Re} \langle a|b\rangle &= \frac{1}{2}(\langle a|b\rangle + \langle b|a\rangle) \\ &= \frac{1}{2} \times 2 \langle \psi|\{\check{A}, \check{B}\}|\psi\rangle \\ &= \langle \psi|\{\check{A}, \check{B}\}|\psi\rangle\end{aligned}\quad (5.8.10)$$

where

$$\langle \psi|\{\check{A}, \check{B}\}|\psi\rangle = \langle \psi|(A - \langle A \rangle)(B - \langle B \rangle)|\psi\rangle \quad (5.8.11)$$

which is the contracted form of (5.8.5). Our uncertainty equation then becomes, which is (5.8.4)

$$\boxed{(\Delta A)^2(\Delta B)^2 \geq (\langle \psi|\{\check{A}, \check{B}\}|\psi\rangle)^2 + \left(\frac{1}{2i} \langle \psi|[A, B]|\psi\rangle\right)^2} \quad (5.8.12)$$

Eq (5.8.12) is Generalized Uncertainty Principle or Generalized Uncertainty Equation. But (5.6.2) and (5.8.12) are not the same. In the former one, we see that the real part is dropped. Indeed, for a regular uncertainty equation, the real part can be dropped.

The given reason for the drop is usually stated as the (anti-commutator) part is not of use. And dropping it off does not affect the inequality. The Anti-commutator part is often zero (or positive in some states), so we are good to drop it here to achieve the celebrated uncertainty relation. Therefore, we have

$$\boxed{(\Delta A)^2(\Delta B)^2 \geq \left( \frac{1}{2i} \langle \psi | [A, B] | \psi \rangle \right)^2} \quad (5.8.13)$$


---

Eq (5.8.13) can be written as<sup>10</sup>

$$\boxed{(\Delta A)^2(\Delta B)^2 \geq \frac{1}{4} |\langle [A, B] \rangle|^2} \quad (5.8.14)$$


---

## 5.9 Achieving Minimum Uncertainty

In the last section, we derive out equation using the Schwarz Inequality

$$\langle a|a \rangle \langle b|b \rangle \geq |\langle a|b \rangle|^2 \quad (5.9.1)$$

which, however, comes from a more basic definition of

$$a \cdot b = |a||b| \cos \theta \quad (5.9.2)$$

This is for  $\mathbb{R}^3$ , where now,  $\mathbf{a}$  and  $\mathbf{b}$  are vectors. Squaring on the both sides, we see

$$(a \cdot b)^2 = (a \cdot a)(b \cdot b) \cos^2 \theta \leq (a \cdot a)(b \cdot b) \quad (5.9.3)$$

the inequality is because of  $\cos^2 \theta$ . This inequality becomes equality when both vectors are parallel, so  $a = \alpha b$ . Following this we can say that Schwarz Equality

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<sup>10</sup>It would be a good exercise to check it

can be achieved for  $\psi$  for  $\Delta A = \alpha \Delta B$ . This way, we follow what we did in previous section, we reach at Eq 5.8.12, which however, here is ;

$$(\Delta A)^2(\Delta B)^2 = (\langle \psi | \{\check{A}, \check{B}\} | \psi \rangle)^2 + \left( \frac{1}{2i} \langle \psi | [A, B] | \psi \rangle \right)^2 \quad (5.9.4)$$

In the last equation, we dropped the real (anti-commutator) part because of the inequality it was in. Here, we can't do that. Though, we can set it to zero

$$(\langle \psi | \{\check{A}, \check{B}\} | \psi \rangle)^2 = 0 \quad (5.9.5)$$

so, the state in which this part is zero will have minimum possible uncertainty that we are trying to configure. Furthermore,

$$\langle \{\check{A}, \check{B}\} \rangle = 0 \quad (5.9.6)$$

now we will replace out A and B with  $\hat{x}$  and  $\hat{p}$ , and since  $\Delta A = \alpha \Delta B$  which sets out  $\Delta x = \alpha \Delta p$

$$\begin{aligned} \langle \{\check{x}, \check{p}\} \rangle &= \langle \psi | \Delta \check{x} \Delta \check{p} + \Delta \check{p} \Delta \check{x} | \psi \rangle \\ &= \alpha \langle \psi | \Delta \check{x}^2 | \psi \rangle + \langle \psi | \Delta \check{p} \Delta \check{x} | \psi \rangle \end{aligned} \quad (5.9.7)$$

From the commutator relation<sup>11</sup>  $[x, p] = i\hbar$ , we have  $\Delta \check{p} \Delta \check{x} = \Delta \check{x} \Delta \check{p} - i\hbar$ , and we put it to the calculation

$$\begin{aligned} &\alpha \langle \psi | \Delta \check{x}^2 | \psi \rangle + \langle \psi | \Delta \check{x} \Delta \check{p} | \psi \rangle - i\hbar \\ &= \alpha \langle \psi | \Delta \check{x}^2 | \psi \rangle + \alpha \langle \psi | \Delta \check{x}^2 | \psi \rangle - i\hbar \\ &= 2\alpha \langle \psi | \Delta \check{x}^2 | \psi \rangle - i\hbar \end{aligned} \quad (5.9.8)$$

so

$$2\alpha \langle \psi | \Delta \check{x}^2 | \psi \rangle = i\hbar \quad (5.9.9)$$

what can be observed is that  $\alpha$  needs to cancel the  $i$ , hence it must be complex. We now define the  $\alpha = i\beta$  where  $\beta \in \mathbb{R}$ . So

$$\Delta \check{p} = i\beta \Delta \check{x} \quad (5.9.10)$$

---

<sup>11</sup> $[x, p] = [\Delta \check{x}, \Delta \check{p}] = i\hbar$

If this condition is satisfied, we get the minimum uncertainty because the real part is now zero, and the relation is

$$(\Delta x)^2(\Delta p)^2 = \left( \frac{1}{2i} \langle \Psi | [x, p] | \Psi \rangle \right)^2 \quad (5.9.11)$$

Furthermore, Eq (5.9.10) can be written in position space using Fourier transformation and we get

$$\begin{aligned} |(p - \langle p \rangle) \Psi| &= i\beta |(x - \langle x \rangle) \Psi| \\ \left( \frac{\hbar}{i} \frac{\partial}{\partial x} - \langle p \rangle \right) \Psi &= i\beta |(x - \langle x \rangle) \Psi| \end{aligned} \quad (5.9.12)$$

Solving the differential equation, we obtain

$$\Psi = \left( \frac{\beta}{\hbar\pi} \right)^{\frac{1}{4}} e^{\frac{i\langle p \rangle x}{\hbar}} e^{-\frac{a(x - \langle x \rangle)^2}{2\hbar}} \quad (5.9.13)$$

We achieved the state with minimum uncertainty. This wave packet would have non-zero expectation values for position and momentum. Since this has minimum uncertainty, it is an ideal state for stability.

## 5.10 Energy-Time Uncertainty

Is time observable? It is an open question in physics. Though sometimes time can be used as an operator, it is never done in quantum mechanics in the sense of observables. In string theory, we can say that time is an operator by introducing the proper time. However, it is not fit for us to call it an operator. An operator called "time-evolution operator," but that is a different one that we will study later.

For a wave propagating, we say the total number of wave is represented by

$$N = \frac{\omega T}{2\pi} \quad (5.10.1)$$



where  $\omega$  is frequency and  $T$  is time period. Now

$$\begin{aligned}\Delta N \approx 1 &\rightarrow \frac{\Delta\omega T}{2\pi} = 1 \\ \Delta\omega T &= 2\pi\end{aligned}\tag{5.10.2}$$

For a photon, energy is described by

$$\begin{aligned}E &= \hbar\omega \\ \Delta E &= \hbar\Delta\omega\end{aligned}\tag{5.10.3}$$

From Eq. (5.10.2), we can do

$$\Delta E T = 2\pi\hbar.\tag{5.10.4}$$

Now we have completed our small setup and introduced two operators; one is our Hamiltonian and another an arbitrary one which is the function of position and momentum.

$$A = \hat{H}, B = Z(\hat{x}, \hat{p})\tag{5.10.5}$$

where  $Z$  does not have direct time dependence. We compute the uncertainty between these two operators as

$$(\Delta H)^2(\Delta Z)^2 \geq \left( \langle \psi | \frac{1}{2i} [H, Z] | \psi \rangle \right)^2\tag{5.10.6}$$


---

Let's take a moment aside and ask what is  $\frac{d\langle Z \rangle}{dt}$  ?

$$\begin{aligned}\langle Z \rangle &= \langle \psi | Z | \psi \rangle \\ \frac{d}{dt} \langle Z \rangle &= \left\langle \frac{d}{dt} \psi | Z | \psi \right\rangle + \langle \psi | Z \frac{d}{dt} \psi \rangle\end{aligned}\tag{5.10.7}$$

from our past calculations about  $\frac{d}{dt} \psi$ , we can do

$$\begin{aligned}\frac{d}{dt} \langle Z \rangle &= \frac{i}{\hbar} \langle \psi | [H, Z] | \psi \rangle \\ &= \frac{i}{\hbar} \langle [H, Z] \rangle\end{aligned}\tag{5.10.8}$$

We now see that the result from Eq. (5.10.8) is similar to that of Eq. (5.10.6). So, a simple instinct tells us that

$$(\Delta H)^2(\Delta Z)^2 \geq \left( \frac{\hbar}{2i^2} \frac{d}{dt} \langle Z \rangle \right)^2 \quad (5.10.9)$$

$$\geq \left( \frac{\hbar}{2} \right)^2 \left( \frac{d}{dt} \langle Z \rangle \right)^2 \quad (5.10.10)$$

and at the end of the day

$$\Delta H \Delta Z \geq \frac{\hbar}{2} \left| \frac{d}{dt} \langle Z \rangle \right| \quad (5.10.11)$$

We intend to introduce a time configuration where

$$\Delta t \approx \frac{\Delta Z}{\left| \frac{d}{dt} \langle Z \rangle \right|} \quad (5.10.12)$$

$\Delta Z$  is the time needed  $\langle Z \rangle$  to change by  $\Delta Z$ . And, hence we stand near to the uncertainty between Hamiltonian and a time construct as

$$\Delta H \Delta t \geq \frac{\hbar}{2}. \quad (5.10.13)$$

Moreover,  $\Delta T$  is the time which is taken by  $\psi(x, t)$  to show orthogonality with  $\psi(x, 0)$ . Eq. (5.10.13) can be written as

$$\Delta E \Delta t \geq \frac{\hbar}{2} \quad (5.10.14)$$

**Note;** The uncertainty of energy in an isolated environment and system does not change and hence is constant.

Coming back the Eq. (5.10.8), if we substitute at the place of arbitrary operator  $Z$  with our Hamiltonian operator  $H$ , which is time independent for now, then we see

$$\frac{d}{dt} \langle H \rangle = \frac{i}{\hbar} \langle \psi | [H, H] | \psi \rangle = 0 \quad (5.10.15)$$

That result is often stated as **Energy Conservation**. So, there is no change in overall energy as we go in forward time. We can also see,

$$\frac{d}{dt} \langle H^2 \rangle = \frac{i}{\hbar} \langle \psi | [H, H^2] | \psi \rangle = 0 \quad (5.10.16)$$

There can, however, another good calculation for  $\Delta H$

$$\begin{aligned} \frac{d}{dt} (\Delta H)^2 &= \frac{d}{dt} (\langle H^2 \rangle - \langle H \rangle^2) \\ \frac{d}{dt} (\Delta H)^2 &= 0 \end{aligned} \quad (5.10.17)$$

$$\Delta H = 0 \quad (5.10.18)$$

That is a clear argument that energy is always conserved.

We follow a quick quantum exercise to clear out any misunderstanding that will happen after this chapter. We can see that there are operators which adjust the wave-functions. There is a similar operator called translation operator.

The translation is the change in coordinates of space. If a wave function at position  $x$  is translated by  $a$ , the new position of the wave function is  $x + a$ .

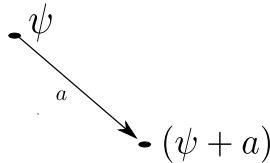


Figure 5.1: Translation of wave-function demonstrated.

The translation operator - there is not only one translation operators, there are many versions of it in quantum mechanics - is

$$e^{\frac{i\hat{p}a}{\hbar}} \quad (5.10.19)$$

and  $\hat{p}$  is our operator

$$\frac{\hbar}{i} \frac{\partial}{\partial x}$$

inserting in the Eq. (5.10.19) and inserting left to a wave function which is a function of position ( $\psi(x)$ )

$$e^{\frac{i\hat{p}a}{\hbar}} \psi(x) = e^a \frac{\partial}{\partial x} \psi(x) \quad (5.10.20)$$

Use Taylor expansion here, which is

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!} (x-a)^n \quad (5.10.21)$$

where n denotes the  $n^{th}$  derivative. Expanding Eq. (5.10.20) using Taylor expansion becomes

$$\begin{aligned} & \sum_{n=0}^{\infty} \frac{1}{n!} \left( a \frac{\partial}{\partial x} \right)^n \psi(x) \\ &= \psi(x) + a \frac{d\psi(x)}{dx} + \frac{1}{2} a^2 \frac{d^2\psi(x)}{dx^2} + \dots \\ &= \psi(x+a) \end{aligned} \quad (5.10.22)$$

You will realize that this expansion is the translated wave function to a new position, which is  $x+a$ . So, the  $e^{\frac{i\hat{p}a}{\hbar}}$  translates any wavefunction by 'a'.

# Chapter 6

## Angular Momentum and Spin

In this chapter, we ought to discuss angular momentum and spin in quantum mechanics. These discussions are essential for modeling the perfect quantum models and digging deeper into field theory. We will aim to talk in quantum language; along the way, we will discuss some classical aspects also. This chapter also relates the hyperfine and fine splittings that we see in our hydrogen and other atoms, which is also a very fine example of atomic physics.

