Introduction to Wave Mechanics

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Chapter 1

Motivation, Motivation, Motivation .....

In these notes we will develop a theory, which is deeply rooted in experiment and can only be understood using a new mathematical language. It not only describes how nature works in all microscopic physical systems, but also in macroscopic physical systems.

It is most important, however, when the characteristic length scale of the physical system is smaller than $10^{-4}\,m$.

This theory is called **quantum mechanics**.

The physical world we will discover in our studies is a strange and fascinating place where nature operates in a way that seems to defy the intuition we have built up living among macroscopic systems. We will not endeavor to explain why nature works in this particular way since it is my strong belief, as we will see in this book, that it is not possible to do so within the context of this theory. We will, however, be able to correctly predict the outcomes of an amazingly wide range of experiments in many different fields of physics, chemistry and biology.

Let me emphasize my strong belief that theories in physics should only endeavor to make predictions about experimental measurements and not attempt to provide reasons for *why* nature works in these particular ways, that is, why we must choose to start with certain postulates.

Feynman put it best.....

> We know how the electrons and light behave. But what can I call it? If I say they behave like particles I give the wrong impression; also if I say they behave like waves. They behave in their own inimitable way, which technically could be called a quantum mechanical way. They behave in a way that is like nothing that you

> have seen before. Your experience with things that you have seen before is incomplete. The behavior of things on a very small scale is simply different. An atom does not behave like a miniature representation of the solar system with little planets going around in orbits. Nor does it appear like a cloud or fog of some sort surrounding the nucleus. It behaves like nothing you have ever seen before.
>
> There is one simplification at least. Electrons behave in this respect exactly the same way as photons; they are both screwy, but in exactly the same way.
>
> The difficulty really is psychological and exists in the perpetual torment that results from your saying to yourself "but how can it really be like that?", which is a reflection of an uncontrolled but vain desire to see it in terms of something familiar. I will not describe it in terms of an analogy with something familiar; I will simply describe it...
>
> I am going to tell you what nature behaves like. If you will simply admit that maybe she does behave like this, you will find her a delightful and entrancing thing. Do not keep saying to yourself, if you can avoid it, Õ but how can it really be like that?" because you will get "down the drain", into a blind alley from which nobody has yet escaped.
>
> Nobody knows how it can be like that.

and we can add an addendum .....

> and "nobody knows why it is like that"

We will not be able to reduce the quantum universe to everyday ways of thinking(usually called *common sense*). In fact, in order to understand the ideas and implications of the theory we will have to adjust all of our ways of thinking at the most fundamental level.

Imagine, for a moment, that you are attempting to understand a new culture. If you are serious about it, the first thing you would do is to learn the language appropriate to that culture so that you can put your experiences in the proper context. Understanding the universe of quantum phenomena is much like a understanding a new culture where the appropriate language is mathematics and the experiences we are attempting to put into context are experiments.

As we shall see, we will have to use a mathematical language to describe the

quantum world since ordinary language, which was developed to explain everyday occurrences(experiments on macroscopic objects), will turn out to be totally inadequate.

Since it makes no sense to attempt any understanding of the nature of quantum phenomena without first learning to speak and use the language of the quantum world, we will spend the first several chapters of this book learning the appropriate mathematics, in particular, the subject of linear vector spaces.

The adjustment of our ways of thinking at the fundamental level that will be needed is not simply a mathematical matter, however. The development of the necessary mathematical language will not come into conflict with our everyday modes of thinking in any major way. Although, the mathematics of linear vector spaces is very elegant, you will be able to understand it without much difficulty and without having your basic view of the world changed at any fundamental level.

You will be troubled, however, when we apply the mathematics to physical systems that develop according to quantum ideas. We will attach physical meaning to the mathematical formalism in ways that will conflict with your well-developed views(I will call these classical views) about how the world works.

After studying wave mechanics in these notes, we will rethink(more advanced notes covering full quantum thoery) the mathematics and the quantum theory using the Dirac language, which, as we shall see, incorporates the very nature of the quantum world in an intrinsic and natural way. Since we are attempting to develop a physical theory, we will link all the mathematical concepts that we introduce to physical concepts as we proceed.

Dirac was able to link the physical structure of quantum mechanics with the mathematical structure in a unique way. His mathematical language incorporates the physical meaning directly into the formalism and the calculational methods. The language explicitly exhibits the physics and clearly exposes the internal logic of quantum mechanics. Once we understand the language, every equation will directly convey its physical meaning without the need for further explanation or any need for inadequate models.

It is very important to understand that the Dirac language is not simply a new notation for quantum mechanics(as many physicists seem to think). It is a way of thinking about quantum mechanics. It will allow us to use the physical ideas of quantum mechanics to develop the appropriate mathematical language rather than the other way around. This will allow the very mathematical quantum theory to be more closely connected to experiment than any other physical theory.

These statements about the importance of understanding the mathematical language appropriate to the physics under consideration do not only apply to the

quantum world. It is true for all areas of physics and other sciences. One should always learn the appropriate language before studying any field that relies on that language for its understanding.

As I stated above, these notes will cover various aspects of the **original** formulations of quantum mechanics. We will concentrate on the development of the theory in terms of the position and the momentum, namely, wave mechanics.

1.1. Basic Principles and Concepts of Quantum Theory

There are many equivalent formulations of quantum mechanics, namely,

1. Schrodinger wave mechanics
2. Heisenberg matrix mechanics

Dirac developed a general formalism for the quantum theory, which includes wave mechanics, matrix mechanics, and other formulations as special cases. We shall first develop Schrodinger wave mechanics and then generalize it to the Dirac formalism, which is very abstract, in later chapters of this book.

In these notes, the quantum formalism will be applied mainly to non-relativistic systems ($v \ll c = 3 \times 10^{10}\, cm/s$).

1.1.1. Mathematical Methods

We will have to use various mathematical techniques in order to formulate quantum mechanics and in order to solve the resulting equations. Some of these techniques you have learned in a Mathematical Methods in Physics course, some you have learned in Mathematics courses such as Linear Algebra, and Multivariable Calculus and some we will develop in this book.

The techniques we will need are linear operators in Hilbert space (an extension of linear algebra), partial differential equations, special functions of mathematical physics (Legendre polynomials, spherical harmonics, Bessel functions), Fourier transforms, use of Green's functions, integral equations, contour integration in the complex plane, group theory and group representations, etc. We will cover many of these techniques in detail as we proceed.

As we proceed we will cover many applications of quantum theory to physical systems in the areas of atomic and molecular physics.

We will use the following two definitions:

1. *macroscopic phenomena* - observable with the naked eye or with an ordinary microscope; length scale $\geq 10^{-4}\, cm$(1 micron).

2. *microscopic phenomena* - atomic and subatomic; length scale $\leq 10^{-8}\,cm = 0.1\,nm$.

1.1.2. Classical Concepts

We cannot throw out all of classical physics for it works well when dealing with macroscopic phenomena. Furthermore, quantum theory relies on various formulations of classical physics, namely,

1. Classical mechanics (action principle, Lagrangian formulation, Hamiltonian formulation)
2. Classical electromagnetism (Maxwell's equations, Lorentz force law
3. Thermodynamics and Statistical Mechanics
4. Special Relativity (important when speed comparable to c)

Classical physics accurately describes macroscopic phenomena.

1. Classical mechanics:

$$\begin{aligned} &\vec{p} = linear\ momentum \quad , \quad \vec{p} = m\vec{v} \quad , \quad \text{non-relativistic} \\ &\vec{F} = \frac{d\vec{p}}{dt} \\ &\vec{p} = \frac{m\vec{v}}{\sqrt{1 - \frac{v^2}{c^2}}} \quad , \quad \text{relativistically correct} \end{aligned} \tag{1.1}$$

2. Types of forces and how they are produced:
   (a) Electromagnetism (Maxwell's equations, Lorentz force law)
   (b) Gravitation (Newton's law of gravitation for weak gravitational fields, Einstein's general theory of relativity)
3. Thermodynamics and Statistical Mechanics - describes average properties of systems containing many particles.

There are no logical inconsistencies in classical physics, however, microscopic phenomena do not obey the laws of classical physics.

Quantum physics is the theory describing microscopic phenomena and macroscopic phenomena. It approaches the laws of classical physics for non-quantum macroscopic phenomena.

1. Quantum mechanics - gives the equations of motion for a system (new non-classical concepts are needed).
2. Types of interactions among microscopic particles:

(a) range of interaction extends to macroscopic distances
   i. electromagnetism
   ii. gravitation

(b) interactions that are negligible at macroscopic distances or they act only when particles are microscopically separated
   i. strong interactions (holds the protons and neutrons of a nucleus together)
   ii. weak interactions (responsible for the beta-decay of nuclei)

These are the only interactions known today. In the 1970s electromagnetism and weak interactions were unified into the electroweak interactions. In the 1980s, the electroweak interaction and the strong interaction were unified as part of the standard model.

3. Quantum Statistical Mechanics - approaches classical statistical mechanics at sufficiently high temperatures.

1.1.3. The Fundamental Principle of Quantum Mechanics

To introduce this principle, let us consider the experimentally observed alpha-decay of certain nuclei. We crudely describe an atom in this way:

1. radius of volume occupied by *orbiting* electrons = $10^{-8}\,cm$
2. radius of volume occupied by nucleus = $10^{-13}\,cm$

where $1 = 10^{-8}\,cm$ and $1\ fermi = 10^{-13}\,cm$.

As we shall see, we have no idea what is meant by the words *orbiting* in this context. Such occurrences will be in *emphasis font*.

The nucleus contains nucleons (protons and neutrons) bound together by the strong interaction, which overcomes the electrostatic repulsion of the protons (the gravitational attraction is negligible).

We also have the following data and definitions:

electron charge = $-1.60 \times 10^{-19}\,coul = -4.80 \times 10^{-10}\,esu$
proton charge = -(electron charge)
neutron charge = 0
electron mass = $9.11 \times 10^{-28}\,gm$
proton mass ≈ neutron mass = $1.67 \times 10^{-24}\,gm$
(the neutron is slightly more massive than the proton)
Z = atomic number of the nucleus = number of protons
  = number of electrons in a neutral atom
A = mass number of the nucleus = number of nucleons

Notation:

$$_Z\,(chemical\,symbol)^A \leftrightarrow {}_{92}U^{232} = uranium\,232 \leftrightarrow {}_{90}U^{228} = thorium\,228$$

An α-particle is a helium-4 nucleus or ${}_2He^4$. Certain nuclei spontaneously emit an α-particle (α-decay)

$$_{92}U^{232} \rightarrow {}_{90}Th^{228} + \alpha \leftrightarrow A = 232 = 228 + 4 \leftrightarrow Z = 92 = 90 + 2 \qquad (1.2)$$

or we have the setup shown in Figure 1.1 below.