### 6.1 Angular Momentum and Spherical Coordinates

#### Three-Dimensions

So far, we have been doing the two-dimensional cases and have been defining every operator for only two-dimension (one spatial+one time). However, we can define the quantum mechanics in three-dimensional also. Just there, we have to change the dimensions and smoothness related to it. The position operator for three dimensions (where all three are spatial) is

$$\hat{Q}(x, y, z) = Q(x, y, z). \quad (6.1.1)$$

Same we can define the momentum operator<sup>1</sup> as

$$\vec{p} = -i\hbar \vec{\nabla} \quad (6.1.2)$$

where  $\vec{\nabla}$  is gradient which is written as

$$\nabla = \frac{d}{dx} + \frac{d}{dy} + \frac{d}{dz} \quad (6.1.3)$$

and  $x, y, z$  are our dimensions. Since,  $p_x$  is one of the component of  $\vec{p}$ , we can write that with  $Q_x = x$

$$p_x = -i\hbar \frac{d}{dx}, \rightarrow [x, p_x] = i\hbar. \quad (6.1.4)$$

however, different components of position must commute

$$[x, y] = 0 \quad (6.1.5)$$

hence, momentum should also commute

$$[p_x, p_y] = 0 \quad (6.1.6)$$

We can write the time-independent wavefunction in terms of three-dimensional representation as

$$E\psi(\vec{Q}) = \frac{-\hbar^2}{2m} \nabla^2 \psi(\vec{Q}) + V(\vec{Q})\psi(\vec{Q}) \quad (6.1.7)$$

where  $\vec{Q}$  is our position. Three-dimensional quantum mechanics is indeed fascinating and a lot more about geometry and spaces. However, we won't be discussing it more, other than the discussed part of it in succeeding chapters, because it is not relevant to most of our discussions.

### Angular Momentum Algebra

We classically define the angular momentum ( $L$ ) as

$$L = \vec{r} \times \hat{p} \quad (6.1.8)$$

---

<sup>1</sup>We need to drop the hat because it will trouble us to write the vector arrow.

$\hat{p}$  is momentum. In quantum mechanics, it is reasonable to see  $L$  as an operator so,  $\hat{L}$ . Since we are doing 3D, the total angular momentum will be

$$\hat{L} = \hat{L}_x + \hat{L}_y + \hat{L}_z \tag{6.1.9}$$

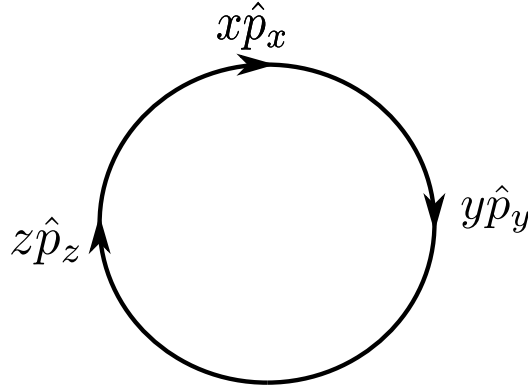


Figure 6.1: Angular momentum in terms of components along the circle.

where we can see the matrix is

$$\hat{L} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ L_x & L_y & L_z \end{vmatrix} \tag{6.1.10}$$

from here one can easily see that

$$\hat{L} = \hat{L}_x + \hat{L}_y + \hat{L}_z = (p_z - zp_y) + (zp_x - xp_z) + (xp_y - yp_x) \tag{6.1.11}$$

and

$$\hat{L}_x = (y\hat{p}_z - z\hat{p}_y) \tag{6.1.12}$$

$$\hat{L}_y = (z\hat{p}_x - x\hat{p}_z) \tag{6.1.13}$$

$$\hat{L}_z = (x\hat{p}_y - y\hat{p}_x) \tag{6.1.14}$$

furthermore,

$$\hat{L}_x = \left( y \frac{\hbar}{i} \frac{d}{dz} - z \frac{\hbar}{i} \frac{d}{dy} \right) \quad (6.1.15)$$

$$\hat{L}_y = \left( z \frac{\hbar}{i} \frac{d}{dx} - x \frac{\hbar}{i} \frac{d}{dz} \right) \quad (6.1.16)$$

$$\hat{L}_z = \left( x \frac{\hbar}{i} \frac{d}{dy} - y \frac{\hbar}{i} \frac{d}{dx} \right) \quad (6.1.17)$$

in momentum space (5.1),

$$\hat{L}_x = \left( \frac{\hbar}{i} \frac{d}{dp_y} \hat{p}_z - \frac{\hbar}{i} \frac{d}{dp_z} \hat{p}_y \right) \quad (6.1.18)$$

$$\hat{L}_y = \left( \frac{\hbar}{i} \frac{d}{dp_z} \hat{p}_x - \frac{\hbar}{i} \frac{d}{dp_x} \hat{p}_z \right) \quad (6.1.19)$$

$$\hat{L}_z = \left( \frac{\hbar}{i} \frac{d}{dp_x} \hat{p}_y - \frac{\hbar}{i} \frac{d}{dp_y} \hat{p}_x \right) \quad (6.1.20)$$

It is obvious to observe that  $\hat{L}_x, \hat{L}_y, \hat{L}_z$  are invariant under adjoint operation, hence they are hermitian. Since they are hermitian, they are also observables.

$$\hat{L}_z^\dagger = (x\hat{p}_y - y\hat{p}_x)^\dagger = \hat{p}_y^\dagger x^\dagger - \hat{p}_x^\dagger y^\dagger = x\hat{p}_y - y\hat{p}_x \quad (6.1.21)$$

It will be an interesting thing to commute the two  $L_i$ , where  $i = x, y, z$ . In that case, the commutator is

$$\begin{aligned} [\hat{L}_x, \hat{L}_z] &= [y\hat{p}_z - z\hat{p}_y, x\hat{p}_y - y\hat{p}_x] \\ &= -[y\hat{p}_z, x\hat{p}_y] + [z\hat{p}_y, y\hat{p}_x] \end{aligned} \quad (6.1.22)$$

It was done by commutator identity. Now, we can do

$$= -(\hat{p}_z[y, \hat{p}_y]x) + (z[\hat{p}_y, y]\hat{p}_x) \quad (6.1.23)$$

$$= i\hbar z\hat{p}_x - i\hbar\hat{p}_z x \quad (6.1.24)$$

$$= i\hbar(z\hat{p}_x - \hat{p}_z x) \quad (6.1.25)$$

$$= i\hbar\hat{L}_y \quad (6.1.26)$$

$$\boxed{[\hat{L}_x, \hat{L}_z] = i\hbar\hat{L}_y} \quad (6.1.27)$$



Likewise, we can do the other commutator algebras

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z \quad (6.1.28)$$

$$[\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x \quad (6.1.29)$$

$$[\hat{L}_x, \hat{L}_z] = -i\hbar\hat{L}_y \quad (6.1.30)$$

It can be easily calculated that the angular components i.e  $L_i$  do not commute in a position space, we answer it straightforward

$$[L_x, L_y]x = -\hbar^2 y \neq 0 \quad (6.1.31)$$

and it would be interesting to calculate the inner product between  $L_i$ , that we leave to the reader, i.e.,

$$\langle L_i | L_j \rangle; i \neq j. \quad (6.1.32)$$

When it comes to choose the basis among  $L_i$  - since any  $L_i$  can be written in form of other we can identify a basis and write angular momentum in that basis - we have to first identify the matrix relation between them. A simple analysis by checking the commutator relations gives us<sup>2</sup>

$$L_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \hbar \quad (6.1.33)$$

$$L_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \hbar \quad (6.1.34)$$

$$L_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \hbar \quad (6.1.35)$$

they all satisfy (6.1.28 - 6.1.30). These  $3 \times 3$  matrices are hermitian and can be checked. Among the matrices, the one which can be chosen as the basis is that the diagonal matrices, as they are good for eigenvalue picking. Fashionably, (6.1.35) is diagonal and can be chosen as the basis. Once, we pick  $L_Z$  as basis in the

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<sup>2</sup>This is the same analysis that we did in finding the Mach-Zehnder Interferometer's beam splitters matrices, which at the point can also be seen as operators.

representation theory of angular momentum, we can calculate the other  $L_i$  in the basis of  $L_z$  using (6.1.12 - 6.1.14) as they are non-commuting objects. However, one can surely pick the  $L_x$  or  $L_y$  as the basis, but the relations (6.1.28 - 6.1.30) would be different in that basis and mathematics would be the same.

We solve the  $[L_x, L_y] = i\hbar L_z$  using the matrix operator

$$\begin{aligned}
[L_x, L_y] &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \hbar \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \hbar - \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \\
&\quad \times \hbar \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \hbar \\
&= \frac{\hbar^2}{2} \begin{pmatrix} i & 0 & -i \\ 0 & -i+i & 0 \\ i & 0 & -i \end{pmatrix} - \frac{\hbar^2}{2} \begin{pmatrix} -i & 0 & -i \\ 0 & i-i & 0 \\ i & 0 & i \end{pmatrix} \\
&= \frac{\hbar^2}{2} \begin{pmatrix} i+i & 0 & -i+i \\ 0 & 0 & 0 \\ i-i & 0 & -i-i \end{pmatrix} \\
&= \frac{\hbar^2}{2} \begin{pmatrix} 2i & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2i \end{pmatrix} = i\hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \hbar
\end{aligned}$$

$$\boxed{[L_x, L_y] = i\hbar L_z} \quad (6.1.36)$$

more generally it is written as

$$[L_i, L_j] = i\hbar \epsilon_{ijk} L_k \quad (6.1.37)$$

where  $i, j, k$  are different space component. Furthermore, in the matrix notation

the total angular momentum  $L$  can be written as

$$L = \begin{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \hbar \\ \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \hbar \\ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \hbar \end{pmatrix} \quad (6.1.38)$$

It can be asked now that what is  $L^2$ ?

Fairly simple to calculate using Dirac notations. If we keep  $|L\rangle$  as  $L$  and product it with  $\langle L|$ , then

$$\langle L|L\rangle = L^2 \quad (6.1.39)$$

we do the calculation, and readers are advised to do this, we get

$$L^2 = 2\hbar^2 \quad (6.1.40)$$

and in matrix notation

$$L^2 = 2\hbar^2 \mathbb{1} \quad (6.1.41)$$

where  $\mathbb{1}$  is the identity matrix ( $3 \times 3$ )

$$\mathbb{1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (6.1.42)$$

Furthermore, we can write the eigenvalues of momentum operators as following

$$L_x |\phi\rangle = \lambda_x |\phi\rangle \quad (6.1.43)$$

$$L_y |\phi\rangle = \lambda_y |\phi\rangle \quad (6.1.44)$$

$$L_z |\phi\rangle = \lambda_z |\phi\rangle \quad (6.1.45)$$

and we can not have simultaneous eigenstates for two (or by means all three) of them. We can check that using commutation;

$$[L_x, L_z] |\phi\rangle = -i\hbar L_y |\phi\rangle = -i\hbar \lambda_y |\phi\rangle \quad (6.1.46)$$

$$(6.1.47)$$

opening the commutator

$$(L_x L_z - L_z L_x) |\phi\rangle = (\lambda_x \lambda_z - \lambda_z \lambda_x) |\phi\rangle \quad (6.1.48)$$

$$\lambda_x \lambda_z = \lambda_z \lambda_x \quad (6.1.49)$$

$$(6.1.50)$$

$$[L_x, L_z] |\phi\rangle = 0 \quad (6.1.51)$$

$$-i\hbar \lambda_y |\phi\rangle = 0 \quad (6.1.52)$$

and that gives us

$$\lambda_z = 0 \quad (6.1.53)$$

$$|\phi\rangle = 0 \quad (6.1.54)$$

moreover,

$$\lambda_x = 0, \lambda_y = 0 \quad (6.1.55)$$

$$\boxed{\lambda_x = \lambda_y = \lambda_z = 0, |\phi\rangle = 0} \quad (6.1.56)$$

that is how all three of them cannot have simultaneous eigenstates.

Because we are randomly picking subjects and discussion them in this chapter, we want to know now what is the commutator

$$[L_x, L^2] ? \quad (6.1.57)$$

In (6.1.41), we say  $L^2 = 2\hbar$ . In spite of that, we can write  $L^2$  also as the following form

$$L^2 = L_x L_y + L_y L_x + L_z L_z \quad (6.1.58)$$

a straightforward answer (yet surprising) to (6.1.57) can be now written as

$$\begin{aligned}
 [L_x, L^2] &= [L_x, L_x L_y + L_y L_y + L_z L_z] \\
 &= [L_x, L_y] L_y + L_y [L_x, L_y] + [L_x, L_z] L_z + L_z [L_x, L_z] \\
 &= i\hbar L_z L_y + i\hbar L_y L_z - i\hbar L_y L_z - i\hbar L_z L_y \\
 &= 0
 \end{aligned} \tag{6.1.59}$$

similarly

$$[L_y, L^2] = 0 \tag{6.1.60}$$

$$[L_z, L^2] = 0 \tag{6.1.61}$$

so,  $L_i$  commutes with  $L^2$  in a less but fancy way, which is expected. An important thing to note is that we can find simultaneous eigenstates for commuting operators:  $[L_i, L^2]$  can have non-vanishing simultaneous eigenstates.

### Central Potential and Polar QM

Our freshly three-dimensional quantum mechanics has a very speculating problem called 'Central Potential Problem.' In 3D, we have potential in terms of distance from the origin, which hints at what central potential can mean. It looks something like this,  $V(\vec{Q}) = V(\vec{r})$ . One classic example can be found in electromagnetism known as 'Coulomb Potential';

$$V(\vec{r}) = -\frac{Ze^2}{4\pi\epsilon_0 r}. \tag{6.1.62}$$

For a stationary state - of which we will discuss in later chapter, however they are time-independent states, means they have observables which don't depend on time - we can write the Schrodinger Equation as

$$\left( \frac{-\hbar^2}{2m_\psi} \nabla^2 + V(\vec{r}) \right) \psi(\vec{r}) = H\psi(\vec{r}) \tag{6.1.63}$$

where  $m_\psi$  is the mass. We can write the  $\nabla^2$  as spherical coordinates  $(r, \theta, \phi)$  as

$$\nabla^2 = \underbrace{\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right)}_{\text{radial component}} + \underbrace{\frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}}_{\text{angular component}} \tag{6.1.64}$$

the notations can be summarized as

$$\begin{aligned}x &= r \sin\theta \cos\phi \\y &= r \sin\theta \sin\phi \\z &= r \cos\theta \\r &= \sqrt{x^2 + y^2 + z^2} \\ \theta &= \cos^{-1} \left( \frac{z}{r} \right) \\ \phi &= \tan^{-1} \left( \frac{y}{x} \right)\end{aligned}$$

Furthermore, using chain rules

$$\frac{\partial}{\partial \phi} = \frac{\partial y}{\partial \phi} \frac{\partial}{\partial y} + \frac{\partial z}{\partial \phi} \frac{\partial}{\partial z} + \frac{\partial x}{\partial \phi} \frac{\partial}{\partial x} \quad (6.1.65)$$

$$\frac{\partial}{\partial \phi} = x \frac{\partial}{\partial y} + 0 - y \frac{\partial}{\partial x} \quad (6.1.66)$$

$$\frac{\partial}{\partial \phi} = x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \quad (6.1.67)$$

using 6.1.17, we can immediately write

$$L_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi} \quad (6.1.68)$$

that is how we can write angular momentum in terms of polar coordinates.

### General Discussion on Angular Momentum

We write the angular momentum magnitude squared as<sup>3</sup>

$$L^2 = -\hbar^2 \left( \frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \sin\theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2} \right) \quad (6.1.69)$$

---

<sup>3</sup>Can be checked using various methods, one include writing explicitly the  $L^2$  in polar coordinates.

with eigenvalue written as

$$\hbar^2 \lambda, \lambda > 0 \tag{6.1.70}$$

As we said, the  $L_i$  and  $L^2$  commute, most of the time we would be wanting to calculate  $L^2$ . An eigenvalue equation would be

$$L^2 \psi_{l,m} = \hbar^2 \lambda \psi_{l,m} \tag{6.1.71}$$

$$L_z \psi_{l,m} = \hbar l(l+1) \psi_{l,m} \tag{6.1.72}$$

and for  $L_z$  it is

$$L_z \psi_{l,m} = \hbar m \psi_{l,m} \tag{6.1.73}$$

it can be also written as it is clear that solutions to angular momentum is in multiples of  $\hbar$ , which is fascinating for now. Where  $m$  follows  $-l \leq m \leq l$ , and  $m \in \mathbb{C}$ . Now, we would like to know what is  $\psi_{l,m}$ , we can deduce it from (6.1.73) and solve the differential equation by the following way

$$\frac{\hbar}{i} \frac{\partial}{\partial \phi} \psi_{l,m} = \hbar m \psi_{l,m} \tag{6.1.74}$$

$$\frac{\partial}{\partial \phi} \psi_{l,m} = im \psi_{l,m} \tag{6.1.75}$$

solving this PDE (partial differential equation) gives us

$$\psi(\phi) = e^{im\phi} C \tag{6.1.76}$$

where  $C$  is a tensor function of  $\theta$  (later would be called Legendre polynomials)

We impose one boundary condition

$$\psi_{l,m}(\theta, \phi) = \psi_{l,m}(\theta, \phi + 2\pi). \tag{6.1.77}$$

Eq (6.1.76) is exponential, and somewhat similar to our matter wave solution. It is a very convenient wave function for writing solutions to PDE and ODE of Schrödinger equations.

We can also extract  $\psi_{l,m}$  by using (6.1.72). We will calculate it using the (6.1.69).

$$\begin{aligned} L^2 \psi_{l,m} &= -\hbar^2 \left( \frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \sin\theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2} \right) \psi_{l,m} \\ &= \hbar^2 l(l+1) \psi_{l,m} \end{aligned} \tag{6.1.78}$$

solving (6.1.78) is easy if we multiply both sides with  $-\sin^2\theta$ . Canceling the  $\hbar^2$  and taking the derivative that has been solved in this section gives us the equation

$$\sin\theta \frac{\partial}{\partial\theta} \left( \sin\theta \frac{dC}{d\theta} \right) + (l + (l + 1)\sin^2\theta - m^2) C = 0 \quad (6.1.79)$$

$$\frac{\partial^2(i^2m^2)}{\partial\phi^2} = -m^2 \quad (6.1.80)$$

Using (6.1.79) and solving it we can get

$$C_l = \sum_k a_k x^k \quad (6.1.81)$$

if we can't tell already,  $C_l$  are Legendre polynomials. What are the coefficients  $a_k$ ? These have an identity

$$\frac{a_{k+2}}{a_k} = -\frac{[l(l+1) - k(k+1)]}{(k+1)(k+2)} \quad (6.1.82)$$

however, it must vanish for  $l = k$ . From the overall calculation, one can deduce the famous result

$$-l \leq m \leq l \quad (6.1.83)$$

and  $m$  can't exceed the number of solutions than  $2l + 1$ .

More generally Legendre polynomials have the differential form

$$\frac{d}{dx} \left[ (1-x^2) \frac{dP_n(x)}{dx} \right] + n(n+1)P_n(x) = 0 \quad (6.1.84)$$

and eigenvalue equation

$$\frac{d}{dx} \left( (1-x^2) \frac{d}{dx} \right) P(x) = -\lambda P(x) \quad (6.1.85)$$

where  $P(x)$  are Legendre polynomials.



## 6.2 Spins and Stern-Gerlach Experiment

Now we turn to an important discussion, however short, of spins and magnetic momenta. Algebra for spins are similar to angular momentum algebra which was introduced in Sec. 6.1.

Magnetic momentum ( $\mu$ ) is written as

$$\mu = rA \quad (6.2.1)$$

where  $r$  is direction and  $A$  is area of the charge, for charged rotating particle, see Figure 6.2.

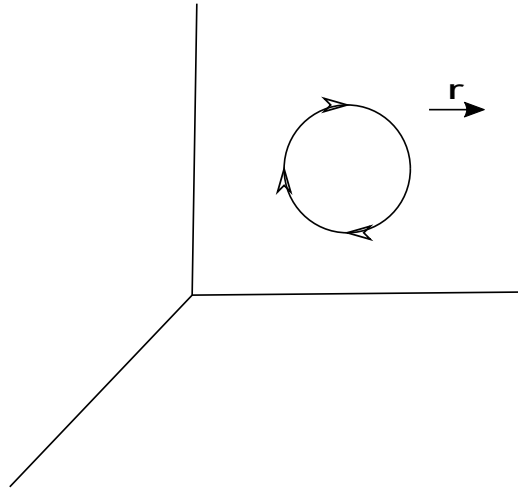


Figure 6.2: Rotating charge in direction  $r$ .

There is also a formulae

$$\mu = \frac{1}{2} \theta v R \quad (6.2.2)$$

and we have

$$L = P \cdot R = mvR \quad (6.2.3)$$

$$\mu = \frac{1}{2m} \theta mvR \quad (6.2.4)$$

$$= \frac{\theta}{2m} L \quad (6.2.5)$$

$$\mu = \frac{\theta L}{2m}, \quad \text{Relationship between angular momentum and magnetic moment,} \quad (6.2.6)$$

in all these,  $R$  is radius. But these are classical equations. If we quantize a regular field we get  $\hbar$  and various other factors. Generally speaking, for electron in quantized way

$$\mu = g \frac{e\hbar S}{2m_e\hbar}, \quad (6.2.7)$$

where  $g$  is **Lande factor**,  $m_e$  is mass of electron and  $S$  is spin. Before we discuss more, we ought to discuss the spins.

Spins are intrinsic properties of rotating particles. It has its immense importance in quantum theories. When we talk about rotating particles, we don't mean only its angular component and linear components. In classical theories, it may be sufficient. But in quantum theories, we have to include spins in talks of rotating (and sometimes non-rotating) particles. Spins never means *rotating*. The definition of spins are a little referred to a quantum property without a pure meaning.

Algebra for spins are similar to angular momentum algebra, discussed in Sec. 6.1. In 3D, spins have component  $(S_x, S_y, S_z)$ . We see that  $S_i$  are similar to  $L_i$ , of course they have differences in algebraic structures and operations. Like for  $L_i, L_j$  and  $L_k$  we have following

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k, \quad (6.2.8)$$

where  $\epsilon$  is showing permutation. Algebras related to this are 6.1.28-6.1.30. Similarly, one can write the spins algebra as

$$[S_i, S_j] = i\hbar\epsilon_{ijk}S_k, \quad (6.2.9)$$

$$[S_x, S_y] = i\hbar S_z \quad (6.2.10)$$

$$[S_y, S_z] = i\hbar S_x \quad (6.2.11)$$

$$[S_x, S_z] = -i\hbar S_y \quad (6.2.12)$$

Important thing to note that while  $L_i$  acts on functions, for that matter wave functions,  $S_i$  acts on vectors. There will be *no* simultaneous eigenstates in this

case either for  $S_i$  and  $S_j$  ( $i \neq j$ ). But there exist simultaneous eigenstates for  $S^2$  and  $S_i$ . We can explicitly write these spin operators as

$$\hat{S}_i = \frac{\hbar}{2} \sigma_i, \quad (6.2.13)$$

where  $\sigma_i$  are Pauli matrices. These are  $2 \times 2$  (square) matrices for values of “i”. And these are

$$\begin{aligned} \sigma_1 = \sigma_x &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \sigma_2 = \sigma_y &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ \sigma_3 = \sigma_z &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \end{aligned} \quad (6.2.14)$$

and<sup>4</sup>

$$\text{Tr} \sigma_i = 0 \quad (6.2.15)$$

So,

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (6.2.16)$$

$$S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (6.2.17)$$

$$S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (6.2.18)$$

and all  $S_i$  are hermitian. So, they are observables. We can also derive the commutation relations for spin operators using the matrices that we discussed now. It should be now a time to check for eigenvalues for  $S_i$ . Before we check that, we want to construct some states as  $S_i$  has two possible eigenvalues (with basically  $\pm$ ). Let us take  $\phi$  as our wave function, with two possible spins  $\pm s$ , we will say what this  $s$  is.

$$|\phi; \pm\rangle \quad (6.2.19)$$

and

$$S_i |\phi; \pm\rangle = s_i |\phi; \pm\rangle \quad (6.2.20)$$

---

<sup>4</sup>Tr is trace, means the sum of diagonal components.

where  $s_i$  is eigenvalue. If we apply the matrix operator of  $S_z$  with some random  $|\phi; \pm\rangle$ , we will find that

$$S_z |\phi; \pm\rangle = \pm \frac{\hbar}{2} |\phi; \pm\rangle, \quad (6.2.21)$$

here to note that angular momentum had explicitly  $\hbar$  in the eigenvalue (that is what makes it “quantum”) and here in spins, we have  $\hbar/2$ . And in some sense  $\pm$  is indicating the helicity of the spin. (In general, we can say a spin is up or down.) We can still discuss a lot about spins themselves, but we ought to study *Stern-Gerlach Experiment*, which is a theory around this topic. So spins can have two values  $\hbar/2$  and  $-\hbar/2$  and for brevity, let us write that  $\phi_+$  represents a state with spin “+” and  $\phi_-$  represents a state with spin “-”.

A Stern-Gerlach machine will take  $\phi$  and produce either  $\phi_+$ , or  $\phi_-$ . In this way, we have a efficient way to measure the spin of a system (or for that matter, wave function). Consider the following figure;

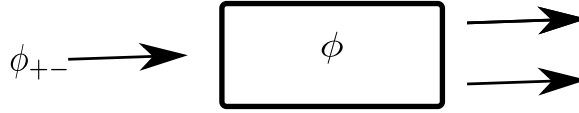


Figure 6.3: A Stern-Gerlach machine, where we put  $\phi_{+-}$  and get either spin up or spin down. One of these will be blocked in the machine and only one will ray out.

and we mention a very important property

$$\langle \phi_+ | \phi_- \rangle = 0, \quad (6.2.22)$$

and that means, they are orthogonal. And

$$\langle \phi_+ | \phi_+ \rangle = 1. \quad (6.2.23)$$

When applying the operators, we have

$$S_z \phi_+ = \frac{\hbar}{2} \phi_+ \quad (6.2.24)$$

$$S_z \phi_- = -\frac{\hbar}{2} \phi_- \quad (6.2.25)$$

It should be noted that eigenvalues of spin angular momentum are all either integral or half-integral. While angular momentum eigenvalues are only integral. So, for the case of spin angular momentum the possibilities are more general than orbital angular momentum.

We make now some general remarks about spins. Angular momentum (orbital) is well defined because its connection with the rotation operator (which causes the rotation around an origin). But spins lack physical meaning in many sense. We will try to some extent to define it. Consider a spin 0 particle, now it is a special case. Because in this case all the  $m$  are vanishes. For simplicity,  $J = L + S$  and if spins is zero then  $J = L$ . This result is telling us that rotating a particle does not change the particle's orientation, we call those particles (with spin zero) as "spherically symmetric". Indeed a sphere from any orientation is same looking. This is not the case with  $s = 1/2, 1$ . Only observed fermions in nature is of spins  $1/2$ , so orientation for them causes different looks.

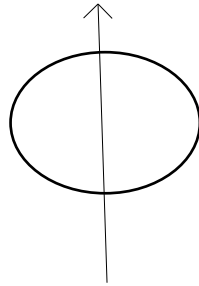


Figure 6.4: Consider this ball, the spin is showing its helicity (we can ignore it), if the arrow of the ball is 0, we can rotate this ball around the axis and the ball will be same. However, if the case is that of spin  $1/2$ , then ball will be upside down.

However, we gather that a macroscopic object with no angular momentum is non-symmetric, but if it cool down so the quanta become non-associated with the state, the state will have to become "spherically symmetric" It may contradict the result we discussed above but it is a classical result.

For  $s = 1/2$  we have already introduced the spinor formalism where

$$S^2 |\zeta\rangle = \frac{1}{4} \hbar^2 |\zeta\rangle \quad (6.2.26)$$

$$S|\zeta\rangle = \frac{\hbar}{2}\sigma_i \quad (6.2.27)$$

where  $|\zeta\rangle$  is some arbitrary state. Spinor formalism has been discussed in above discussions. As we said, this  $s = 1/2$  will change the sign on one rotation and it can be observed easily with a phase space state.

### 6.3 Quantum Effects in Orbitals

Generally, atoms experience four kinds of quantum effects in their orbitals. They are

1. Bohr Energy  $\rightarrow \alpha^2 m_e c^2$
2. Hyperfine Splitting  $\rightarrow \alpha^4 m_e c^2 \left(\frac{m_e}{m_p}\right)$
3. Spin-Orbit Coupling  $\rightarrow \alpha^4 m_e c^2$
4. Lamb Shift  $\rightarrow \alpha^5 m_e c^2$

where  $m_e, m_p$  are mass of electron and proton respectively. We would not discuss them here as it might divert us from the objective of this book.