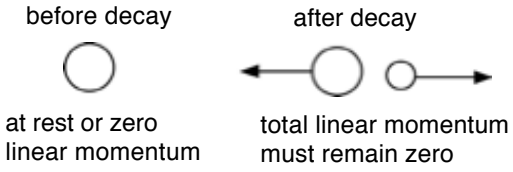


Figure 1.1: Decay Picture 1

Experimental Observation: Let N_0 (very large number $\approx 10^{23}$) identical U^{235} nuclei be observed at $t = 0$. Then, the α-decays of these nuclei will *not* occur at the same time. Furthermore, the alpha particles emitted in the decays will *not* go in the same direction as in Figure 1.2 below.

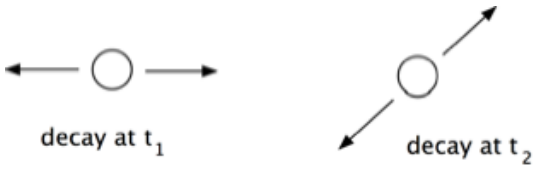


Figure 1.2: Decay Picture 2

Let $N(t)$ be the number of U^{235} nuclei (not yet decayed) present at time t. It is observed that

$$N(t) = N_0 e^{-\gamma t} \quad , \quad \gamma = \text{ constant(dimensions } 1/\text{time)} \qquad (1.3)$$

as shown in Figure 1.3 below.

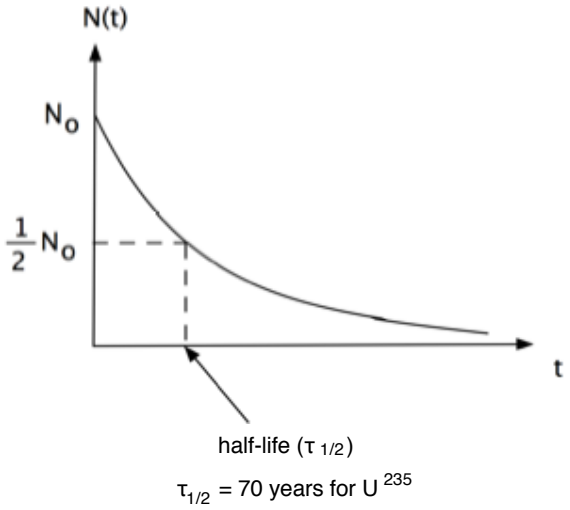


Figure 1.3: Decay Data

Therefore,

$$\frac{dN(t)}{dt} = -\gamma N_0 e^{-\gamma t} = -\gamma N(t) \tag{1.4}$$

$$\frac{(-dN)}{N} = \gamma dt \tag{1.5}$$

$$\rightarrow \frac{\#\text{ decays in dt}}{\#\text{ present at time t}}$$

$$= \text{ probability of a decay between t and t + dt}$$

Therefore, γ = probability of decay per unit time. Note that

$$N(\tau_{1/2}) = \frac{N_0}{2} = N_0 e^{-\gamma \tau_{1/2}} \tag{1.6}$$

$$\Rightarrow \frac{1}{2} = e^{-\gamma \tau_{1/2}} \Rightarrow \tau_{1/2} = \frac{\ell n(2)}{\gamma} \tag{1.7}$$

Thus, systems in the *same* initial state will, in general, develop differently in time, that is, U^{235} nuclei live for different lengths of time. Since the initial states are *identical* (there does not exist any way to distinguish the initial states), it is impossible to predict when a given nucleus will decay.

However, there does exist a definite probability of a decay per unit time. This means that we should be able to predict how many decays will occur in a given time interval when we observe a sample of many U^{235} nuclei.

This decay process may be viewed in another way. Before the decay, the

α–particle is *located* in the U^{235} nucleus. After the decay, the α–particle is separated from the residual nucleus and is traveling in a certain direction. It is impossible to predict the α–particle's position (*inside* U^{235} or separated from Th^{228} as a function of time, and it is impossible to predict the α–particle's velocity direction as a function of time. One may only hope to find the *probability* that the α–particle will be at a given position at a given time and the *probability* that the α–particle will be traveling at a given velocity at a given time.

This leads us to the **Basic Principle of Quantum Mechanics**:

> One can only predict the *probability* of finding a particle at a given position at a given time and the *probability* of finding a particle with given momentum (momentum is easier to deal with than velocity) at a given time. The result of measuring a given particle's position or momentum at a certain time cannot be predicted in general - only the results of measuring the position or momentum of many *identically-prepared* particles at a certain time can be predicted.

Note that this is contrary to the *Classical Doctrine*, which states that a particle's position and momentum at any time is *completely determined* by the particle's initial state (specified by the initial position and momentum). In quantum mechanics, a complete specification of the particle's initial state (we will discuss later exactly what must be given for a complete quantum mechanical specification of a state) does not determine a particle's position and momentum at all later times - only the probability that the particle will have a certain position and momentum can be predicted for observations made at later times.

Note (1): You might argue that if the U^{235} nuclei (which we have stated to be in identical initial states so that there does not exist any way to distinguish the states) decay at different times, then there *must* be some difference in the initial states. You might argue that there exists some *hidden variable* (which we have not as yet succeeded in determining) which has different values in the different nuclei and which determine when a given nucleus will decay. This certainly a possibility. However, no one has ever found such a variable so that the time at which the decay will occur can be predicted with certainty. In these notes, we will take the point of view (standard quantum theory) that such hidden variables do not exist. In fact, there now exists much experimental evidence that hidden variables cannot exist (more about this later).

Note (2): How does classical physics fit into this description? How is classical determinism (observed in macroscopic phenomena) compatible with this prob-

abilistic interpretation of nature? This is easy to deal with. For *macroscopic objects*, the *probability of observing the classical trajectory (position and momentum as a function of time) to an accuracy of better than* $\approx 10^{-4}\,cm$ *is almost unity (negligible uncertainty).* This is known as the *Correspondence Principle*, which implies that quantum physics approaches classical physics for macroscopic objects (more about this later).

The central problem in quantum mechanics is therefore the following:

> Given a particle with known interactions: in terms of the initial state of the particle, find the probability of observing the particle at a given position as a function of time and find the probability of observing the particle with a given momentum as a function of time.

Before giving rules for determining these probabilities for physical systems, let us review some simple probability concepts.

1.2. Simple Ideas about Probability

1.2.1. Discrete Distributions

Let a variable take on certain discrete values $u_1, u_2, u_3, \ldots$. Suppose N measurements of the variable are made. Let N_i = of measurements in which the result u_i was obtained.

1.2.1.1. Definition

The probability of observing u_i is

$$\wp(u_i) = \frac{N_i}{N} \tag{1.8}$$

in the limit as $N \to \infty$ (N_i also $\to \infty$ unless $wp(u_i) = 0$). We must also have $\wp(u_i) \geq 0$.

The probability of observing u_k *or* u_{k+1} *or* ..... *or* $u_{k+\ell} = \sum_{i=k}^{k+\ell} \wp(u_i)$. The probability of observing *some* value is given by

$$\sum_{all\ i} \wp(u_i) = \sum_{all\ i} \frac{N_i}{N} = \frac{1}{N} \sum_{all\ i} N_i = \frac{N}{N} = 1 \tag{1.9}$$

which is called the *normalization condition.*

1.2.2. Continuous Distributions

Let the variable u be capable of taking on any value in the interval $[a, b]$. Suppose N measurements of the variable are made. Let $dN(u)$ = # of measurements in which the variable was in the interval $[u, u + du]$. $dN(u)$ is *not* meant to represent the differential of some function $N(u)$.

1.2.2.1. Definition

The probability of observing the variable in the interval $[u, u + du]$ is given by

$$\lim_{N\to\infty} \wp(u)du = \frac{dN(u)}{N} \tag{1.10}$$

$$\wp(u) = \frac{\text{probability}}{\text{unit interval of } u} = \text{ probability density} \tag{1.11}$$

The probability of measuring u in the interval $[u_1, u_2]$ is

$$prob\,([u_1, u_2]) = \int_{u_1}^{u_2} \wp(u)du \tag{1.12}$$

Since all measurements yield values in $[a, b]$, we have the normalization condition

$$\int_a^b \wp(u)du = 1 \tag{1.13}$$

1.2.2.2. Example A

It is equally probable to measure u anywhere in the interval $[0, a]$. Therefore,

$$\wp(u)du = Adu \quad \text{for } u \in [0, a] \quad , \quad A = \text{ constant}$$

But

$$\int_0^a \wp(u)du = 1 = A\int_0^a du = Aa \to A = \frac{1}{a} \to \wp(u) = \frac{1}{a}\ for\ u \in [0, a]$$

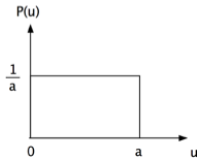


Figure 1.4: Example A Probability Distribution

1.2.2.3. Example B

Consider the Gaussian distribution in the interval ($u \in [-\infty, \infty]$) given by

$$\wp(u) = Ae^{-(u-u_0)^2/2\sigma^2} \tag{1.14}$$

where u_0, σ, A are constants and $\sigma > 0$. This looks like Figure 1.5 below.

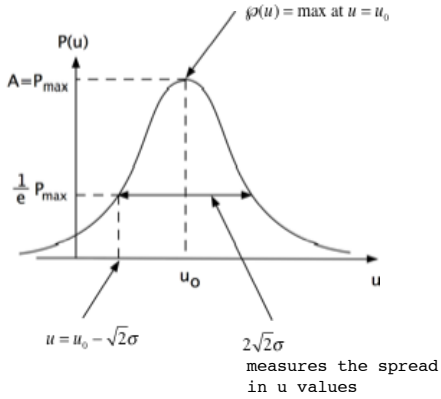


Figure 1.5: Example B Probability Distribution

We then have

$$\int_{-\infty}^{\infty} \wp(u)du = 1 = A\int_{-\infty}^{\infty} e^{-(u-u_0)^2/2\sigma^2}du \tag{1.15}$$

If we let

$$v = \frac{u-u_0}{\sqrt{2}\sigma} \rightarrow dv = \frac{du}{\sqrt{2}\sigma} \tag{1.16}$$

we get

$$1 = A\sigma\sqrt{2}\int_{-\infty}^{\infty} e^{-v^2}dv \tag{1.17}$$

Trick for doing the integral:

$$\begin{aligned}\left(\int_{-\infty}^{\infty} e^{-v^2}dv\right)^2 &= \int_{-\infty}^{\infty} e^{-x^2}dx\int_{-\infty}^{\infty} e^{-y^2}dy = \int_{-\infty}^{\infty} dx\int_{-\infty}^{\infty} dy e^{-(x^2+y^2)} \\ &= \int_0^{\infty} 2\pi r e^{-r^2}dr = -\pi\int_0^{\infty} d(e^{-r^2}) = \pi \\ &\Rightarrow \int_{-\infty}^{\infty} e^{-v^2}dv = \sqrt{\pi}\end{aligned} \tag{1.18}$$

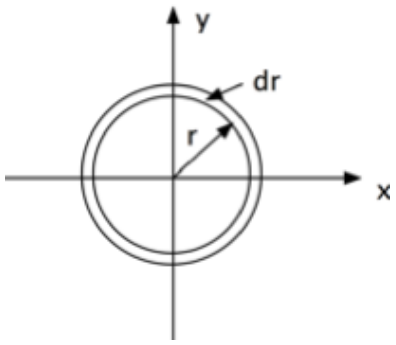


Figure 1.6: Integration Region

where we have done the integral by integrating over the entire $x-y$ plane using circular rings $r^2 = x^2 + y^2$ as shown in Figure 1.6 below:

Therefore,

$$1 = A\sigma\sqrt{2\pi} \rightarrow A = \frac{1}{\sqrt{2\pi}\sigma} \tag{1.19}$$

$$\wp(u) = \frac{1}{\sqrt{2\pi}\sigma} e^{-(u-u_0)^2/2\sigma^2} \tag{1.20}$$

The probability of measuring u between a and b is

$$\int_a^b \wp(u)du = \text{ area under Gaussian curve between a and b} \tag{1.21}$$

This can be evaluated numerically.

We now return to considerations of general distributions $\wp(u)$.

1.2.2.4. Definition

The average value (or expectation value) of $u = \langle u \rangle$:

Discrete	Continuous
$\langle u \rangle = \frac{1}{N} \sum_{all\ i} u_i N_i = \sum_{all\ i} u_i \wp(u_i)$	$\langle u \rangle = \frac{1}{N} \int_{all\ u} u dN(u) = \int_{all\ u} u\wp(u)du$

In general, the *average value* (*expectation value*) of some function of u, $f(u)$, is given by

Discrete	Continuous
$\langle f(u) \rangle = \sum_{all\ i} f(u_i)\wp(u_i)$	$\langle f(u) \rangle = \int_{all\ u} f(u)\wp(u)du$

The values measured for u will, of course, not all be equal to $\langle u \rangle$. One would like a measure of the spread in observed u values around $\langle u \rangle$. Such a measure is the *root-mean-square (rms)* or *standard* deviation given by

$$\begin{aligned}\Delta u &= \sqrt{\langle (u - \langle u \rangle)^2 \rangle} \\ &\Rightarrow (\Delta u)^2 = \left\langle u^2 \right\rangle - 2 \langle (u \langle u \rangle \rangle + \left\langle \langle u \rangle^2 \right\rangle - \left\langle u^2 \right\rangle - \langle u \rangle^2\end{aligned}$$

Clearly, if $\Delta u = 0$, then the only value measurements of u will yield is $u = \langle u \rangle$ since we have

$$(\Delta u)^2 = \left\langle (u - \langle u \rangle)^2 \right\rangle = \sum_i \wp(u_i) (u_i - \langle u \rangle)^2 = 0$$

which, because every term in the sum is positive, says that $u_i = \langle u \rangle$ for all i.

1.2.2.5. Example A

Equally probable anywhere in $[0, a]$.

$$\begin{aligned}&\wp(u) = \frac{1}{a} \; for \; u \in [0, a] \quad , \quad \wp(u) = 0 \; elsewhere \\ &\langle u \rangle = \int_0^a u \frac{1}{a} du = \frac{a}{2} \quad , \quad \left\langle u^2 \right\rangle = \int_0^a u^2 \frac{1}{a} du = \frac{a^2}{3} \\ &\Delta u = \sqrt{\langle u^2 \rangle - \langle u \rangle^2} = \frac{a}{\sqrt{12}}\end{aligned}$$

1.2.2.6. Example B

Gaussian distribution.

$$\begin{aligned}\langle u \rangle &= \int_{-\infty}^{\infty} u \frac{1}{\sqrt{2\pi}\sigma} e^{-(u-u_0)^2/2\sigma^2} du = \int_{-\infty}^{\infty} (v + u_0) \frac{1}{\sqrt{2\pi}\sigma} e^{-v^2/2\sigma^2} dv \\ &= \int_{-\infty}^{\infty} v \frac{1}{\sqrt{2\pi}\sigma} e^{-v^2/2\sigma^2} dv + u_0 \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}\sigma} e^{-v^2/2\sigma^2} dv = 0 + u_0 = u_0 \\ (\Delta u)^2 &= \int_{-\infty}^{\infty} (u - u_0)^2 \frac{1}{\sqrt{2\pi}\sigma} e^{-(u-u_0)^2/2\sigma^2} du = \int_{-\infty}^{\infty} v^2 \frac{1}{\sqrt{2\pi}\sigma} e^{-v^2/2\sigma^2} dv \\ &= \frac{2\sigma^2}{\sqrt{\pi}} \int_{-\infty}^{\infty} w^2 e^{-w^2} dw\end{aligned}$$

Another trick:

$$I = \int_{-\infty}^{\infty} e^{-\lambda w^2} dw = \frac{1}{\sqrt{\lambda}} \int_{-\infty}^{\infty} e^{-u^2} du = \frac{\sqrt{\pi}}{\sqrt{\lambda}}$$

$$\frac{dI}{d\lambda} = -\frac{1}{2}\frac{\sqrt{\pi}}{\lambda^{3/2}} = \int_{-\infty}^{\infty} \frac{d}{d\lambda} e^{-\lambda w^2} dw = -\int_{-\infty}^{\infty} w^2 e^{-\lambda w^2} dw$$

$$\int_{-\infty}^{\infty} w^2 e^{-\lambda w^2} dw = \frac{1}{2}\frac{\sqrt{\pi}}{\lambda^{3/2}}$$

Putting $\lambda = 1$ we get

$$\int_{-\infty}^{\infty} w^2 e^{-w^2} dw = \frac{\sqrt{\pi}}{2} \Rightarrow (\Delta u)^2 = \frac{2\sigma^2}{\sqrt{\pi}} \int_{-\infty}^{\infty} w^2 e^{-w^2} dw = \sigma^2$$

These probability distributions can be generalized to several variables.

In quantum mechanics (where we will focus on one particle systems) we want to find expressions for the following:

1. $\wp(x, y, z; t)d^3x = \wp(x, y, z; t)dxdydz$ = probability of observing particle with coordinates in $(x, x + dx), (y, y + dy), (z, z + dz)$ at time t
2. $\tilde{\wp}(p_x, p_y, p_z; t)d^3p = \tilde{\wp}(p_x, p_y, p_z; t)dp_x dp_y dp_z$ = probability of observing particle with momentum in $(p_x, p_x + dp_x), (p_y, p_y + dp_y), (p_z, p_z + dp_z)$ at time t

Finding these expressions is the central problem of quantum (wave) mechanics.

1.2.2.7. Additional note

We use continuous distributions for definiteness. The n^{th} $(n = 0, 1, 2, 3, \ldots)$ moment of the probability distribution $\wp(u)$ is defined to be

$$\langle u^n \rangle = \int du\, u^n \wp(u) \tag{1.22}$$

1.2.2.8. Theorem (without proof)

If 2 distributions $\wp_1(u)$ and $\wp_2(u)$ have the same moments for all n, then $\wp_1(u) = \wp_2(u)$, that is, the moments uniquely determine the distribution.

Experimental evidence of the so-called Wave-Particle Duality suggests how to calculate these probabilities. This duality refers to the observation that what we usually regard as a wave phenomenon (for example, the propagation of light) sometimes exhibits wave properties and sometimes exhibits particle properties while what we usually regard as a particle(for example, an electron) sometimes exhibits particle properties and sometimes exhibits wave properties!!!

1.2.3. Review of Waves and Diffraction

Let $\vec{x} = (x, y, z), |\vec{x}| = r$ locate a point in space with respect to some origin (position vector) (see Figure 1.7 below). Let $\hat{n}$ = a unit vector ($|\hat{n}| = 1$ pointing in a *fixed* direction. $\hat{n}$ is dimensionless (it has no units). Let $\eta(\vec{x}, t)$ be some physical quantity defined at each point $\vec{x}$ at some time t. We refer to $\eta(\vec{x}, t)$ as a *disturbance*. In this discussion, we will generalize slightly and let $\eta(\vec{x}, t)$ take on complex values. For example, $\eta(\vec{x}, t)$ can refer to one of the Cartesian components of the electric field $\vec{E}(\vec{x}, t)$ or the magnetic field $\vec{B}(\vec{x}, t)$.

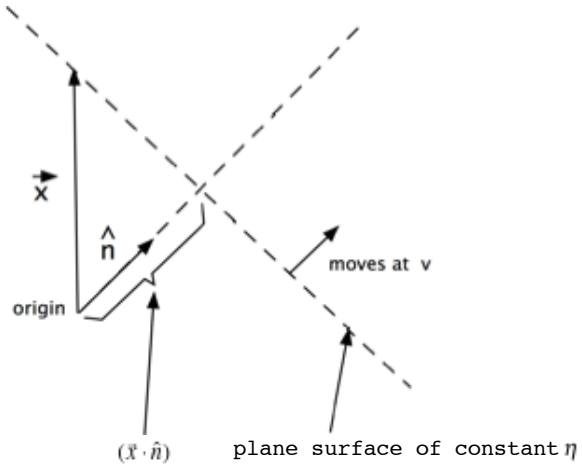


Figure 1.7: Plane Wave Relationships

1.2.3.1. Definition

$\eta(\vec{x}, t)$ is a *plane wave* if it can be written in the form

$$\eta(\vec{x}, t) = F(\vec{x} \cdot \hat{n} - vt) \tag{1.23}$$

where F is some arbitrary function of one variable, where $\hat{n}$ is some fixed unit vector and v = a real constant, $v > 0$. Clearly, v has units

$$\frac{\vec{x} \cdot \hat{n}}{t} \rightarrow \text{ units of velocity} \tag{1.24}$$

Consider the points in space for which $\vec{x} \cdot \hat{n} - vt$ = a constant (η remains constant at these points). Therefore

$$\vec{x} \cdot \hat{n} = \text{ constant } + vt = \text{ projection of } \vec{x} \text{ onto the } \hat{n} \text{ direction} \tag{1.25}$$

This projection moves with constant speed v. All points on the plane perpendicular to $\hat{n}$ have the same value of $\vec{x} \cdot \hat{n}$. These relationships are shown in Figure 1.7 above.