# Chapter 7

## Pictures and Harmonic Oscillator

This is a two-fold chapter. First we discuss the Schrödinger picture and Heisenberg picture. Then we turn to what is quantum mechanics generally for, study of oscillators and study of models. In what follows, model means a configuration for wave-functions. There are many models to study about which includes very interesting scenario called “Harmonic Oscillator”. It is interesting because it is not only confined to quantum mechanics, but has its root in quantum field theory, classical field theory, statistical physics, string theory and many more.

### 7.1 Heisenberg Picture

Discussed in section 4.9, a unitary operator is

$$U^\dagger U = 1, \tag{7.1.1}$$

and we showed that time-evolution operator is a unitary operator. In doing so, we need to make our operators to be time-dependent in what follows. A Schrödinger picture is a simple mechanism of quantum mechanics which incorporate the time-dependency of states, but not necessarily of operators. Operators become constant there.

Heisenberg introduced another formulation for quantum mechanics. In which, we take operators to be time-dependent while states are constant (fixed).

Pictures	States	Operators
Schrödinger Scheme	Moving	Fixed
Heisenberg Scheme	Fixed	Moving

Table 7.1: A table of both schemes and their representations for ket states and observables.

When we speak of operators, we are speaking of *dynamical observables*. And we speak of states, we mean ket states like  $|\psi\rangle$ . In table 7.1, we mention the distinction between the both pictures. Writing the Heisenberg formulation is mainly done in matrix elements, that we have discussed in past chapters. Heisenberg idea and Schrödinger idea is connected in some sense that we will see in some time.

Introduced in 4.9, time evolution operator, which is unitary, given by

$$\mu(t) = e^{-iH_S t/\hbar}, \quad (7.1.2)$$

where  $t$  represents time. Take any dynamical operator  $\hat{A}$  which can be Schrödinger operator if  $\hat{A}_S$  and Heisenberg operator if  $\hat{A}_H$ . As per definition,  $\hat{A}_S$  operators are timely-fixed and  $\hat{A}_H$  operators are otherwise moving. We can relate both using the unitary operator

$$\hat{A}_H(t) = \mu^\dagger(t, 0) \hat{A}_S \mu(t, 0), \quad (7.1.3)$$

such that  $\hat{A}_H(t=0) = \hat{A}_S$ , where in (7.1.3) we can define  $\mu(t, 0)$  in such a way that

$$\psi(t = \tau) = \mu(t = \tau, 0) \psi(0), \quad (7.1.4)$$

which take the wave function from  $t = 0$  to  $t = t$  which we have already seen in Schrödinger picture. However, in Heisenberg picture states are fixed. It is clear that, for instance  $\hat{H}$

$$\hat{H}_H(t) = \mu^\dagger(t, 0) \hat{H}_S \mu(t, 0). \quad (7.1.5)$$

Before we move on, it should be cleared that

$$[A_H, B_H] = C_H \quad (7.1.6)$$

$$[A_S, B_S] = C_S, \quad (7.1.7)$$



hence commutators in either representation are same.

Both the schemes are mathematically equivalent. However, they were developed for the case where we have control over states and dynamic operators. It is clear that Schrödinger picture is well developed in differential mathematics. It is same with Heisenberg picture, we have differential equation for Heisenberg operators<sup>1</sup>

$$i\hbar \frac{d}{dt} \hat{A}_H = i\hbar \left( \frac{\partial}{\partial t} \mu^\dagger \hat{A}_S \mu + \mu^\dagger \hat{A}_S \frac{\partial}{\partial t} \mu + \mu^\dagger \frac{\partial}{\partial t} \hat{A}_S \mu \right), \quad (7.1.8)$$

where from (7.1.2)

$$\frac{\partial}{\partial t} \mu = H_S \mu, \quad (7.1.9)$$

and

$$\frac{\partial}{\partial t} \mu^\dagger = -H_S \mu^\dagger, \quad (7.1.10)$$

after this, (7.1.8) becomes

$$i\hbar \frac{d}{dt} \hat{A}_H = -H_S \mu^\dagger \hat{A}_S \mu + \mu^\dagger \hat{A}_S H_S \mu + \mu^\dagger i\hbar \frac{\partial}{\partial t} \hat{A}_S \mu. \quad (7.1.11)$$

and reduces to

$$\boxed{i\hbar \frac{d}{dt} \hat{A}_H = [\hat{A}_H, H_H] + i\hbar \frac{\partial \hat{A}_H}{\partial t}}. \quad (7.1.12)$$

One interesting development one see from Heisenberg scheme is its connection with classical mechanics. It is one of the ways from which one first get to know about ‘‘Poisson Brackets’’. Which are defined as

$$\{a, b\}_{P.B} = \sum_r \left( \frac{\partial a}{\partial q_r} \frac{\partial b}{\partial p_r} - \frac{\partial a}{\partial p_r} \frac{\partial b}{\partial q_r} \right), \quad (7.1.13)$$

where  $p_r$  and  $q_r$  are two canonical variables. (When one goes from classical theory, one also go from Poisson brackets to commutator relations. The former is of great importance in classical mechanics and the latter in quantum mechanics.)

We can related the Poisson bracket and commutator

$$\boxed{i\hbar \{a, b\}_{P.B} = [a, b]}. \quad (7.1.14)$$

From which, one immediately realizes

$$\{x, p\}_{P.B} = \mathbb{1}. \quad (7.1.15)$$

<sup>1</sup>For brevity, we ignore the brackets of variables.

## 7.2 Energy Levels

Now we change our topic to discuss the energy levels of a system. Consider a System S, for which we have Hamiltonian  $H_n$  with eigenvalue  $E_n$  where, let say,  $n \geq 0$ . If  $n = 0$ , we say  $E_0$  is ground state energy. The reason it is ground state that it gives lowest possible energy for the system. Reader can sense that we are talking about states of the system. When  $n > 0$ , we will call it excited states.

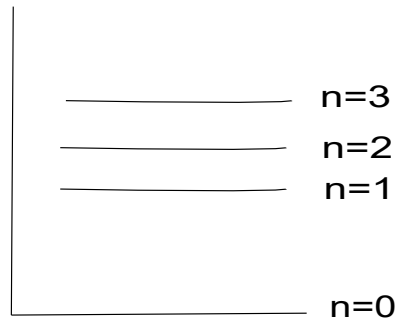


Figure 7.1: A system has energy levels, the ground state is lowest energy and other states are  $n > 0$  “excited states”.

In some cases, vacuum state is ground state. If more than one ground state is found in a system, we call it degenerate system. And so we say that a system oscillates between these energy levels. “Oscillations” are the words that are very important in quantum mechanics as well as quantum field theory. We will treat oscillations as something to do with energy levels which would create the excitations (or otherwise) in any quantum system. Of course, this needs some operators and we call them “ladder operators”. One can denote them  $a_n$  and  $a_n^\dagger$ . The former is “lowering operator” and the latter is “raising operator”. One have, for a system in  $n$ th state

$$a_n |\Psi_n\rangle = |\Psi_{n-1}\rangle \quad (7.2.1)$$

$$a_n^\dagger |\Psi_n\rangle = |\Psi_{n+1}\rangle. \quad (7.2.2)$$

We also have a number  $N$  such that

$$N = a_n^\dagger a_n, \quad (7.2.3)$$

and commutators

$$\left[ a_n, a_n^\dagger \right] = 1, \quad (7.2.4)$$

$$\left[ N, a_n^\dagger \right] = a_n^\dagger, \quad (7.2.5)$$

$$\left[ N, a_n \right] = -a_n. \quad (7.2.6)$$

## 7.3 A Basic Harmonic Oscillator

In quantum mechanics, we study models. Models of different kind and situations, each preserving the basic quantum laws. One of them is Harmonic Oscillator. In any basic book, one see that harmonic oscillators (or more simply simple harmonic oscillators (S.H.M)) are oscillating system. Most basic can be a moving spring or whatever.

The energy for a classical harmonic oscillator is given by

$$E = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}, \quad (7.3.1)$$

but for the harmonic oscillator as quantum system, we write the Hamiltonian

$$H = \frac{\hat{p}^2}{2m} + \frac{m\omega^2 \hat{x}^2}{2}. \quad (7.3.2)$$

The next thing to consider in any system is the question; “What are the eigenfunctions for these operators?” So we search for wave functions of these kinds of systems. In this case of harmonic oscillators, our wave function should resemble the properties under underlying operations of harmonic oscillators. First, we need to identify what are the ladder operators for such harmonic system. One can find that, they are<sup>2</sup>

$$\begin{aligned} a &= \sqrt{\frac{m\omega}{2\hbar}} \left( \hat{x} + \frac{i}{m\omega} \hat{p} \right) \\ a^\dagger &= \sqrt{\frac{m\omega}{2\hbar}} \left( \hat{x} - \frac{i}{m\omega} \hat{p} \right) \end{aligned} \quad (7.3.3)$$

---

<sup>2</sup> $a$  and  $a^\dagger$  are not hermitian as their adjoints are equal.

It turns out that wave function for Harmonic oscillators are

$$\Psi_n(x) = \frac{1}{\sqrt{2^n n!}} \cdot \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \cdot e^{-\frac{m\omega x^2}{2\hbar}} \cdot A_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right), \quad n = 0, 1, 2, \dots, \quad (7.3.4)$$

where  $A_n$  are Hermite polynomials

$$A_n(z) = (-1)^n e^{z^2} \frac{d^n}{dz^n} \left( e^{-z^2} \right). \quad (7.3.5)$$

We mention here few Hermite Polynomials results

$$\begin{aligned} H_0(x) &= 1 \\ H_1(x) &= 2x \\ H_2(x) &= 4x^2 - 2 \\ H_3(x) &= 8x^3 - 12x \\ H_4(x) &= 16x^4 - 48x^2 + 12 \\ H_5(x) &= 32x^5 - 160x^3 + 120x \\ H_6(x) &= 64x^6 - 480x^4 + 720x^2 - 120 \\ H_7(x) &= 128x^7 - 1344x^5 + 3360x^3 - 1680x \\ H_8(x) &= 256x^8 - 3584x^6 + 13440x^4 - 13440x^2 + 1680 \\ H_9(x) &= 512x^9 - 9216x^7 + 48384x^5 - 80640x^3 + 30240x \\ H_{10}(x) &= 1024x^{10} - 23040x^8 + 161280x^6 - 403200x^4 + 302400x^2 - 30240 \\ H_{11}(x) &= 2048x^{11} - 56320x^9 + 506880x^7 - 1774080x^5 + 2217600x^3 - 665280x. \end{aligned} \quad (7.3.6)$$

The energy eigenvalues are given by

$$E_n = \hbar\omega \left( n + \frac{1}{2} \right), \quad (7.3.7)$$

and ground state energy is given by a peculiar observation that it is  $\hbar\omega/2$  more than **Zero-Point Energy**. And this property contradicts what we see in classical oscillators where it is zero. Also that position and momentum are not fixed in ground state, however, uncertainty principle does not let that happen. Wave function for the ground state is centered at origin, see 7.2. Other things to note for the energies of these kinds of oscillators are that every energy level is equally spaced and are properly quantized ( $\hbar$  factors).

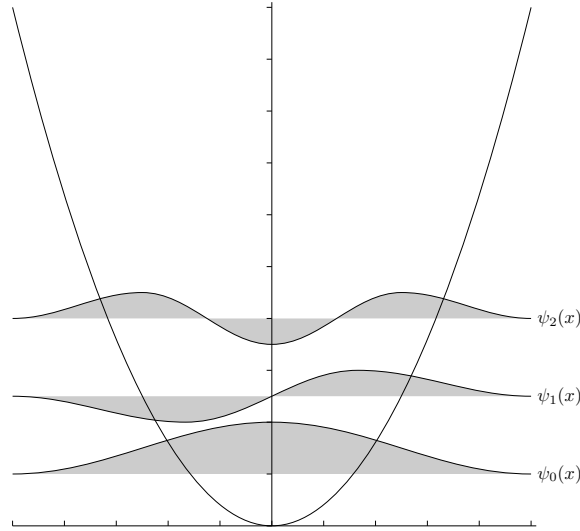


Figure 7.2: Wave functions for harmonic oscillator, where  $n$  is representing state.

The ground state wavefunction is given by setting  $n = 0$  in (7.3.4), which in  $1D$  is given by the first-order differential equation

$$\left(x + \frac{\hbar}{m\omega} \frac{d}{dx}\right) \psi_0 = 0, \quad (7.3.8)$$

which results in

$$\psi_0(x) = C \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-m\omega x^2/2\hbar}. \quad (7.3.9)$$

Before discussing the application of such system, it is interesting to note that dynamical variables like  $x$  and  $p$  can also be written in terms of ladder operators. They can be written in harmonic oscillators as

$$\begin{aligned} \hat{x} &= \sqrt{\frac{\hbar}{2m\omega}} (a^\dagger + a), \\ \hat{p} &= i\sqrt{\frac{\hbar m\omega}{2}} (a^\dagger - a). \end{aligned} \quad (7.3.10)$$

The applications of these oscillators and operators are not limited to quantum mechanics, in fact, every other physics beyond quantum mechanics nowadays need these oscillating machine in the theory.

Most interesting example is Quantum Field Theory. In quantum field theory, we discuss about various types of quantization involved which quantizes a classical field. Two important quantization process is *canonical quantization* and *path-integral formulation*. Both uses the oscillator technique, however, the former exploit it extensively. We do not have the scope (in this book) to discuss either, however we can talk it very briefly.

---

To establish a canonical quantization of  $\phi$ , we have some procedure. (We will not mention them here.) An important one is to write the commutation relations for  $x$  and  $p$  for the field. Then find the oscillators of the field, after establishing a *vacuum*  $|\phi;0\rangle$ . These oscillators will excite the vacuum to first excited state or it can oscillate the excited state to lower state (or vacuum for some examples). Conventionally, they are  $a_n$  and  $a_n^\dagger$ , where  $n$  is some integer. They are also called annihilation operator and creation operator respectively. Then we do some ordering, and our Lagrangian (see appendix A)  $\mathcal{L}$  is ready. For  $\phi$ , when quantized, the action is given in terms of

$$\mathcal{L} = -\frac{1}{2} (-\partial^2\phi^2 + (m\phi)^2), \quad (7.3.11)$$

and given the Euler-Lagrange, we can write;

$$\partial^2\phi + m^2\phi = 0, \quad (7.3.12)$$

which is a simple linear equation and shows a Schrödinger equation for wave function  $\phi$ . For a set of scalar fields, we can write the Lagrangian for  $\phi$  as

$$\mathcal{L} = -\frac{1}{2} \sum_i^N (\partial^2\phi_i^2 + m^2\phi_i^2) - \frac{1}{8}\lambda \left( \sum_i^N \phi_i \right)^2, \quad (7.3.13)$$

which of course is interacting field.