Thus, the surfaces on which $\eta(\vec{x},t)$ has a fixed value are plane surfaces perpendicular to $\hat{n}$ which move at speed v in the $\hat{n}$ direction (hence the name plane wave).

v = phase velocity of the plane wave, i.e., the velocity
of the planes of constant phase$(\vec{x}\cdot\hat{n})$
$\hat{n}$ = direction of propagation

That is what a wave is!!

Now

$$\frac{\partial\eta}{\partial t} = F'\frac{\partial(\vec{x}\cdot\hat{n}-vt)}{\partial t} = -vF'$$

Similarly,

$$\frac{\partial\eta}{\partial x} = F'\frac{\partial(\vec{x}\cdot\hat{n}-vt)}{\partial x} = F'\frac{\partial(xn_x+yn_y+zn_z-vt)}{\partial x} = n_xF'$$
$$\frac{\partial^2\eta}{\partial x^2} = n_xF''\frac{\partial(\vec{x}\cdot\hat{n}-vt)}{\partial x} = n_x^2F''$$

and

$$\frac{\partial^2\eta}{\partial y^2} = n_y^2F'' \quad , \quad \frac{\partial^2\eta}{\partial z^2} = n_z^2F''$$

Therefore,

$$\frac{\partial^2\eta}{\partial x^2}+\frac{\partial^2\eta}{\partial y^2}+\frac{\partial^2\eta}{\partial z^2} = (n_x^2+n_y^2+n_z^2)F'' = (\hat{n}\cdot\hat{n})F'' = F'' = \frac{1}{v^2}\frac{\partial^2\eta}{\partial t^2}$$
$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}-\frac{1}{v^2}\frac{\partial^2}{\partial t^2}\right)\eta = \left(\nabla^2-\frac{1}{v^2}\frac{\partial^2}{\partial t^2}\right)\eta = 0$$

which is the *classical wave equation.* It is obeyed by any plane wave of the form $\eta(\vec{x},t) = F(\vec{x}\cdot\hat{n}-vt)$ where v = phase velocity of the plane wave.

Note that:

1. The classical wave equation is linear, that is, if $\eta_1(\vec{x},t)$ and $\eta_2(\vec{x},t)$ are separately solutions of the wave equation, then any linear superposition (combination)
$$a_1\eta_1(\vec{x},t)+a_2\eta_2(\vec{x},t) \tag{1.26}$$
where a_1 and a_2 are constants, is also a solution.

2. If $\eta(\vec{x},t)$ is a complex solution of the wave equation, then $Real(\eta(\vec{x},t))$ and $Imag(\eta(\vec{x},t))$ separately satisfy the wave equation (because $1/v^2$ is real).

3. The classical wave equation has solutions other than plane wave solutions, for example, the linear superposition of 2 plane waves traveling in different directions

$$\eta(\vec{x},t) = F_1(\vec{x}\cdot\hat{n}_1 - vt) + F_2(\vec{x}\cdot\hat{n}_2 - vt) \tag{1.27}$$

is a solution.

1.2.3.2. Definition

$\eta(\vec{x},t)$ is a *spherical wave* if it can be written in the form

$$\eta(\vec{x},t) = \begin{cases} \frac{1}{r}G(r-vt) & \rightarrow \text{ spherical outgoing wave} \\ \frac{1}{r}G(r+vt) & \rightarrow \text{ spherical incoming wave} \end{cases} \tag{1.28}$$

where, $r = |\vec{x}|$, G is some arbitrary function of one variable and where v is a real constant $(v > 0)$ abd v has dimensions of velocity.

Now consider the points in space for which $r \mp vt =$ constant (G remains constant at these points). We consider $r - vt$ and $r + vt$ as 2 separate cases. Therefore, $r =$ constant $\pm\, vt \rightarrow$ a sphere(centered at $r = 0$ that moves (*outward* or *inward*) with speed v. Thus the constant phase surfaces on which $(\eta(\vec{x},t))$ has a fixed value are spheres (with center at the origin) which move (*outward* or *inward*) with speed v. $v =$ phase velocity of the spherical wave. The $1/r$ factor was used in the definition of $\eta(\vec{x},t)$ so that $\eta(\vec{x},t)$ obeys the classical wave equation for $r \neq 0$.

We prove this as follows. First consider a function $f(r)$. We need to calculate $\nabla^2 f(r)$ where $r = |\vec{x}| = \sqrt{x^2+y^2+z^2}$. We have

$$\begin{aligned} &\frac{\partial r}{\partial x} = \frac{x}{r} \quad , \quad \frac{\partial r}{\partial y} = \frac{y}{r} \quad , \quad \frac{\partial r}{\partial z} = \frac{z}{r} \\ &\frac{\partial f}{\partial x} = \frac{df}{dr}\frac{\partial r}{\partial x} = \frac{df}{dr}\frac{x}{r} \\ &\frac{\partial f}{\partial y} = \frac{df}{dr}\frac{\partial r}{\partial y} = \frac{df}{dr}\frac{y}{r} \\ &\frac{\partial f}{\partial z} = \frac{df}{dr}\frac{\partial r}{\partial z} = \frac{df}{dr}\frac{z}{r} \end{aligned}$$

and

$$\begin{aligned} \frac{\partial^2 f}{\partial x^2} &= \frac{\partial}{\partial x}\left(\frac{df}{dr}\frac{x}{r}\right) = \frac{df}{dr}\frac{1}{r} + x\frac{df}{dr}\frac{\partial}{\partial x}\left(\frac{1}{r}\right) + \frac{\partial}{\partial x}\left(\frac{df}{dr}\right)\frac{x}{r} \\ &= \frac{df}{dr}\frac{1}{r} + x\frac{df}{dr}\frac{\partial}{\partial r}\left(\frac{1}{r}\right)\frac{\partial r}{\partial x} + \frac{x}{r}\frac{\partial}{\partial r}\left(\frac{df}{dr}\right)\frac{\partial r}{\partial x} \\ &= \frac{df}{dr}\frac{1}{r} + x\frac{df}{dr}\left(-\frac{1}{r^2}\right)\frac{x}{r} + \frac{x}{r}\frac{\partial}{\partial r}\left(\frac{d^2 f}{dr^2}\right)\frac{x}{r} \end{aligned}$$

and similarly for $\partial^2 f/\partial y^2$ and $\partial^2 f/\partial z^2$. We then obtain

$$\begin{aligned}\nabla^2 f &= \frac{d^2 f}{dr^2}\left(\frac{x^2}{r^2}+\frac{y^2}{r^2}+\frac{z^2}{r^2}\right)+\frac{df}{dr}\left(\frac{3}{r}-\frac{x^2}{r^3}-\frac{y^2}{r^3}-\frac{z^2}{r^3}\right)\\ &= \frac{d^2 f}{dr^2}+\frac{2}{r}\frac{df}{dr}\end{aligned} \tag{1.29}$$

But

$$\frac{1}{r}\frac{d^2}{dr^2}\left(rf(r)\right) = \frac{1}{r}\frac{d}{dr}\left(f+r\frac{df}{dr}\right) = \frac{1}{r}\left(r\frac{d^2 f}{dr^2}+2\frac{df}{dr}\right) \tag{1.30}$$

Therefore,

$$\nabla^2 f = \frac{1}{r}\frac{d^2}{dr^2}\left(rf(r)\right) \tag{1.31}$$

for $r \neq 0$ since things are not defined at $r = 0$. Now for

$$\eta(\vec{x},t) = \frac{1}{r}G(r \mp vt) \tag{1.32}$$

and

$$\begin{aligned}&\frac{\partial \eta}{\partial t} = \frac{1}{r}G'(\mp v) \rightarrow \frac{\partial^2 \eta}{\partial t^2} = \frac{1}{r}G''(\mp v)^2 = v^2\frac{1}{r}G''\\ &\nabla^2\eta = \frac{1}{r}\frac{\partial^2}{\partial r^2}\left(r\eta(r)\right) = \frac{1}{r}\frac{\partial^2}{\partial r^2}\left(G(r \mp vt)\right) = \frac{1}{r}G''\\ &\nabla^2\eta - \frac{1}{v^2}\frac{\partial^2\eta}{\partial t^2} = 0\end{aligned} \tag{1.33}$$

so that spherical waves also obey the classical wave equation (for $r \neq 0$). The $1/r$ factor is required physically of course to account for the $1/r^2$ decrease in the intensity of the spherical wave with distance.

1.2.3.3. Definition

A function $\eta(\vec{x},t)$ has a *definite frequency* if it is of the form

$$\eta(\vec{x},t) = f_+(\vec{x})e^{i\omega t} + f_-(\vec{x})e^{-i\omega t} \tag{1.34}$$

where $f_\pm(\vec{x})$ are arbitrary functions of $\vec{x}$ and where ω is a real number such that $\omega \geq 0$. ω = an angular frequency. Now

$$e^{\pm i\omega t} = \cos\omega t \pm i\sin\omega t \tag{1.35}$$

so that this $\eta(\vec{x},t)$ is a linear superposition of $\cos\omega t$ and $\sin\omega t$.

In addition, since $e^{\pm 2\pi i} = +1$, at any point $\vec{x}$, this function $\eta(\vec{x},t)$ repeats itself in time after a time interval T (*period* of $\eta(\vec{x},t)$), where $\omega T = 2\pi$ or

$$T = \frac{2\pi}{\omega} \tag{1.36}$$

independent of $\vec{x}$. The *frequency* of $\eta(\vec{x},t)$ is then

$$f = \frac{1}{T} = \frac{\omega}{2\pi} \tag{1.37}$$

1.2.3.4. Plane Wave of Definite Frequency

We have

$$\eta(\vec{x},t) = f_+(\vec{x})e^{i\omega t} + f_-(\vec{x})e^{-i\omega t} = F(\vec{x}\cdot\hat{n} - vt) \tag{1.38}$$

Therefore, we can write

$$f_\pm(\vec{x})e^{\pm i\omega t} = f_\pm(\vec{x})e^{\pm i\frac{\omega}{v}vt} = A_\pm e^{\pm i\frac{\omega}{v}(vt-\vec{x}\cdot\hat{n})} = A_\pm e^{\pm i(\omega t - \frac{\omega}{v}\vec{x}\cdot\hat{n})} \tag{1.39}$$

where $A_\pm$ are constants so that it fits the standard functional form. If we let $\omega/v = k$ and $\vec{k} = k\hat{n}$ = propagation vector so that $\vec{k}$ is parallel to $\hat{n}$ = direction of wave propagation, then

$$\eta(\vec{x},t) = A_+e^{+i(\omega t - \vec{k}\cdot\vec{x})} + A_-e^{-i(\omega t - \vec{k}\cdot\vec{x})} \tag{1.40}$$

Now let $\hat{n} = \hat{z}$ (propagation in the $z-$direction) for definiteness. Therefore,

$$\eta(\vec{x},t) = A_+e^{+i(\omega t - kz)} + A_-e^{-i(\omega t - kz)} \tag{1.41}$$

At a given time, $\eta(\vec{x},t)$ repeats itself in z after a distance λ (wavelength of $\eta(\vec{x},t)$) where $k\lambda = 2\pi$ or

$$k = \frac{2\pi}{\lambda} \quad , \quad \lambda \text{ independent of } t \tag{1.42}$$

Now

$$k = \frac{2\pi}{\lambda} = \frac{\omega}{v} = \frac{2\pi f}{v} \rightarrow \lambda f = v \tag{1.43}$$

or

$$\text{wavelength} \times \text{frequency} = \text{phase velocity} \tag{1.44}$$

Note: $e^{\pm i(\omega t - kz)}$ has *phase* $(\omega t - kz)$. This phase is constant when

$$\omega t - kz = \text{ constant} \tag{1.45}$$

or when

$$z = -\frac{\text{constant}}{k} + \frac{\omega}{k}t = -\frac{\text{constant}}{k} + vt \tag{1.46}$$

Therefore, the planes of constant phase move with velocity $\omega/k = v$ in the $+z$ direction; hence the name phase velocity for v.

1.2.3.5. Spherical Waves of Definite Frequency

Spherical waves of definite frequency are given by

$$\begin{aligned}\eta(\vec{x},t) &= f_+(\vec{x})e^{i\omega t} + f_-(\vec{x})e^{-i\omega t} = \frac{1}{r}G(r \mp vt) \\ &= \frac{1}{r}\left[A_+e^{+i\frac{\omega}{v}(vt\mp r)} + A_-e^{-i\frac{\omega}{v}(vt\mp r)}\right] \\ &= A_+\frac{e^{+i(\omega t \mp kr)}}{r} + A_-\frac{e^{-i(\omega t \mp kr)}}{r}\end{aligned} \tag{1.47}$$

where

$$\frac{\omega}{v} = k = \frac{2\pi}{\lambda} \tag{1.48}$$

as in the plane wave case.

There exists a relationship between plane waves of definite frequency and spherical waves of definite frequency.

Consider the functions defined by the integrals

$$I_{\pm} = \int\limits_{\substack{\text{infinite}\\ \text{plane}}} \mathrm{dA} \frac{e^{\pm ikR}}{R} e^{-\varepsilon R} \qquad \text{(a definition!)} \tag{1.49}$$

where $e^{-\varepsilon R}$ is a *convergence factor* and we will take the limit $\varepsilon \to 0^+$ *after* the integration has been done. If we were to take $\varepsilon \to 0^+$ inside the integral, then $e^{-\varepsilon R} \to 1$ and the resulting integral is undefined or so it seems (as will be seen below).

Since all area elements on the circular ring shown in Figure 1.8 below have the same R

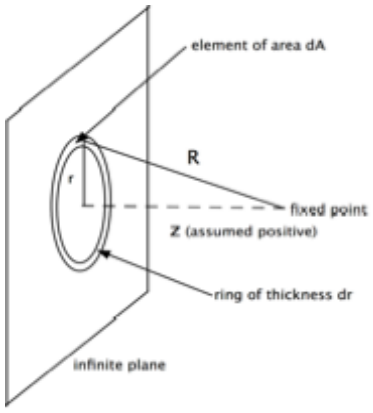


Figure 1.8: Integration Details

we can write (using Figure 1.8)

$$I_{\pm} = \int\limits_{r=0}^{r=\infty} 2\pi r dr \frac{e^{\pm ikR}}{R} e^{-\varepsilon R} \tag{1.50}$$

which is just integrating over the rings.

Now $R = \sqrt{x^2 + y^2}$ with z fixed during the integration. Therefore,

$$dR = \frac{\partial R}{\partial r} dr = \frac{1}{R} r dr \tag{1.51}$$

with R going from $R = z$ (when $r = 0$) to $R = \infty$ (when $r = \infty$). Therefore

$$I_{\pm} = \int_{r=0}^{r=\infty} 2\pi dR e^{(\pm ik - \varepsilon)R} = \frac{2\pi}{\pm ik - \varepsilon} e^{(\pm ik - \varepsilon)R} \Big|_{R=z}^{R=\infty} \tag{1.52}$$

The value at the upper limit vanishes because $e^{\pm ik(\infty)} e^{-\varepsilon(\infty)} = 0$ v for $\varepsilon > 0$. If we had let $\varepsilon = 0$ at the beginning of the calculation, then the value at the upper limit would have been $e^{\pm ik(\infty)}$, which is undefined (it just keeps on oscillating). Thus,

$$I_{\pm} = \lim_{\varepsilon \to 0^+} \frac{2\pi}{\pm ik - \varepsilon} e^{(\pm ik - \varepsilon)z} = \pm \frac{2\pi i}{k} e^{\pm ikz} \tag{1.53}$$

so that we get the amazing result (limit $\varepsilon \to 0^+$ understood)

$$e^{\pm ikz} = \pm \frac{k}{2\pi i} \int_{\substack{\text{infinite} \\ \text{plane}}} \mathrm{dA} \frac{e^{\pm ikR}}{R} e^{-\varepsilon R} \tag{1.54}$$

where R = distance from dA to a fixed point located a distance z from the plane. This then implies that

$$\begin{aligned} & C_+ e^{+i(\omega t - kz)} + C_- e^{-i(\omega t - kz)} \\ & = \frac{k}{2\pi i} \int_{\substack{entire\,plane \\ \perp\, to\, z-axis \\ at\, z=0}} dA\, e^{-\varepsilon R} \left[C_+ \frac{e^{+i(\omega t - kR)}}{R} + C_- \frac{e^{-i(\omega t - kR)}}{R} \right] \end{aligned} \tag{1.55}$$

Thus, a plane wave propagating in the $+z$ direction is equal to a linear superposition of spherical outgoing waves emanating from each point on a plane perpendicular to the $z-$axis, that is,

$$e^{+i(\omega t - kz)} = \frac{k}{2\pi i} \int_{\substack{entire\,plane \\ \perp\, to\, z-axis \\ at\, z=0}} dA\, e^{-\varepsilon R} \left[\frac{e^{+i(\omega t - kR)}}{R} \right] \tag{1.56}$$

1.2.3.6. Note A

A classical physical quantity(for example, $\vec{E}$ or $\vec{B}$) is a real quantity. Therefore, $\eta_{physical}(\vec{x}, t)$ = *real* linear superposition of $\cos(\omega t - \vec{k} \cdot \vec{x})$ and $\sin(\omega t - \vec{k} \cdot \vec{x})$ is a plane wave of definite frequency, and $\eta_{physical}(\vec{x}, t)$ = *real* linear superposition of $\cos(\omega t - \vec{k} \cdot \vec{x})/r$ and $\sin(\omega t - \vec{k} \cdot \vec{x})/r$ is a spherical wave of definite frequency.

For definiteness, let us consider plane waves (similar results hold for spherical

waves).

A real linear superposition of $\cos(\omega t - \vec{k}\cdot\vec{x})$ and $\sin(\omega t - \vec{k}\cdot\vec{x})$ can be written as

$$\eta_{physical}(\vec{x},t) = A\cos(\vec{k}\cdot\vec{x} - \omega t + \phi) \quad , \quad A,\phi \text{ real} \tag{1.57}$$

We let

$$\eta(\vec{x},t) = Ae^{i\phi}e^{i(\vec{k}\cdot\vec{x}-\omega t)} = Ze^{i(\vec{k}\cdot\vec{x}-\omega t)} \quad , \quad Z = \text{ complex number} \tag{1.58}$$

so that

$$\eta_{physical}(\vec{x},t) = A\cos(\vec{k}\cdot\vec{x} - \omega t + \phi) = Real(\eta(\vec{x},t)) \tag{1.59}$$

Therefore, it is sufficient that we consider $\eta(\vec{x},t) = Ze^{i(\vec{k}\cdot\vec{x}-\omega t)}$ in our discussions. When $\eta_{physical}(\vec{x},t)$ is required, we need only take the real part of $\eta(\vec{x},t)$. We do this because $\eta(\vec{x},t)$ is simpler than $\eta_{physical}(\vec{x},t)$ to manipulate in calculations.

The analogous result for a spherical wave is obvious:

$$\eta(\vec{x},t) = Z\frac{e^{i(kr-\omega t)}}{r} \quad \text{outgoing wave} \tag{1.60}$$

$$\eta(\vec{x},t) = Z\frac{e^{-i(kr-\omega t)}}{r} \quad \text{incoming wave} \tag{1.61}$$

with

$$\eta_{physical} = Real(\eta) \tag{1.62}$$

The linear superposition of spherical outgoing waves which gives a plane wave can therefore be used in the earlier form(1.55) with $C_+ = 1$ and $C_- = 0$

$$e^{+i(\omega t-kz)} = \frac{k}{2\pi i}\int_{\substack{entire\,plane \\ \perp\, to\, z-axis \\ at\, z=0}} dA\, e^{-\varepsilon R}\left[\frac{e^{+i(\omega t-kR)}}{R}\right] \tag{1.63}$$

As I said, we shall do our calculations with $\eta(\vec{x},t)$ and $\eta_{physical}(\vec{x},t)$ is recovered at any stage of the calculation simply by taking the real part.

1.2.3.7. Note B

If $\eta(\vec{x},t) = F(\vec{x})e^{-i\omega t}$ has definite frequency, where $F(\vec{x}) = A(\vec{x})e^{i\psi(\vec{x})}$ and A,ψ are real, then we have

$$\eta_{physical}(\vec{x},t) = \text{Real}(\eta(\vec{x},t)) = A(\vec{x})\cos(\omega t - \psi(\vec{x})) \tag{1.64}$$

The intensity of a wave = magnitude of energy flow per unit time per unit area. This means that

$$\text{intensity } \propto (\eta_{physical}(\vec{x},t))^2 = \text{ intensity at } \vec{x} \text{ and } t \tag{1.65}$$

For example, the Poynting vector $\vec{S} = c\left(\vec{E} \times \vec{B}\right)/4\pi$ gives the energy flow per unit time per unit area or the intensity. For a plane wave of definite frequency propagating in free space (vacuum), $|\vec{E}| = |\vec{B}|$ and $\vec{E} \perp \vec{B}$ with $\vec{E} \times \vec{B}$ n the direction of propagation.