---

## 7.4 Infinite Square Well

Infinite Square Well is, yet, another model of interest in quantum mechanics. It is also known as “particle in a box” and “infinite potential well”. The model is

too simple that it can be solved exactly without any approximations (we have also used it in the past in book). So, it is just two walls and a particle between them. Particle always attains the positive energy. So the particle's energy can not be zero, hence it will not sit. Particle can be found anywhere between the well, the positions would be called "spatial nodes"

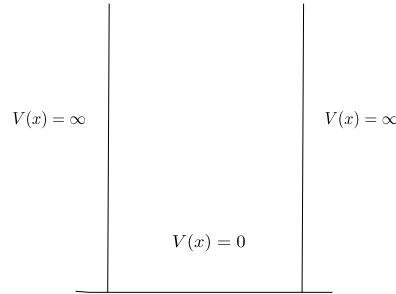


Figure 7.3: A 1D potential well, where inside well  $V(x) = 0$  and otherwise  $V(x) = \infty$ .

We can write it as

$$V(x) = \begin{cases} 0, & x_c - \frac{L}{2} < x < x_c + \frac{L}{2} \\ \infty, & \text{otherwise} \end{cases} \quad (7.4.1)$$

where  $L$  is the length of well (or box). Because the potential inside the box is zero (constant), particles are free to move anywhere in the region. We should also note that infinite potential at the boundary pushes the box so the particle does not escape the box. Overall, this is an interesting and simple model.

Particle can never be at infinite potential, which is a similar case of classical mechanics.

We will also assume that

$$\psi(x) = 0 \text{ for } x < L, x > L \quad (7.4.2)$$

and since we want the wave function to be continuous, we should also impose some boundary conditions

$$\psi(x = 0) = 0, \quad (7.4.3)$$

$$\psi(x = L) = 0. \quad (7.4.4)$$

Our task is now to search for wavefunctions related to infinite square well. Since in the interval  $x \in [0, L]$ , potential is zero we can write the Schrödinger equation as

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi, \quad (7.4.5)$$

where  $E > 0$  and  $E$  can be written in terms of wave-number

$$E = \frac{\hbar^2 k^2}{2m}, \quad (7.4.6)$$

so the Schrödinger equation becomes

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \quad (7.4.7)$$

for which the solution wave function is

$$\psi(x) = a \sin kx + b \cos kx, \quad (7.4.8)$$

where  $a, b$  are two constants. We can find these constants by simply observing that (7.4.3) implies that

$$\psi(0) = a \sin k0 + b \cos k0, \quad (7.4.9)$$

and that further implies that  $b = 0$ . So wave function solution simplifies to

$$\psi(x) = a \sin kx. \quad (7.4.10)$$

To know about the constant  $a$ , we need to work with another boundary condition i.e.  $\psi(x = L) = 0$ . Hence

$$\psi(x = L) = a \sin kx = 0, \quad (7.4.11)$$

that further goes

$$kL = n\pi, \quad k_n = \frac{n\pi}{L}. \quad (7.4.12)$$

So

$$\psi_n(x) = A \sin\left(\frac{n\pi x}{L}\right) \quad (7.4.13)$$

where  $A$  is the normalization constant and we assume that  $n > 0$ , though it can be negative as well. Doing the normalization, we get

$$\Psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \quad (7.4.14)$$



$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2mL^2}, \quad n = 1, 2, \dots \quad (7.4.15)$$

We can check that in equation

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2} \quad (7.4.16)$$

every  $n$  values gives different energy level. So, there is no chance of being degeneracy in infinite square well.

We can write the ground state with  $n = 1$ , which will have energy  $E \neq 0$ .

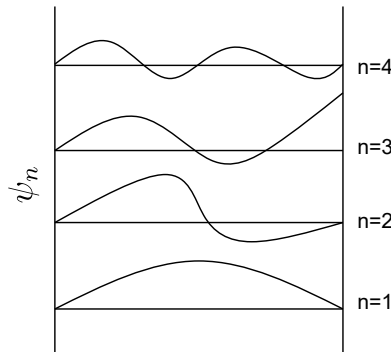


Figure 7.4: Wave functions of infinite square well. Each  $\psi_n$  with nodes  $n - 1$ .

## 7.5 Finite Square Well

In last section, we discussed infinite square well. In infinite square well, we had a well with  $V(x) = 0$  and with infinite potential boundaries. Potentials are important elements of models. And potential well too. It is important to note that energy inside the potential well can not be converted into other forms of energy. Because we have trapped it there at the minimum of potential well.

There are few more interesting potential wells to discuss. We will discuss in this section, two of them - Dirac Delta Potential Well and Finite Square Well.

Finite square well is another simple model of quantum mechanics. Generally, one can speak that finite square well is an extension of infinite square well but with finite potential wells. In infinite square well, we just had to calculate things about states inside the box. But in finite square well, as it will permit the wave function to extend beyond the boundaries, we need to calculate the outside the box as well.

Well, yes, the boundary conditions would differ in this case. But we won't do any boundary conditions in this case, which we recommend however, strongly to reader.

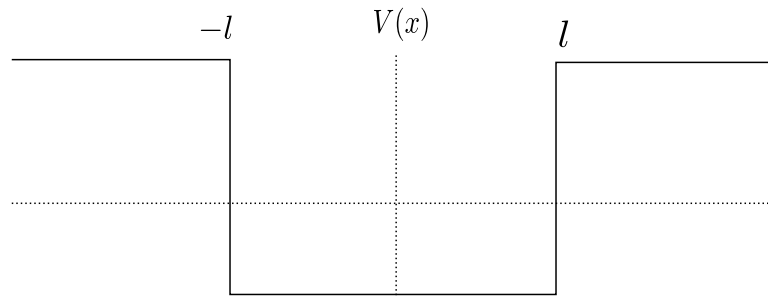


Figure 7.5: Finite Potential Well

Outside the box in finite square box (or well) is not the case with infinite potential but with finite potential. In finite square well case, potential requirements are

$$V(x) = \begin{cases} 0, & |x| \geq l \\ -V_0, & |x| \leq l \end{cases} \quad (7.5.1)$$

where  $V_0$  is always positive. We need to find the states outside the box, without defining boundary conditions in case. We have  $V(x) = V_0$  in that case. So overall energy will be  $E - V_0$ , then the Schrödinger equation is

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}(E - V_0)\psi \quad (7.5.2)$$

We need to focus on bound states, i.e states with  $V_0 > E$ .

## 7.6 Scattering

In last three sections, we learned about Harmonic oscillators, infinite square well and finite square well. We can add in this list a number of other important and consequential models, but we will not do it here.

We should now move to other important topics as well. In this section, we will overview briefly about scattering and resonant transmission in quantum mechanics, where we will also analyze the incoming and outgoing waves.

Scattering is a consequential study of physics. It has its wide applications, mainly in field theory and particle phenomenology. In quantum mechanics, it would mean a little different when we say “scattering”.

Scattering in quantum field theory is quite interesting (however, this book is not about that). Though we can - at least - introduce scattering in terms of field theory.

A simple scattering process is

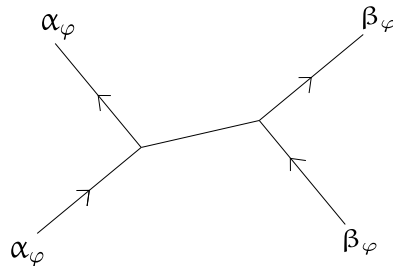
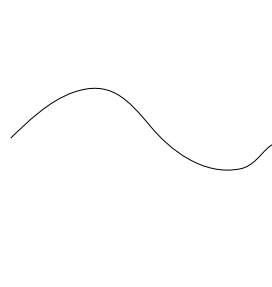


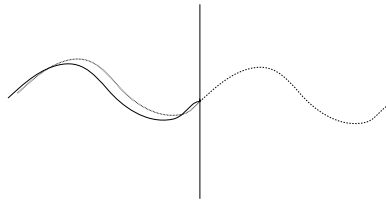
Figure 7.6: A Feynman diagram among many, a tree level  $2 \rightarrow 2$ , for  $\alpha_\varphi \beta_\varphi \rightarrow \alpha_\varphi \beta_\varphi$ . It is important to note that this is not the *only* way to draw diagrams, we can map this diagram (conformally) to some disk or sphere and work on those diagrams also.

Let us suppose, we have a barrier (of potential), we direct a wave towards it. As shown in below figure

Scattering comes into play when the indicated *wave* hit the wall.



When the *wave* hit the wall, there are two things to consider (one is **scattering** and other is tunneling.) the incident wave will **suffer** the collapse and it would



either transmit through the wall or get reflected, as indicated in figure. For convention, we will write  $A$  as incident wave,  $B$  as transmitted wave and  $C$  as reflected wave.

We now can ask how much  $A$  would be transmitted and how much of it would be reflected?

It is, however, a simple question. Before moving on, we need to define the potential in this case

$$V(x) = \begin{cases} v(x), & x \in [0, L] \\ \infty, & x < 0 \\ 0, & x > L \end{cases} \quad (7.6.1)$$

where  $L$  is the length from the origin to well. We will also need a wave function to incident on it. By choice, we take  $e^{-ikx}$  which is also a zero potential solution. So, in the region of  $v(x)$  the reflected wave should be just  $e^{ikx}$ . The change between the incident and reflected wave is perhaps because of “phase shift  $\delta$ ”. Phase shift can be understood by saying that “it is the shift in the phase”. Well, every wave have their phases. The shift in those phases will be denoted by  $\delta$ .

Note that probability flux of both waves shall be same, however the direction is only opposite. Energy of both waves would be same.

Scattering is not much interesting at this time. Where it is important is in Quantum Field Theory. In QFT, scattering deals with cross sections, **S-matrix**, and so on. Waves scattering importance comes in quantum mechanics in the cases of square well(s) as well.

## Node Theorem

Node theorem is a simple theorem in quantum mechanics associated to nodes of wave-functions. Our aim should be understand this theorem not rigorously, as it is not.

Recall the infinite square well (or finite well or even harmonic oscillators), the bound states wave functions  $\psi_n$  have  $n - 1$  nodes.

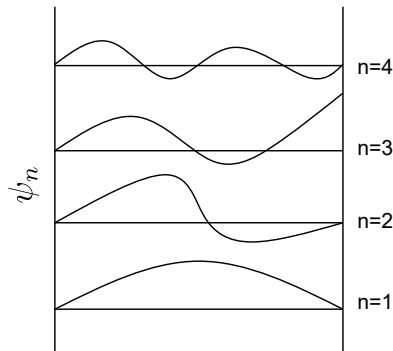


Figure 7.7: Wave functions of infinite square well. Each  $\psi_n$  with nodes  $n - 1$ .



# Chapter 8

## System and Interactions

Back a few sections, we discussed the orbital angular momentum and spins. Both are extensive in the sense of atomic physics and quantum mechanics. In this chapter, we will focus on the sum of both angular momentum(s), which is called **Total Angular Momentum**,  $J$ . We will also discuss the Clebsh-Gordon Coefficients<sup>1</sup>.

### 8.1 Total Angular Momentum

We might want to recall few things about angular momentum and spins.

- Angular momentum, represented by  $L$ , is given by

$$L_z \psi = \hbar m \psi \quad (8.1.1)$$

and  $L^2$  by the eigenvalue equation

$$L^2 \psi = \hbar^2 l(l+1) \psi \quad (8.1.2)$$

$$[L_i, L^2] = 0 \quad (8.1.3)$$

---

<sup>1</sup>Consider reading *arXiv* : 1907.09930.

- Spins are also intrinsic property in quantum mechanics. We represent it by  $S$ .

$$S_z |\phi; \pm\rangle = \pm \frac{\hbar}{2} |\phi; \pm\rangle \quad (8.1.4)$$

We can write the total angular momentum as the sum of both  $L$  and  $S$ . Why does this matter?

The answer is straightforward: the total angular momentum, as we have seen, is accountable for a lot of trivial commutation. Furthermore, the total angular momentum is overall angular momentum that can tell us more deeply about the system as a whole rather than the individual angular momentum.

$$\hat{J} = \hat{L} + \hat{S} \quad (8.1.5)$$

When we couple the momentum, we call the basis of work as “Coupled basis”. Uncoupled basis are in form of quantum numbers  $(l, n, m_l, m_s)$ . However, in the couple basis, we tensor product the  $l$  multiplets and  $s$  multiplets to have  $J$  multiplets.

The coupled basis can be denoted by  $(l, n, J, J_m)$ . Why not  $J_s$ ?

When we write coupled basis, it helps us to draw the spectrum for the system also, which we will see in the upcoming time. The eigen-equation for  $J^2$  can be written as

$$J^2 \Psi = j(j+1) \hbar^2 \Psi \quad (8.1.6)$$

where  $\Psi$  is a coupled state. The multiplets equation be can written as

$$(l_{mt}) \times (s_{mt}) = \sum J_{mt} \quad (8.1.7)$$

$$\rightarrow (l_{mt}) \times \left( \pm \frac{1}{2} \right) = \left( l + \frac{1}{2} \right) \times \left( l - \frac{1}{2} \right) \quad (8.1.8)$$

where subscript  $mt$  is used to depict multiplets. Note that  $l$  multiplets have  $m$  in it, so total angular momentum would be ranging through all the  $m$ .

We can better understand it if we take an example. Let us suppose we have two electrons with spins  $\pm \frac{1}{2}$ . (We are not indulging with  $l$  here.)