Therefore,

$$\begin{aligned}\overline{\text{intensity}} \;&\propto \frac{1}{T}\int_0^T dt\,(\eta_{physical}(\vec{x},t))^2 = \frac{1}{T}\int_0^T dt\,(A(\vec{x})\cos(\omega t - \psi(\vec{x})))^2 \\ &= \frac{1}{\omega T}(A(\vec{x}))^2 \int_0^{\omega T} d(\omega t)\cos^2(\omega t - \psi(\vec{x})) \\ &= \frac{(A(\vec{x}))^2}{2\pi}\int_0^{2\pi} du\cos^2(u - \psi(\vec{x})) = \frac{(A(\vec{x}))^2}{2} = \frac{1}{2}|\eta(\vec{x},t)|^2 \end{aligned} \tag{1.66}$$

Thus,

$$\overline{(\eta_{physical}(\vec{x},t))^2} = \frac{1}{2}|\eta(\vec{x},t)|^2 \tag{1.67}$$

which is independent of t since $\eta \propto e^{-i\omega t}$. Clearly we have the result

$$\overline{\text{intensity}} \propto |\eta(\vec{x},t)|^2 \tag{1.68}$$

1.2.4. Diffraction of Waves

Referring to Figure 1.9 below, we choose the origin of the coordinate system to lie in the region containing the aperture.

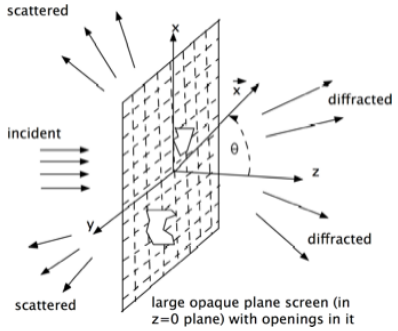


Figure 1.9: Opaque Screen with Holes

We assume a wave incident from the $z < 0$ region given by

$$\eta_{incident}(\vec{x},t) = e^{i(kz-\omega t)} \tag{1.69}$$

In general, the screen will affect the incident wave so that there will be scattered waves (back into the $z < 0$ region) and diffracted waves (waves in the $z > 0$ region).

Now

$$\eta_{incident}(\vec{x},t) = e^{+i(\omega t - kz)} = \frac{k}{2\pi i}\int_{\substack{entire\\ z=0\,plane}} dA\, e^{-\varepsilon R}\left[\frac{e^{+i(\omega t - kR)}}{R}\right] \tag{1.70}$$

This would be the wave for $z > 0$ if no screen were present. This plane wave is a linear superposition of spherical outgoing waves emanating from each point in the $z = 0$ plane. The *Kirchhoff approximation* for the diffracted wave is simply a linear superposition of spherical outgoing waves emanating from each point *in the openings* in the screen with each of these spherical waves having a coefficient equal to the coefficient in the expansion of $\eta_{incident}(\vec{x},t) = e^{i(kz-\omega t)}$. Note that the diffracted wave contains no spherical waves emanating from points on the opaque screen itself.

$$\eta_{diffracted}(\vec{x},t) = \frac{k}{2\pi i}\int_{\substack{openings\\ in\,the\\ opaque\\ screen}} dA\, e^{-\varepsilon R}\left[\frac{e^{+i(\omega t - kR)}}{R}\right] \tag{1.71}$$

where R is the distance from dA to the point $\vec{x}$.

This result seems reasonable, but note that we have proved nothing!!! To prove that this gives a good approximation for $\eta_{diffracted}(\vec{x},t)$ requires an analysis of the solutions to the classical wave equation and the boundary values of these solutions at the screen and in the openings. The Kirchhoff approximation is a good one under the following conditions:

1. $r >> \lambda \rightarrow kr >> 1$ and $r >>$ linear dimensions of the region containing the apertures. Thus, we must be far from the apertures for the above expression for $\eta_{diffracted}(\vec{x},t)$ to be valid.

2. $\theta << 1$, that is $\eta_{diffracted}(\vec{x},t)$ should be evaluated with the above expressions only when $\vec{x}$ makes a small angle with the $z-$axis.

3. $\lambda <<$ linear dimensions of the region containing the apertures (high frequency limit). We will apply the above expression to situations in which this condition is sometimes violated - in such cases our results will only be qualitatively accurate.

4. If the wave is described by a vector field ($\vec{E}$ and $\vec{B}$), then there exist relationships among the various components. These relationships have not been taken into account in the Kirchhoff approximation and therefore this approximation has neglected all polarization effects.

Note: When the apertures on the screen are finite, the integral is over a finite area and the limit $\varepsilon \to 0^+$ may be taken inside the integral (with $e^{-\varepsilon R} \to 1$) because the resulting integral will be well-defined and exist.

One must do the integral before letting $\varepsilon \to 0^+$ only when the integration extends over an infinite area(which is unphysical anyway!).

1.2.4.1. Application

We now discuss diffraction by two small holes in the opaque screen. The experimental configuration is shown in Figure 1.10 below.

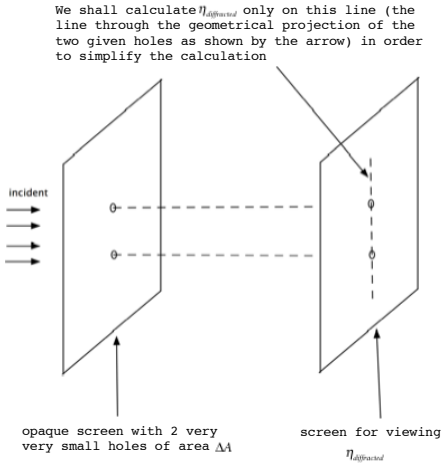


Figure 1.10: Two Small Holes

Looking from the side we get the diagram in Figure 1.11:

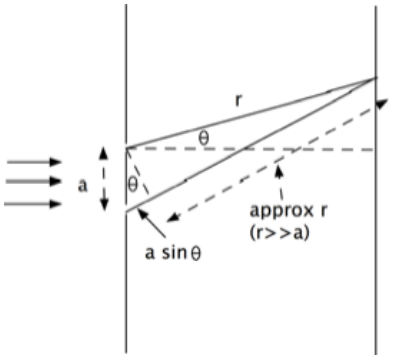


Figure 1.11: Side View

We have

$$\eta_{diffracted}(\vec{x},t) = +\frac{k}{2\pi i}\int\limits_{\text{openings}} \mathrm{dA} e^{-\varepsilon R}\frac{e^{i(kR-\omega t)}}{R}$$
$$= +\frac{k}{2\pi i}\int\limits_{\text{openings}} \mathrm{dA}\frac{e^{i(kR-\omega t)}}{R} \tag{1.72}$$

where we have taken the limit inside the integral. For small openings this gives

$$\eta_{diffracted}(\vec{x},t) = +\frac{k}{2\pi i}\left[\frac{e^{i(kR-\omega t)}}{r}\Delta A + \frac{e^{i(k(r+a\sin\theta)-\omega t)}}{r+a\sin\theta}\Delta A\right]$$
$$= \frac{k}{2\pi i}\Delta A\frac{e^{i(kR-\omega t)}}{r}\left[1+\frac{e^{ika\sin\theta}}{1+\frac{a}{r}\sin\theta}\right] \tag{1.73}$$

Since $r >> a\sin\theta$ we have

$$|\eta_{diff}| = \frac{k}{2\pi}\frac{\Delta A}{r}\left|1+e^{ika\sin\theta}\right| \tag{1.74}$$

and

$$\overline{\text{intensity}} \propto |\eta_{diff}|^2 = \frac{k^2}{4\pi^2}\frac{(\Delta A)^2}{r^2}(2+2\cos(ka\sin\theta)$$
$$\overline{\text{intensity}} \propto 1+\cos(ka\sin\theta) \tag{1.75}$$

A typical interference pattern is shown below in Figure 1.12.

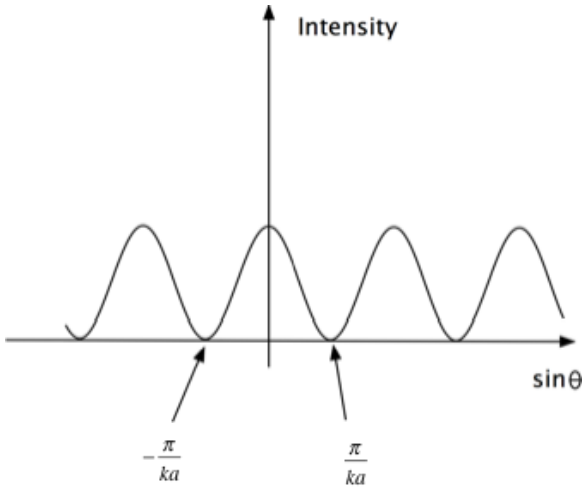


Figure 1.12: Interference Pattern

Note(as shown) that the first zero of the $\overline{\text{intensity}}$ occurs at $\sin\theta = \pi/ka$. Therefore,

$$ka\sin\theta = \frac{2\pi}{\lambda}a\sin\theta = \pi \rightarrow a\sin\theta = \frac{\lambda}{2} \tag{1.76}$$

for the first zero.

1.3. Review of Particle Dynamics

The following discussion is relativistically valid, that is, it holds for particles traveling at any speed $v < c$.

1.3.1. Relativistic Dynamics

$$\vec{F} = \frac{d\vec{p}}{dt} \text{ with } \vec{p} = m\gamma\vec{v} \text{ and } \gamma = \frac{1}{\sqrt{1 - v^2/c^2}} \tag{1.77}$$

where m = particle's rest mass (it is constant and does not change with v).

Non-relativistically ($v \ll c$) implies that $\gamma \approx 1$ and $\vec{p} \approx m\vec{v}$. The kinetic energy (KE) of a particle is defined such that the work done by $\vec{F}$ on the particle equals the change in KE. Thus, the definition of kinetic energy is

$$\Delta K = K - K_0 = \int_{\vec{r}_0}^{\vec{r}} \vec{F}\cdot d\vec{r} = \int_{\vec{r}_0}^{\vec{r}} \frac{d\vec{p}}{dt}\cdot d\vec{r} \tag{1.78}$$

Now, we have that $\vec{p} = m\gamma(v)\vec{v}$ where $\gamma(v) = (1-\beta^2)^{-1/2}$, $\beta = v/c$. Therefore we have

$$K - K_0 = \int_{\vec{r}_0}^{\vec{r}} \frac{d}{dt}(m_0\gamma(v)\vec{v})\cdot\vec{v}dt = m_0\int_0^v \vec{v}\cdot d(\gamma(v)\vec{v}) \tag{1.79}$$

Since the kinetic energy is zero when the velocity is zero we finally have

$$K = m_0\int_0^v \vec{v}\cdot d(\gamma(v)\vec{v}) \tag{1.80}$$

Now since

$$d(\gamma v^2) = d(\gamma\vec{v}\cdot\vec{v}) = \vec{v}\cdot d(\gamma\vec{v}) + \gamma\vec{v}\cdot d\vec{v} \tag{1.81}$$

we can write

$$K = m_0 \int_0^v \left(d(\gamma v^2) - \gamma \vec{v} \cdot d\vec{v}\right) = m_0 \int_0^v d(\gamma v^2) - \frac{1}{2} m_0 \int_0^v \gamma d(v^2)$$

$$= m_0 \gamma v^2 - \frac{1}{2} m_0 c^2 \int_0^{v^2/c^2} \gamma du \frac{du}{\sqrt{1-u}}$$

$$= m_0 \gamma v^2 + m_0 c^2 \left(\frac{1}{\gamma} - 1\right) = m_0 c^2 \left(\gamma \beta^2 + \frac{1}{\gamma}\right) - m_0 c^2$$

$$= m_0 c^2 (\gamma - 1) \tag{1.82}$$

The first thing we should do is check that this makes sense. What is the low velocity limit of this expression?