We can write the 4 configurations of uncoupled states as  $(\alpha, \beta$  for electrons representations) in form of  $(s_\alpha, m_s; s_\beta, m_s)$

- $|\frac{1}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}\rangle (\uparrow\uparrow)$
- $|\frac{1}{2}, \frac{1}{2}; \frac{1}{2}, -\frac{1}{2}\rangle (\uparrow\downarrow)$
- $|\frac{1}{2}, -\frac{1}{2}; \frac{1}{2}, \frac{1}{2}\rangle (\downarrow\uparrow)$
- $|\frac{1}{2}, -\frac{1}{2}; \frac{1}{2}, -\frac{1}{2}\rangle (\downarrow\downarrow)$

Our work is to create a coupled basis  $(s_\alpha, s_\beta, S, M_s)$  where  $S = |s_\alpha + s_\beta|$ . In so, we will only have two values of  $S = 0, 1$  and four values of  $M_s$ . They are

- $|\frac{1}{2}, \frac{1}{2}, 0, 0\rangle$  as  $m_s = 2s + 1 \implies 2 \times 0 + 1 = 1$
- $|\frac{1}{2}, \frac{1}{2}, 1, (1, 0, -1)\rangle$ , there are three  $m_s$  in the square brackets.

this was the coupled eigenstates (wave-functions). This particular example was of **Spin-Spin** coupling. We can do, similar like this, L-L coupling and Spin-Orbit coupling which we introduced at the beginning of the section.

## 8.2 Hamiltonian Corrections

In the last section, we reviewed the addition rule in angular momentum. Straight-forwardly it is a simple law of making two uncoupled states a coupled state. In the last section, we talked about spin-spin coupling for two spins of  $\pm 1/2$ . There are a few practical applications of spin-spin coupling - which, however, we will not see here.

One example would be from organic chemistry, where we observe the spin-spin coupling in the hydrogen atom's NMR (Nuclear Magnetic Resonance) spectrum.

Before we proceed, let me point out important points.

- Spin-Spin, Spin-Orbit and many like Pauli equation, Darwin correction, relativistic correction, Dirac equation, Hyperfine correction, Lamb shift are a few corrections to Hamiltonian of a system. These corrections appear in a system because of the splitting in the spectra they carry.
- It is somewhat important to include them in any system.

We can not talk about each of them in detail. But concerning the vast importance of some of them, we will talk about them in the coming sections.

### 8.2.1 Pauli Equation

Pauli equation is written as

$$H_{Pauli}|\Psi\rangle = \left[ \frac{1}{2m}(\boldsymbol{\sigma} \cdot (\mathbf{p} - q\mathbf{A}))^2 + q\phi \right] |\Psi\rangle = i\hbar \frac{\partial}{\partial t} |\Psi\rangle \quad (8.2.1)$$

where  $\phi - q\mathbf{A} = \Pi$  ( $\Pi$  is kinetic momentum,  $\phi$  is canonical momentum) and  $\boldsymbol{\sigma}$  are Pauli matrices. It would be important to note that  $\Psi$  can be considered as two component spinor (of which we will learn more in Dirac equation, as it is called Dirac spinor).  $\phi$  is the scalar potential,  $q$  is the charge,  $\mathbf{A}$  is the vector potential.

Because of the coupling to EM

$$\phi \rightarrow \Pi = \phi - \frac{q}{c}\mathbf{A} \quad (8.2.2)$$

(The bold letters are vectors.) We take the Pauli equation in account when the spins are interacted with the external electromagnetic field. (We can derive the Pauli equation from the equation

$$H = \boldsymbol{\mu} \cdot \mathbf{B} = \frac{e\hbar}{2mc}\boldsymbol{\sigma} \cdot \mathbf{B} \quad (8.2.3)$$

from the section on the dipole moment with the following)

$$\begin{aligned} (\boldsymbol{\sigma} \cdot \mathbf{a})(\boldsymbol{\sigma} \cdot \mathbf{b}) &= (\mathbf{a} \cdot \mathbf{b})\mathbb{1} + i\boldsymbol{\sigma} \cdot (\mathbf{a} \times \mathbf{b}) \\ (\mathbf{r} \cdot \mathbf{p})(\mathbf{a} \cdot \mathbf{p}) &= (\mathbf{p}^2)\mathbb{1} + 0 \\ H &= \frac{\mathbf{p}^2}{2m}\mathbb{1} = \frac{(\boldsymbol{\sigma} \cdot \mathbf{p}^2)(\boldsymbol{\sigma} \cdot \mathbf{p})}{2m} \end{aligned} \quad (8.2.4)$$

Note that in Pauli equation, we have the case

$$v \ll c \quad (8.2.5)$$

whereas, in Dirac equation we will observe the relativistic effects.

### 8.2.2 Dirac Equation

Dirac equation is the relativistic equation which governs some purposes of quantum electrodynamics as well. Dirac equation is written as a dispersion relation

$$\boxed{E^2 = (pc)^2 + (mc^2)^2} \quad (8.2.6)$$

*we may have heard about the famous equation;  $E = mc^2$ , - we have dropped the bold letters convention - the Dirac equation is a little stretched equation of the same famous equation. One, to find the  $H$  correction, needs to do the following*

$$H = \sqrt{p^2 c^2 + m^2 c^4} \quad (8.2.7)$$

$$= mc^2 \left( 1 + \frac{p^2}{m^2 c^2} \right) \quad (8.2.8)$$

extracting the square root

$$H = mc^2 \left( 1 + \frac{1}{2} \frac{p^2}{m^2 c^2} - \frac{1}{8} \frac{p^2 p^2}{m^4 c^4} + \dots \right) \quad (8.2.9)$$

Which it not satisfactory. We need to find another fact to eliminate the square root, a better way. We have such one

$$H_{Dirac} = c\alpha \cdot p + \beta mc^2 \quad (8.2.10)$$

where  $c$  is a constant and  $\alpha$  matrices

$$\alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} \quad (8.2.11)$$

and  $\beta$  matrices are

$$\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (8.2.12)$$

We can write the Schrödinger equation for the *Dirac spinor* (two-component)

$$H_{Dirac} \Psi_{Dirac} = i\hbar \frac{\partial \Psi}{\partial t} \quad (8.2.13)$$

and when the Dirac equation is coupled to electromagnetism,  $p$  couples to  $A$ .

### 8.2.3 Darwin Correction

Last time, we briefly talked about the correction in a basic Hamiltonian. We did the Dirac correction and Pauli correction, which were relativistic and non-relativistic, respectively. Both were related to the spins and their coupling to either exterior electromagnetic field or making it to be in the sea of Dirac ideas of spinor in relativistic limits.

In this subsection, we will continue our exploration of these corrections. In our list of corrections, we will be discussing the Relativistic and Darwin correction and, then Spin-Orbit coupling.

Before we go further, let us clarify that we will continue the scheme of being brief in these discussions as these discussions are part of a more diverse-d edition of quantum mechanics and field theory as well.

Darwin's correction comes from the Dirac equation and can be written as

$$H_{Darwin} = \frac{\pi e^2 \hbar^2}{2m_e^2 c^2} \delta(r) \quad (8.2.14)$$

and, in fact, only of concern when  $l = 0$ .  $\delta(r) = \nabla^2 V / 4\pi e^2$ . Expectation value can be written as

$$\langle \Psi_{nlm} | H_{Darwin} | \Psi_{nlm} \rangle = \frac{\pi e^2 \hbar^2}{2m_e^2 c^2} |\Psi_{nlm}(x)|^2 \quad (8.2.15)$$

where we will assume that  $\psi$  vanishes at the origin for  $l = 0$ .

$$\langle \Psi_{n00} | H_{Darwin} | \Psi_{n00} \rangle = \frac{\pi e^2 \hbar^2}{2m_e^2 c^2} |\Psi_{n00}(0)|^2 \quad (8.2.16)$$

It turns out that the wave function can be determined (by following the discussion we had on polar coordinates)

$$|\Psi_{n00}(0)|^2 = \frac{1}{\pi n^3 a_0^3} \quad (8.2.17)$$

where  $a_0$  is the Bohr radius. In this way the expected value is

$$\langle H_{Darwin} \rangle_{n00} = \frac{4e^2 \hbar^2}{8n^3 a_0^3 m^2 c^2} = \frac{e^2 \hbar^2 \alpha^2 m^2 c^2}{2n^3 a_0 m^2 c^2 \hbar^2} = \frac{2nE_n^2}{mc^2} \quad (8.2.18)$$

And this actually replaces the  $l = 0$  term in the spin-orbit correction (which should be zero) and making the equation correct.

Darwin correction is related to the zitterbewegung of the relativistic electron. A straightforward example of this correction is in the Hydrogen atom.

*“Sir Charles Galton Darwin (1887-1962), a British physicist, was a grandson of the Charles Darwin of evolution fame. Sir Charles was the first, with Gordon, to work out the exact energy levels of Hydrogen according to the Dirac equation and thereby discovered the eponymous term in the levels. He worked out the Lagrangian and Hamiltonian for a classical motion of several interacting charges correct to  $O(v^2/c^2)$ . He also worked on statistical mechanics (Darwin-Fowler method). Later in life, he took part in the Manhattan project.”*

*Darwin’s work was referred to in the original Foldy-Wouthuysen article: Phys Rev. 78 no.1, 29-36, 1950.*

## 8.2.4 Relativistic Correction

The fun (and the pun) begins here. The relativistic correction is for energy levels. We will briefly discuss a few relativity concepts and basic principles before we try to understand the topic itself.

- In basic sense, we calculate the relativistic effects when the speed is close to that speed of light ( $c = 3 \times 10^8 m/s$ ).  $v = c$ .
- Consider a uniformly moving object and suddenly, an increase in energy makes the object to reach the speed of light. What happens when it goes with the speed of light?

Relativity is a vast subject, which has been basically divided into two studies; Special Relativity and General Relativity. We would only need special one here. General relativity is a part of an ever-longing study of gravity, initiated by Einstein first. On that subject, we are still pondering, and since it does not fit with quantum mechanical principles, we (physicists and mathematicians) are in another hurry of some unified theory. When we move from non-relativistic arena to relativistic arena, the energy of the electron changes to

$$mc^2 + \frac{p_e^2}{2m} \rightarrow (p^2 c^2 + m^2 c^4)^{1/2} = mc^2 \left( 1 + \frac{p^2 c^2}{m^2 c^4} \right)^{1/2} \quad (8.2.19)$$

and we get when  $p^2 = 0$  (nilpotent of index 2)

$$(p^2 c^2 + m^2 c^4)^{1/2} = mc^2 + \frac{1}{2} \frac{p^2 c^2}{mc^2} - \frac{1}{8} \frac{p^4 c^4}{m^3 c^6} + \dots \quad (8.2.20)$$

$$\approx mc^2 + \frac{p^2}{2m} - \frac{p^4}{8m^3 c^2} \quad (8.2.21)$$

the correction is the last term.

Hence, the relativistic correction is

$$H_{RC} = \frac{p^4}{8m_e^3 c^2} \quad (8.2.22)$$

where  $m_e$  is the corrected mass, which however does not concern us.

### 8.2.5 Spin-Orbit Correction

The main reason for the spin-orbit coupling is the interaction between the magnetic moment with the intrinsic (orbital) moment of the electron.

Spin-Orbit is a relativistic effect observed when the electron's spin interacts with the orbital. The Hamiltonian received in this interaction

$$H_{spin-orbit} = \frac{e^2}{2m_e^2 c^2} \frac{1}{r^3} \vec{S} \cdot \vec{L} \quad (8.2.23)$$

where  $1/r^3$  is written as the expectation value

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{Z^3}{n^3 l(l+1/2)(l+1)} \quad (8.2.24)$$

where  $Z$  is the effective atomic number.

$$\langle \mathbf{L} \cdot \mathbf{S} \rangle = \frac{1}{2} (\langle \mathbf{J}^2 \rangle - \langle \mathbf{L}^2 \rangle - \langle \mathbf{S}^2 \rangle) = \frac{\hbar^2}{2} (j(j+1) - \ell(\ell+1) - s(s+1)) \quad (8.2.25)$$

The total energy correction observed is

$$\Delta E = \frac{\beta}{2} (j(j+1) - \ell(\ell+1) - s(s+1)) \quad (8.2.26)$$

where

$$\beta = \beta(n, l) = Z^4 \frac{\mu_0}{4\pi} g_s \mu_B^2 \frac{1}{n^3 a_0^3 \ell(\ell+1/2)(\ell+1)} \quad (8.2.27)$$

**Concluding Notes on Interactions;** So far we have observed many interactions which result into further corrections in the (*premature*) Hamiltonian. There are definitely more interactions that can be studied, for instance Hyperfine splitting or Lamb shift. However, we will not do them here.

These interactions are not just theoretical or conjugated, they exist and are easily observed in the laboratory.

## 8.2.6 Clebsch-Gordan Coefficients

We are now in the state of discussing how two total angular momentum (of two particles) are coupled to a total-total angular momentum.

For something like

$$J = j_1 + j_2 \quad (8.2.28)$$

where

$$j_1 = L_1 + S_1 \quad (8.2.29)$$

$$j_2 = L_2 + S_2 \quad (8.2.30)$$

we write the equation for  $J$  in bracket notation

$$|JM\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} |j_1 m_1 j_2 m_2\rangle \langle j_1 m_1 j_2 m_2 | JM\rangle \quad (8.2.31)$$

where  $M$  is

$$M = m_1 + m_2 \quad (8.2.32)$$

Clebsch-Gordan coefficient are written as

$$\Psi_{JM} = \sum_{M=M_1+M_2} C_{M_1 M_2}^J \Psi_{M_1 M_2} \quad (8.2.33)$$

These coefficients can be calculated easily. We do not show how. But we include a chart to provoke the reader to learn about it more as it is a broad subject even in particle physics.

In Mathematica, one can compute these coefficients using the command:  
 “ClebschGordon[{ $j_1, m_1$ }, { $j_2, m_2$ }, { $j, m$ }]”.







# Chapter 9

## Entanglement and EPR

Now we go to the topic for which quantum mechanics is (in)famous, Entanglement. This has a history, which has characters like Einstein as well deferring the theory as unreal and unnatural. Our investigation (of course, briefly) would be about the entangled states set out by Bell and locality.

Before we start discussing the entangled states, we might want to introduce tensor products in states.

**Tensor Products:** for two vector spaces  $V$  and  $W$  we write the tensor product as  $V \otimes W$ . Let us say that  $e_i$  is the basis of  $V$  and  $f_j$  is of  $W$ . After tensor product

$$v \otimes w = \left( \sum_i v_i e_i \right) \otimes \left( \sum_j w_j f_j \right) = \sum_{i,j} v_i w_j e_i \otimes f_j \quad (9.0.1)$$

$$\dim(V \otimes W) = \dim(V) \times \dim(W) \quad (9.0.2)$$

For the tensor product  $V \otimes W$ , we can write the wave function

$$\Psi = \sum_i \alpha_i v_i \otimes w_i \quad (9.0.3)$$

which is written as a superposition of  $v \otimes w$ , where  $v \in V, w \in W$ .