Using

$$\gamma = \left(1 - \beta^2\right)^{-1/2} \to 1 + \frac{1}{2}\beta^2 = 1 + \frac{1}{2}\frac{v^2}{c^2} \tag{1.83}$$

we have

$$K = m_0 c^2 (\gamma - 1) \to m_0 c^2 \frac{1}{2}\frac{v^2}{c^2} = \frac{1}{2} m_0 v^2 \tag{1.84}$$

as expected.

If we rearrange this result we have

$$\begin{aligned} \gamma m_0 c^2 &= K + m_0 c^2 \\ &= \text{Energy(motion)} + \text{Energy(rest)} \\ &= \text{Total Energy} = E \end{aligned} \tag{1.85}$$

The total energy is conserved.

What is the connection to momentum? Some algebra gives the following results:

$$\frac{pc}{E} = \frac{\gamma m_0 v c}{\gamma m_0 c^2} = \frac{v}{c} = \beta \tag{1.86}$$

and

$$\left(\frac{E}{c}\right)^2 - \vec{p}^2 = m_0^2 c^2 = \text{ invariant} \tag{1.87}$$

We now turn our attention to the so-called *wave-particle duality* exhibited by physical systems - a given physical system sometimes exhibits wave-like properties and sometime exhibits particle-like properties. This experimentally observed duality will suggest how to calculate the probabilities $\wp(\vec{x}, t) d^3x$ and $\tilde{\wp}(\vec{p}, t) d^3p$.

1.4. Wave-Particle Duality of Light

These results actually apply to all electromagnetic radiation.

1. The wave nature of light is manifest in the diffraction (interference) patterns observed when light passes through apertures in an opaque screen.

2. The particle nature of light is exhibited in the photoelectric effect (as well as many other experiments).

In the experiment shown in Figure 1.13 below, the incident light causes photoelectrons to be emitted at the cathode (alkali metal plate held at negative potential). The voltage V gives rise to a current I as the photoelectrons are collected at the surrounding anode.

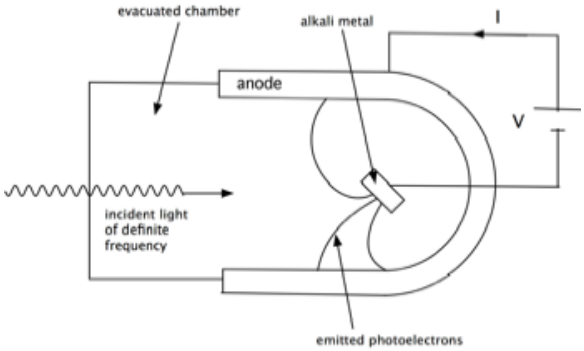


Figure 1.13: Experimental Setup

For a given metal and *fixed* frequency ν, the dependence of I on V is observed to be as shown in Figure 1.14 below:

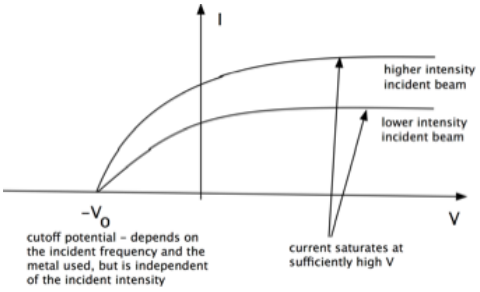


Figure 1.14: Experimental Data

The photoelectrons leaving the metal have different kinetic energies. When V is sufficiently high, all electrons leaving the metal will be collected at the anode.

A further increase in V will not, therefore, increase I because the number of electrons leaving the metal per unit time is determined by the incident intensity.

As V is lowered (but still positive), the slower electrons emitted from the metal will not reach the anode (ordinarily all the electrons would be attracted to the anode for $V > 0$, however, the electrons already traveling to the anode tend to repel newly emitted photoelectrons.

As V is made negative, still fewer photoelectrons reach the surrounding conductor. However, a non-zero current can still flow because those electrons emitted with very high kinetic energy can overcome the negative potential difference.

At $V = -V_0$, those electrons emitted with the maximum kinetic energy will barely be able to overcome the negative potential difference and then $V < -V_0$ will therefore give zero current.

Thus, V_0 is a measure of the maximum kinetic energy of the emitted photoelectrons (charge $q = -e, e > 0$) so that

$$(KE)_{at\,metal} + qV_{at\,metal} = (KE)_{at\,surrounding\,conductor} + qV_{at\,surrounding\,conductor}$$
$$(KE)_{at\,metal} = (KE)_{at\,surrounding\,conductor} + q(V_{at\,surrounding\,conductor} - V_{at\,metal})$$
$$(KE)_{at\,metal} = (KE)_{at\,surrounding\,conductor} + qV$$

When photoelectrons barely get to anode $(KE)_{at\,surrounding\,conductor} = 0$ so that

$$(KE)_{at\,metal} = -eV \tag{1.88}$$

and we have

$$(KE)_{\max} = eV_0 \tag{1.89}$$

V_0 versus frequency ν (for a given metal) is shown in Figure 1.15 below.

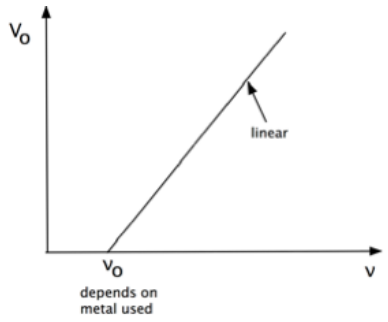


Figure 1.15: V_0 versus ν

For $\nu < \nu_0$, no current flows (regardless of how intense the incident light beam is).

The classical wave theory of light cannot explain these observations. Indeed, the classical theory requires that the electric field $|\vec{E}|$ increases as the intensity of the light increases (intensity $\propto |\vec{E}|^2$). Since the light's electric force on an electron in the metal is $q\vec{E}$, the maximum kinetic energy of emitted photoelectrons should increase as the light beam is made more intense. Furthermore, since $|\vec{E}|$ is independent of ν, the photoelectron's maximum kinetic energy should not depend on ν. In particular, a current should flow for any frequency of the light, provided the light beam is intense enough. But the observations show that $(KE)_{\max} = eV_0$ is independent of the intensity but depends on ν current flowing for $\nu < \nu_0$!

One additional point: Since the energy of the classical wave is distributed over the entire wave front, a single localized electron in the metal should absorb only a small part of this energy (the energy incident on the effective area of the electron). Thus, for a beam of very low intensity, there should be a time lag between the time the light first impinges on the metal and the time the photoelectrons are emitted (a time interval during which an electron in the metal can absorb enough energy to escape from the metal). No such time lag has ever been observed!

To explain the photoelectric effect, *Einstein*, in 1905, proposed the *photon concept* - a concept which attributes particle-like properties to light.

1.4.1. Einstein's Photon Hypothesis

1. The energy in a light beam is not continuously distributed over space but is localized in small bundles called photons. The energy of each photon is proportional to the light wave's frequency

$$E_{photon} = h\nu \tag{1.90}$$

   where h is a proportionality constant, called Planck's constant (introduced in 1900 by Planck to describe black body radiation).

2. The intensity of the light beam is proportional to the mean number of photons traveling per unit area per unit time.

3. An electron bound in the metal can absorb a photon and thereby gain its energy. The probability that a single electron absorb 2 photons is negligible, and an electron bound in the metal can only absorb a whole photon, never part of a photon.

It is easy to see that these 3 assumptions explain the photoelectric effect completely.

$$\underbrace{\left\{\begin{array}{l}\text{energy absorbed}\\ \text{by one electron}\end{array}\right\}}_{h\nu} = \left\{\begin{array}{l}\text{energy for electron}\\ \text{to get to metal surface}\end{array}\right\}$$

$$+\underbrace{\left\{\begin{array}{l}\text{energy for electron}\\ \text{to leave metal surface}\end{array}\right\}}_{W_0(\text{work function of metal})>0} + \left\{\begin{array}{l}\text{electron's KE}\\ \text{after leaving metal}\end{array}\right\}$$

The electrons which absorb a photon at the metal's surface(none wasted) have the maximum possible kinetic energy

$$h\nu = W_0 + (KE)_{\max} \rightarrow eV_0 = (KE)_{\max} = h\nu - W_0 \tag{1.91}$$

This gives the required linear relationship between $(KE)_{\max}$ and ν. It also shows that $(KE)_{\max}$ is independent of the incident intensity. Note that for $\nu < W_0/\hbar$ no electron will absorb enough energy to leave the surface. Thus, the cutoff frequency $\nu_0 = W_0/\hbar$ and $\nu < \nu_0$ imply that no photoelectrons will be emitted. When the light beam's intensity is increased, more photons hit the surface of the metal per unit time and therefore more electrons will leave the surface per unit time when $\nu > \nu_0$.

Also note that the emission of photoelectrons with no time delay is an immediate consequence of the localization of the photon and its energy.

By measuring the slope of the V_0 versus ν curve and by knowing the electron charge $q = -e$ one finds the experimental result

$$h = 6.63 \times 10^{-27} erg - sec \tag{1.92}$$

It is interesting to note that the human eye can detect a single photon in the visible range ($\nu \approx 10^{15} sec^{-1}$) or

$$E = h\nu \approx 7 \times 10^{-12} erg = 4.4\ eV \tag{1.93}$$

Now since light waves propagate at c, photons must travel at speed c. Two relations we wrote down earlier, namely,

$$\frac{pc}{E} = \frac{v}{c} \quad , \quad \left(\frac{E}{c}\right)^2 - p^2 = m_0^2 c^2 \tag{1.94}$$

then say that the rest mass of the photon is zero and $E = pc$. We then have

$$p = \frac{E}{c} = \frac{h\nu}{c} = \frac{h}{\lambda} \tag{1.95}$$

where p is the magnitude of photon momentum.