Note that if we can calculate the  $\Psi$  in terms of  $v$  or  $w$  only, then  $\Psi$  is not entangled. It has to be dependent on each other, as entanglement suggests.

Let us say that  $V$  has basis  $e_1, e_2$  and  $W$  has basis  $f_1, f_2$ , then the most general state is

$$\Psi_A = a_{11}e_1 \otimes f_1 + a_{12}e_1 \otimes f_2 + a_{21}e_2 \otimes f_1 + a_{22}e_2 \otimes f_2 \quad (9.0.4)$$

which can be put under in a matrix  $E$

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \quad (9.0.5)$$

where we put forward a condition: matrix  $E$  determinant should not be zero, if it is for a non-entangled state. You may check it yourself, by comparing the coefficients.

## 9.1 Entangled State

In last lecture, we briefly touched entanglement. Entanglement, in simple words, is an event seen frequently in quantum mechanics about coupled states. What are these coupled states at first? Why they become dependent of each other after getting entangled? Does causes on one produces result on another? What is EPR paradox?

These are the questions which we will address today. As explained earlier,  $\Psi$  a entangled state of two spin particles is

$$\Psi = \frac{1}{2} \left( |+\rangle_x \otimes |+\rangle_y + |-\rangle_x \otimes |-\rangle_y \right) \quad (9.1.1)$$

but we will take a much simpler entangled state (of the same setting) for discussion. Consider two particles with spins either up or down. The important catch of entangled states is that if one particle is found with spin up, then the other particle is (strongly) spin down. This only happens with entangled particles.

Note that it is also not important that how much separated the two particles are, once they are entangled, they communicate with each other at an impossible

speed which, perhaps, break the relativity conjecture that no information can travel faster than speed of light.

Entanglement will still hold if we take the two particles are either horizons of the universe.

Entangled Electrons See these two particles these are entangled particles, came

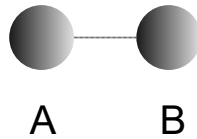


Figure 9.1: Two particles are entangled to each other.

close together and are synced up. It can be aided that these two particles come from decay of a spin 0 particles, hence A and B will be spin  $\pm 1/2$  particles. Now we take A and B far apart and we find that spin of A is up. The spin of B must be



Figure 9.2: We take the particle apart. Measure first particle's spin, suppose that it is "up"

down.



Figure 9.3: One state is observed up, we will not disturb the other state.

### 9.1.1 Bell-Basis States

Bell-Basis states are entangled states of two particles (qubits - if we talk specifically computations) which is a simplest construction for entanglement. We will

work out these basis states in this lecture. In a general entangled state  $\Psi_0$ , we have

$$\langle \Psi_0 | \Psi_0 \rangle = 1 \quad (9.1.2)$$

so if one particle wave function is collapsed (from the superposition) in one of the basis (will explained soon), other's wave function collapses as well.

So we create four dimensional basis with  $|\Psi_0\rangle$

$$\frac{1}{2} (|+\rangle \otimes |+\rangle + |-\rangle \otimes |-\rangle) \quad (9.1.3)$$

we write the basis as

$$|\Psi_i\rangle = (1 \otimes \sigma_i) |\Psi_0\rangle, \quad i = 1, 2, 3 \quad (9.1.4)$$

$\sigma_i$  unitary matrices are have been introduced before. For  $\Psi_1$ , we can create the state

$$|\Psi_1\rangle = (1 \otimes \sigma_1) |\Psi_0\rangle \quad (9.1.5)$$

$$|\Psi_1\rangle = \frac{1}{\sqrt{2}} (|+\rangle |-\rangle + |-\rangle |+\rangle) \quad (9.1.6)$$

$$\langle \Psi_0 | \Psi_1 \rangle = 0 \quad (9.1.7)$$

Similarly, we can construct other states  $|\Psi_2\rangle, |\Psi_3\rangle$

$$|\Psi_2\rangle = \frac{i}{\sqrt{2}} (|+\rangle |-\rangle - |-\rangle |+\rangle) \quad (9.1.8)$$

$$|\Psi_3\rangle = \frac{1}{\sqrt{2}} (|+\rangle |+\rangle - |-\rangle |-\rangle) \quad (9.1.9)$$

and they are orthogonal to  $\Psi_0$

$$\langle \Psi_0 | \Psi_i \rangle = 0 \quad (9.1.10)$$

which resembles the function

$$\langle \Psi_i | \Psi_j \rangle = \delta_{ij} \quad (9.1.11)$$

In can be seen that

$$|-\rangle |-\rangle = \frac{1}{\sqrt{2}} (|\Psi_0\rangle - |\Psi_3\rangle) \quad (9.1.12)$$

(it is easy to check)

$$|+\rangle|-\rangle = \frac{1}{\sqrt{2}}(|\Psi_1\rangle + i|\Psi_2\rangle) \quad (9.1.13)$$

$$|-\rangle|+\rangle = \frac{1}{\sqrt{2}}(|\Psi_1\rangle - i|\Psi_2\rangle) \quad (9.1.14)$$

$$|+\rangle|+\rangle = \frac{1}{\sqrt{2}}(|\Psi_0\rangle + |\Psi_3\rangle) \quad (9.1.15)$$

these are called “**Bell-Basis states**”.

## 9.2 EPR Paradox

In the last section, we discussed Bell states and entanglement. We saw how constructive it is for quantum mechanics. And sure it is a perfect principle of physics. However, rationally questioning it is.

It (entanglement and wave function) was fairly obnoxious to Einstein, Rosen, and Podolsky that they wrote a paper asking some good-old questions about entanglement and quantum mechanics. Quoting quantum mechanics as *incomplete*. The paradox (the paper) is called EPR, published in PRL 1935.

It was also a fair call to “locality and non-locality” in quantum mechanics. In this small section, we will try to cover the EPR Paradox and how the paradox was received technically. With philosophy, of course.

From the view of EPR, we can take out that if a particle’s eigenvalue is definite it should not be that another eigenvalue should be undefined. But that is our critical Heisenberg’s uncertainty relation. So, EPR says that  $\psi$  the wave function is not yet complete.

EPR paper also emphasized on locality and non-locality in quantum mechanics. Locality means that in a theory, if one thing happens at one location then there can’t be immediate effects from it at another location. It is easy to see that quantum entanglement is non-local.

The only way out of this paradox - which was mainly that definite results on particle A created two wave function for particle B, where A and B were entangled - for most of the physicists, including Einstein, was to assume some hidden variables so that quantum entanglement never happens. Bell theorem suggests that we can construct local hidden variables can be introduced to finish the incomplete reality.

Bell theorem suggests that we can construct local hidden variables can be introduced to finish the incomplete reality.



# Chapter 10

## Perturbation and Relativity

Perturbation Theory is a well-defined method to calculate and study deeply about a system. However, this book does not carry sufficient merit to discuss perturbation techniques and methods. We do provide suggested readings for it.

In this chapter, we briefly comment on perturbation theory. Then we finally close up the book introducing relativity for further reading of the subject.

### 10.1 Perturbation Theory

The idea is simple, and we start with a simple Hamiltonian  $H$  to describe a system, and then we add a small perturbative Hamiltonian  $\delta H$  representing a disturbance to the original system. The resulting system is *perturbed system*. The Hamiltonian becomes

$$H' = H + \epsilon\delta H \tag{10.1.1}$$

$H'$ ,  $\delta H$ ,  $H$  are all hermitian as Hamiltonian(s).  $\epsilon$  is a small parameter which we will call “order”. Before we proceed, we need to discuss *degeneracy*. Degeneracy means at the same level. In quantum mechanics, we have different states at the

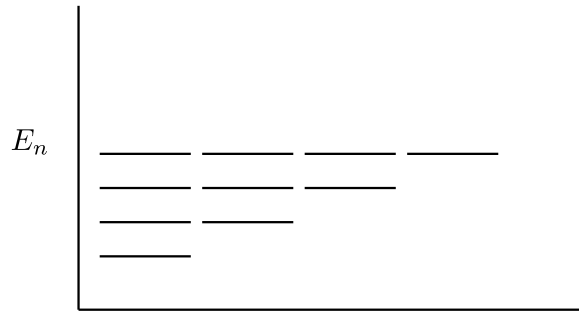


Figure 10.1: The bottom state is ground state, the energy responds for one state, so it is a non-degenerate level. However (for  $n=1$ ), it is two states so this level, so a degenerate level. And so on.

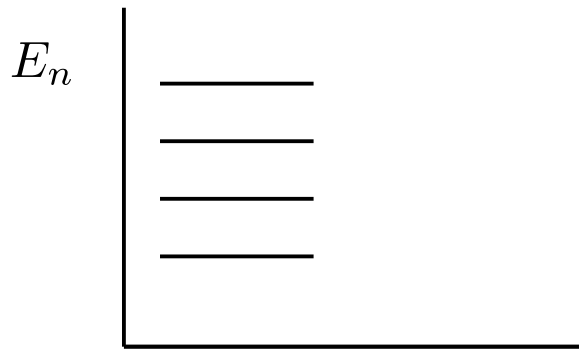


Figure 10.2: A non-degenerate system.

same energy level. For instance, consider a system with the following energy

$$E_n \psi_n = C_n H_n \psi_n \quad (10.1.2)$$

where  $C_n$  are constants of state  $\psi_n$ . If  $E_n$  corresponds for more than one  $\psi$  states (let it be  $\psi_n$  and  $\psi_m$ ,  $m \neq n$ ), then it is called “degenerate level”.

Where comes the perturbation? What effects  $\delta H$  does it bear to a system?

A vast majority of quantum systems can not be solved exactly. We need to approximate the answer to some degrees. So we part away two parts

$$H = H_0 + \epsilon \delta H \quad (10.1.3)$$

where  $H_0$  is the solvable solution.

$$\hat{H}_0 \psi^{(n)}(x) = E^{(n)} \psi^{(n)}(x) \quad (10.1.4)$$

$n$  are the order.

$$\hat{H} \psi(x) = E \psi(x) \quad (10.1.5)$$

Since we can write the things in small parameters, we write

$$\begin{aligned} \psi(x) &= \psi_0(x) + \varepsilon \psi_1(x) + \varepsilon^2 \psi_2(x) + \dots \\ E &= E_0 + \varepsilon E_1 + \varepsilon^2 E_2 + \dots \end{aligned} \quad (10.1.6)$$

which is an eigenvalue equation,

$$\begin{aligned} (\hat{H}_0 + \varepsilon \hat{V}) (\psi_0(x) + \varepsilon \psi_1(x) + \varepsilon^2 \psi_2(x) + \dots) = \\ (E_0 + \varepsilon E_1 + \varepsilon^2 E_2 + \dots) (\psi_0(x) + \varepsilon \psi_1(x) + \varepsilon^2 \psi_2(x) + \dots) \end{aligned} \quad (10.1.7)$$

Now we can solve order by order  $\varepsilon$ .

## 10.2 Relativity Begins

So far, we have dealt with non-relativistic quantum mechanics, i.e.,  $v \ll c$ , but relativity is of much importance in quantum mechanics. And since the common notion that quantum mechanics and relativity do not go hand to hand is famous, which is *absolutely* wrong, however, we will see how early physicists (which included Dirac, Feynman and many others like Pauli) developed a relativistic version of quantum mechanics, which initially founded quantum field theory approach to systems.

### 10.2.1 Jumping into it

Now, once we have checked through all preliminary subjects in quantum mechanics non-relativistic-ally, we can introduce a little bit of relativistic physics in

quantum mechanics. Contrary to wide immature belief that quantum mechanics and “Relativity” never go along, we see that it does go along if we are nice to it.

Einstein’s formulated relativity is a two-piece theory of special relativity and general relativity. In what follows from here, we will not talk about the latter as it comes under the scrutiny of quantum gravity. Nonetheless, special relativity is not as sensitive as others with quantum mechanics.

This is the motive so far. First, we need to review some basics of relativistic physics. Relativistic effects are important, and cannot be ignored when we are close to that speed of light. Relativistic effects comes with geometries, which include *metric spaces, tensors, manifolds, etc.* However, we can ignore these at the moment. But it can not be ignored once the treatment of topology becomes relevant.

We will cover up some definitions first. Spatial transformations means transformations along one coordinate, for instance, position. In Relativity, Lorentz transformations become prominent, which is defined as a family of transformations from one frame to another frame. The change of “frame” is necessary as in relativity, two frames are observing different universes.

So, we have a set of coordinates in  $D = 4$  dimensions  $(x, y, z, t)$  where  $x, y, z$  are spatial coordinates and  $t$  is only time coordinates. Each of them are one of the four dimensions.

When one wishes to go to  $(x', y', z', t')$  frame from  $(x, y, z, t)$ , one can do the following transformations. These are called Lorentz Transformations.

$$\begin{aligned}x' &= \gamma(x - vt) \\y' &= y \\z' &= z \\t' &= \gamma\left(t - \frac{vx}{c^2}\right)\end{aligned}\tag{10.2.1}$$

And a simple spatial transformation is

$$x' \rightarrow \epsilon x.\tag{10.2.2}$$

When we group together the spatial and Lorentz transformations we get Poincare transformations. (We can see them also as Groups, however, we refrain of it here.

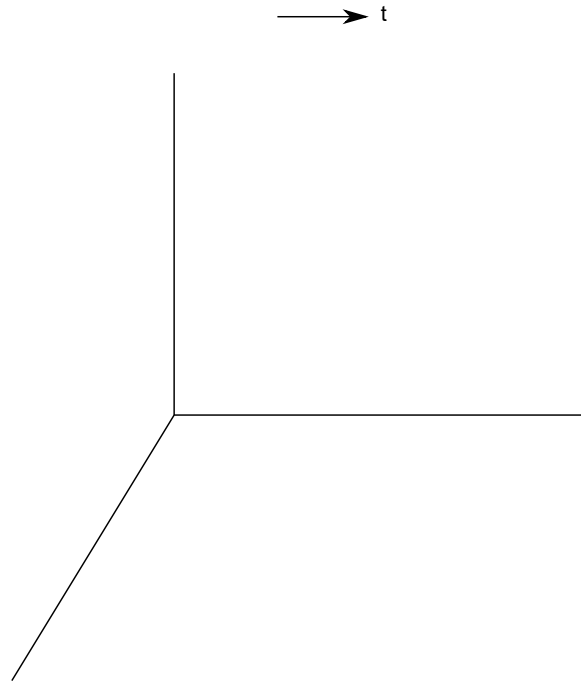


Figure 10.3: xyz-t coordinate frame.  $t$  is always going forward here. The three arrows are for spatial coordinates.

Poincare group would be a large group of all the transformations such as spatial, Lorentz and boosts.)

We do not want to know the physical observation that caused by these relativistic effects. However, they are important too. It is when relativity is inserted into a high-energy region and particularly small-scale important for us now.

Let us define first what are *space-time effects*. The four dimensions that we have specified above constitute space-time. It is seen as a continuous bed-sheet throughout the universe. A location in the space-time is defined by the coordinates (or frames for that matter).

In Relativity, we have a general equation as

$$E^2 = p^2 c^2 + m^2 c^4, \quad (10.2.3)$$

this is called Energy-Momentum relation. So,  $H$  operator can be written as

$$H^2 = \hat{p}^2 c^2 + m^2 c^4, \quad (10.2.4)$$

and this give us Klein-Gordon equation in normal units

$$\left( \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 + \frac{m^2 c^2}{\hbar^2} \right) \psi(t, \mathbf{x}) = 0. \quad (10.2.5)$$

One can now extract the wave function  $\psi$ . Note that it would be a scalar. Reader should also note that in Eq. (10.2.3), there are two solutions, i.e. positive energy and negative energy. While writing the Dirac equation, which is different than Klein-Gordon and relativistic worked by Paul Dirac, these negative energies corresponds to “anti-particles” and their corresponding anti-wave functions. Dirac believed them to be coming from sea and called it “hole theory”. However, explaining these are beyond this book’s objectives.

We do relativity with some geometry and notations. One of them is *four – vector* notation. Such a vector is representative by  $a^\mu$  where  $\mu = 0, 1, 2, 3$ . We assume<sup>1</sup> that 0 corresponds to  $t$  and 1, 2, 3 corresponds to  $x, y, z$  respectively. Hence  $a^0$  is time-like part of the vector and  $a^{x,y,z}$  are space-like dimensions. We also focus on the geometry, for instance, the metric.

Gravity in relativity is seen as an effect of space-time. Riemann had the idea that gravity was, indeed, an effect of space. But, only after the coupling of space-time was initialized, it was found by Einstein and other mathematicians that gravity was an effect of bending in space-time. There are more effective ideas and constructive thoughts in relativity, and we refer the reader to a specific book on relativity to learn more.

### 10.3 Quantum Gravity

It is so ambitious to include a section of ‘quantum gravity in this book. Since it is a very advanced and still on-work work. Quantum gravity is a theory that

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<sup>1</sup>It is a convention and can be changed.

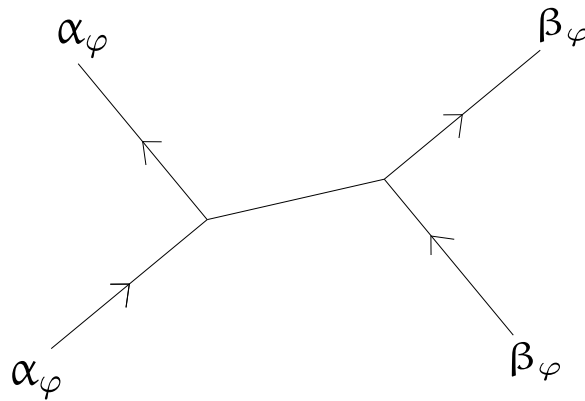


Figure 10.4: A simple Feynman diagram of two scalar scattering. Each particle here has a world-line which has history of that particle.

quantifies gravity at a level where our usual quantum mechanics works. Such kinds of quantization are not possible by a mere ‘quantization process’ that is explained in Appendix B.

The most promising and eloquent theory is “String Theory”. We can not sum up the theory here. The reader must be familiar with quantum field theory, supersymmetry, and relativity (not to mention other mathematical methods) before reading string theory (and superstrings).

In short, our world is made from particles. (We learn about particles, their interactions and amplitudes in high energy physics and particle physics.) These particles interact with each other and hence unfolding a plethora of events. We can draw these interactions (or events) using Feynman diagrams. In string theory, we, somewhat, replace these particles with small *strings*. The way these strings behave determines the matter. It is a hard intuition. These strings can be either open or closed. Strings can do what particles can, they can interact with each other and we can write the string amplitudes for it. (An amplitude is generally a matrix of the interaction.)

In string theory, gravity is inevitable. Since it has gravitons in it and gravitons indicate the presence of gravity. There are, of course, more ways to check gravity. There is not just ‘one’ string theory. String theory has many variations depending on boundary conditions, group theory that represents it, number of supercharges it

has, and number of dimensions present. In a naive sense, we can categorize them into five theories<sup>2</sup>.

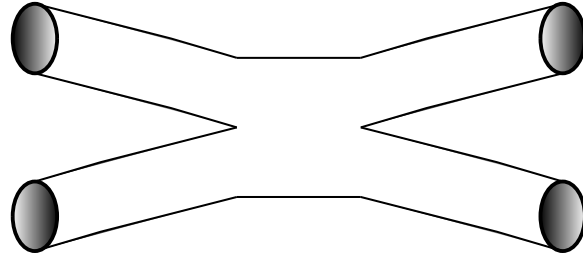


Figure 10.5: A string diagram. Worldlines are replaced with worldsheet.

But it seems that these kind of string theories require supersymmetry<sup>3</sup>, that we have not found yet. But we believe that we will in near future. It also requires the space-time dimensions to be 26, 11, 10 and so on. Despite all these, the theory is beautiful and is convincing. The theoretical beauty has initiated a lot of other physical researches.

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<sup>2</sup>These are the type I theories, type IIA, type IIB theories,  $E_8 \times E_8$  heterotic theory, and  $SO(32)$  theory. Each of these is equivalent to each other by string dualities.

<sup>3</sup>Supersymmetry is a symmetry of particles. It tells us that fermions and bosons, the two possible configuration of statistics in particles, are connected with other each.



# Appendix A

## Lagrangian and Instantons

Instantons are general solutions for non-perturbative system<sup>1</sup>. Actually, they are solution to Euler-Lagrange equations in Euclidean space-time. Firstly, a Euler-Lagrange equation is of kind

$$\frac{\partial \mathcal{L}}{\partial f_i} - \frac{d}{dx} \left( \frac{\partial \mathcal{L}}{\partial f'_i} \right) = 0, \quad (\text{A.0.1})$$

where  $f$  is some function<sup>2</sup>. We solve the differential equation and then we get an equation which, sometimes, is sufficient to know much about the field. In order to learn about that, we need to understand  $\mathcal{L}$  which is called Lagrangian of a system. Generally, it is

$$\mathcal{L} = \frac{1}{2} m \dot{x}^2 - V(x), \quad (\text{A.0.2})$$

where  $V(x)$  is potential of the system and first term is usual kinetic energy. ( $\mathcal{L}$  is different than  $H$  in terms of a minus sign.) Technically,  $\mathcal{L}$  is Lagrangian density,  $L$  is the Lagrangian

$$L = \int \mathcal{L} dx, \quad (\text{A.0.3})$$

---

<sup>1</sup>Non-perturbative system are those system where there is not any inclusion of outside energy. While perturbative system has perturbation, i.e, deviation

<sup>2</sup>In most of the quantum cases, the function is of momentum.

and an action (which encodes basically every thing about the system) is

$$S = \int L dt = \int \int \mathcal{L} dx dt, \quad (\text{A.0.4})$$

and A.0.1 is giving us equation of motion for system of Lagrangian  $\mathcal{L}$ . In simple words, (A.0.1) is just a sophisticated version of  $F = ma$ . We can now write the path integral, which is basically functional integral of the path  $x(t)$ . We can write these path integrals as

$$U = \int [Dx] e^{iS/\hbar}. \quad (\text{A.0.5})$$

Euclidean space-time is a little different than Minkowski space. In Euclidean space time, we do

$$t \rightarrow -i\tau \quad (\text{A.0.6})$$

where  $\tau$  is imaginary time. This is called Euclidean transformation. Under this transformation

$$\mathcal{L} \rightarrow \mathcal{L}_E, \quad (\text{A.0.7})$$

where  $E$  subscript represent Euclidean-ness of the  $\mathcal{L}$  (Euclidean Lagrangian). Under (A.0.6), Eq (A.0.2) changes to

$$\mathcal{L}_E = \frac{m}{2} \left( \frac{dx}{d\tau} \right)^2 + V(x). \quad (\text{A.0.8})$$

The difference is the minus sign which is turning upside down the potential. This is consequence of Euclidean equations of motion. So,

$$S_E = \int \mathcal{L}_E d\tau, \quad (\text{A.0.9})$$

this is Euclidean action.

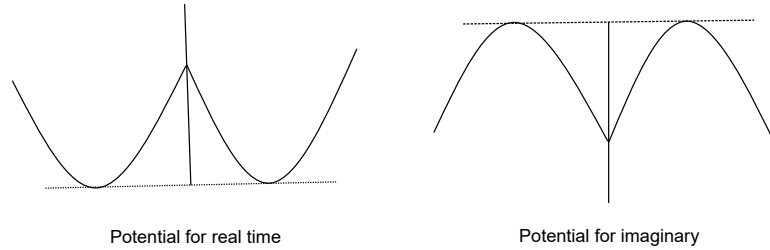


Figure A.1: Potential with minima at  $x = \pm$  gets inverted in imaginary time. This is related to a concept called “Tunneling”.

# Appendix B

## Quantum Field Theory

Quantum field theory (QFT) is not something which can be summarized in one appendix chapter. However, we try to introduce few things about QFTs to the reader.

The idea of field theories is a holistic approach that has its roots in many physics, to name two; high energy physics, and condensed matter physics. However, the latter one uses a slightly different field theory strategy compared to high energy physics, which we will discuss somewhere below. One striking and most important similarity between Quantum Field Theory (QFT) and Statistical Field Theory (SFT) is Renormalization Group. Furthermore, when we have a  $\mathcal{H}$ , a Hilbert space, we can try to generalize the properties of it using ordinary quantum mechanics briefly. But to learn about the fields, which is a broader perspective to understand the physics of a particular regime, we need to consider the theory which will allude us to talk about the generalization of free and interacting models of that regime. So, that is why we speak of field theory in general.

Generally, a field theory is not quantized until it is made because roughly any field theory is an infant classical theory. Some classical field theories, for instance, Einstein's Gravity, face inconsistencies and constraints when we try to quantize them using regular quantization (however, there are some ways to quantize gravity, in string theory, which is a question and part of Quantum Gravity). Some field theories are easily quantized; an elementary example is classical scalar field

theory, which we will denote as  $\phi$ . This scalar field theory for some time will entertain us. In what follows,  $\phi$  is a free field, excluded from any kind of external perturbation and interactions, except in one example it will be otherwise.

Any field theory, take Newton's field, we have some equations of motion describing the field. For a classical version of field theory we can write those equations using "*Hamilton Mechanics*". And for a quantum version, we use "*Lagrangian Mechanics*" (or action). Both are extremely powerful tools. So, how can we write a linear classical theory of  $\phi$  with some mass " $m$ "? For such, we write the Lagrangian (or action)

$$\mathcal{L} = -\frac{1}{2} (-\eta^{\mu\nu} \partial_\mu \partial_\nu \phi + m^2 \phi^2) \quad (\text{B.0.1})$$

where we work in  $(+ - - -)$  signature<sup>1</sup>,  $\partial_\mu = \frac{\partial}{\partial x^\mu}$  and  $\partial^2 = \partial_\mu \partial^\mu$ . It is explicitly mentioned in Lagrangian (B.0.1) that it is a relativistic theory. We can now write the Klein-Gordon equation<sup>2</sup> related to  $\phi$  using "Euler-Lagrange Equation"

$$\eta^{\mu\nu} \partial_\mu \partial_\nu \phi + m^2 \phi = 0. \quad (\text{B.0.2})$$

The Euler-Lagrange equation is a differential equation (much like the Schrödinger equation but more powerful), we write them naively as

$$\frac{\partial \mathcal{L}}{\partial f_i} - \frac{d}{dx} \left( \frac{\partial \mathcal{L}}{\partial f'_i} \right) = 0, \quad (\text{B.0.3})$$

where  $f$  is some function<sup>3</sup>. We solve the differential equation (B.0.3), and then we get an equation which, sometimes, is sufficient to know much about the field. (B.0.2) is a classical solution, and we want to know the quantum properties of the  $\phi$ . There where the "quantization" comes. Quantizing fields go back to electrodynamics. A very successful model of quantization of classical field, at that time, was only "Quantum Electrodynamics" (QED). Quantization can be thought of in mainly two ways: Canonical Quantization and Path Integral Quantization. Both are important ways for quantization. For instance, finding Instantons in quantum

<sup>1</sup>Also  $c = \hbar = 1$ , which are natural units in QFT.

<sup>2</sup>This is a classical solution (??), however, we can say it is a Klein-Gordon equation. But not a *wave* equation. For that, we need to quantize  $\phi$  and then use Euler-Lagrange equation.

<sup>3</sup>In most of the quantum cases, the function is of canonical variables.

theories can be done using path integral approaches, and most of the fields can be easily quantized using canonical variable and oscillators setup. String models, a very proclaimed theory for quantum gravity, can also be quantized in both ways<sup>4</sup>.

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<sup>4</sup>Path integral approach will be replaced by Polyakov integral, a good discussion can be found in.



# Appendix C

## Particle Physics

In this appendix, we will discuss few particle physics. However, we repeat, it is a vast subject and should be taken *more* seriously and comprehensively. In particle physics, we deal with matter and forces. The forces are electromagnetism, weak and strong forces. We do not take gravity here, since that becomes a part of quantum gravity. We do not study quantum gravity in particle physics as so far. The matter, we say, are consists fermions. These fermions can later be categorized into hadrons and leptons. Fermions are *half integer* spins particles. Some fermions are electron, proton, pi-meson, neutron. All these particles create a perfect model that describe the universe called “Standard model”.

Electron is a lepton. Proton, neutron and pi-mesons are hadrons. Leptons are fundamental particles but hadrons are not. The latter are made up of quarks. There are six types of quarks - up, down, top, bottom, strange and charm. When these quarks assemble themselves in certain manner, they form hadrons.





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