$E = h\nu$ and $p = h/\lambda$ relate the particle properties E and $\vec{p}$ to the *wave properties* ν and λ.

There are situations in which the wave properties and the particle properties of light are manifest in different aspects of the same experiment.

Consider the double slit experiment in Figure 1.16 below.

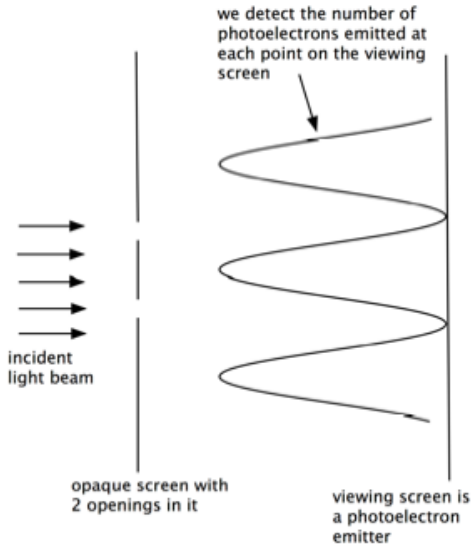


Figure 1.16: Double Slit Experiment

If the incident beam is of very low intensity (say 1 photon per minute), then one can observe individual photoelectrons being emitted from different points on the screen. Each photoelectron is emitted at a point where the photon has struck the screen.

The number of photoelectrons emitted over a period of time at various points on the viewing screen is observed to be given by the wave diffraction pattern. Thus, the probability of a given photon hitting the viewing screen at a given point (this probability is proportional to the number of photons which hit the screen at the given point over some time interval) is given by the wave diffraction pattern.

This is the key point!

> The probability of observing the particle(photon) in a given region is given by the intensity of the wave (diffraction pattern) in that region.

Thus, we have a *statistical connection* between the wave properties and the particle properties!

Is light a wave or a particle? *It is really neither!* It is a physical system in which the probability of observing a photon is determined by the intensity of a wave. Indeed, if light propagation were just a wave phenomenon, then one could not explain the photoelectric effect. On the other hand, if a light beam were actually composed of well-defined localized particles (photons), one could not explain diffraction patterns. For example, consider the two experiments shown in Figure 1.17 below:

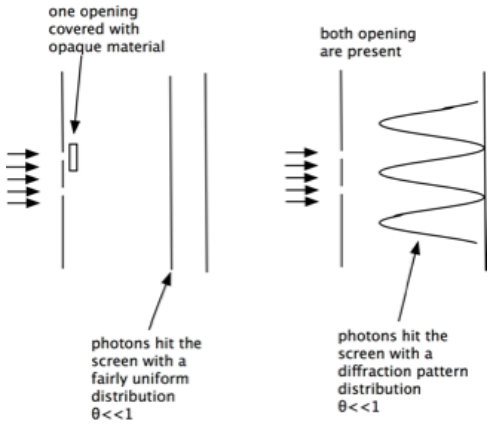


Figure 1.17: Which Slit?

If the light beam were actually composed of localized photons, one could not explain why one opening leads to a uniform distribution while adding another opening (which *increases* the number of ways a photon can get to any point on the viewing screen) yields certain regions of the screen in which the probability of observing a photon *decreases*.

1.4.2. Wave-Particle Duality of Electrons

1. The particle-like properties of an electron are well-known. For example, one can view the trajectory of an electron in a bubble chamber. If the chamber is placed in $\vec{E}$ and $\vec{B}$ fields, then the observed trajectory is just the one determined by Newton's second law with the Lorentz force

$$\frac{d\vec{p}}{dt} = \vec{F} = q(\vec{E} + \frac{\vec{v}}{c} \times \vec{B}) \quad , \quad \vec{p} = m\gamma\vec{v} \tag{1.96}$$

2. The wave-like properties of an electron are exhibited in the diffraction of electrons by a crystal (Davisson and Germer, Phys Rev. 30, 705 (1927)). The experiment is shown in Figure 1.18 below:

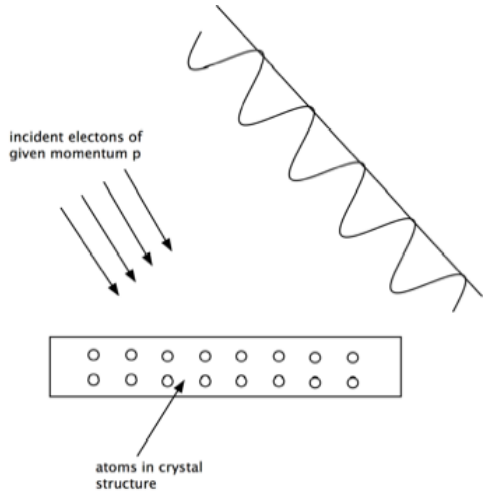


Figure 1.18: Electron Diffraction

The experimental distribution of electrons)shown on the right) is a typical diffraction pattern of a wave having wavelength

$$\lambda = \frac{h}{p} \tag{1.97}$$

which is called the deBroglie wavelength . The probability of observing the particle (electron) is determined (in this experiment) by the intensity distribution of a wave.

This relationship $\lambda = h/p$ or *matter waves* (whatever they might be!) was predicted in 1923 by Louis deBroglie. He argued that matter should exhibit a wave-particle duality just the way light exhibits such a duality - he argued that the relation $\lambda = h/p$ should relate the wave and particle properties for matter as well as for light.

Davisson and Germer confirmed this hypothesis in 1927 when they scattered electrons from a nickel crystal and observed a diffraction pattern distribution.

1.4.2.1. Why isn't the diffraction of macroscopic objects observed?

Consider the experiment shown in Figure 1.19 below. The first minimum occurs for

$$d \sin\theta = \frac{\lambda}{2} \rightarrow \sin\theta = \frac{1}{2}\frac{\lambda}{d} \tag{1.98}$$

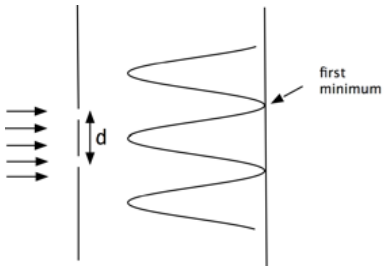


Figure 1.19: Macroscopic Diffraction?

Assume that the incident particles are macroscopic, that is,

$$m = 1\,gm\ ,\ v = 1\,cm/\sec$$
$$\rightarrow p = 1\,gm\cdot cm/\sec \rightarrow \lambda = \frac{h}{p} \approx 7\times 10^{-27} cm$$

so that the first minimum occurs at

$$\sin\theta = \frac{1}{2}\frac{\lambda}{d} \approx \frac{7}{2}\frac{10^{-27}cm}{d} \tag{1.99}$$

For any realistic d, this yields a θ so small that the oscillations in the diffraction pattern cannot be observed. Thus, $\lambda << d$ for macroscopic objects and diffraction patterns cannot be resolved - in this short deBroglie wavelength limit, one obtains classical mechanics. *The wave-particle duality is present. It is just that the wave patterns are too fine to be resolved.*

In addition, if v were as small as $10^{-8}\,cm/sec$ (an atomic distance per second) for macroscopic particles,

$$m \approx 1\,gm,\ p \approx 10^{-8} gm\cdot cm/\sec,\ \lambda \approx 7\times 10^{-19} cm \tag{1.100}$$

Again, for any realistic d, the diffraction pattern still cannot be seen.

All physical systems (light, electrons, neutrons, baseballs, etc) exhibit a so-called *wave-particle duality*! The connection between the wave properties and the particle properties is statistical - *the intensity of the wave in a given region determines the probability of observing the particle in that region.* Wave and particle properties are related by the de Broglie relation $\lambda = h/p$.

Chapter 2

Formulation of Wave Mechanics - Part 1

Using the ideas from Chapter 1, we can now set up a version of quantum theory called *Wave Mechanics*.

2.1. Basic Theory

2.1.1. Postulate 1a

Motivation: probability $\propto |\eta|^2$

Given the initial conditions (to be specified later) and the *particle* interactions (forces acting on the *particle*), there exists a complex-valued function $\psi(\vec{x},t)$, called the wave function or the probability amplitude, such that

1. The quantity
$$\int_{all\ space} d^3x\,|\psi(\vec{x},t)|^2 \tag{2.1}$$
is *finite and non-zero.*

2. The probability is given by
$$\wp(\vec{x},t) = \frac{|\psi(\vec{x},t)|^2}{\int_{all\ space} d^3x\,|\psi(\vec{x},t)|^2} \tag{2.2}$$
Note that no time averages are taken.

From now on $\int_{all\ space} d^3x(.....)$ means an integration over all space.

2.1.1.1. Additional Notes

1. The condition

$$\int d^3x\,|\psi(\vec{x},t)|^2 \text{ is finite and non-zero}$$

is referred to by saying that $\psi(\vec{x},t)$ is *normalizable*.

2. $\wp(\vec{x},t)$ = probability of observing the particle in $(x, x+dx)$, $(y, y+dy)$ and $(z, z+dz)$ at time t.

3.

$$\wp(\vec{x},t) = \frac{|\psi(\vec{x},t)|^2}{\int\limits_{all\ space} d^3x\,|\psi(\vec{x},t)|^2}$$

satisfies the required conditions for a probability density:

$$\wp(\vec{x},t) \geq 0$$
$$\int d^3x \wp(\vec{x},t) = 1 \text{ for all } t$$

4. $\psi(\vec{x},t)$ need not be a continuous function of $\vec{x}$. The only requirement is that it be normalizable. We will, however, assume continuity for physical reasons.

5. A plane wave of definite frequency is not normalizable.

$$\psi(\vec{x},t) = e^{i(\vec{k}\cdot\vec{x}-\omega t)} \Rightarrow |\psi(\vec{x},t)|^2 = 1$$
$$\Rightarrow \int d^3x\,|\psi(\vec{x},t)|^2 = \infty$$

6. $\psi(\vec{x},t)$ must be allowed to take on *complex* values. If $\psi(\vec{x},t=0)$ is real, then the time dependence that will be postulated later will usually yield a $\psi(\vec{x},t>0)$ that is complex.

7. $\psi(\vec{x},t)$ and $\bar{\psi}(\vec{x},t) = Z\psi(\vec{x},t)$, Z complex, determines the same $\wp(\vec{x},t)$.

$$\tilde{\wp}(\vec{x},t) = \frac{\left|\tilde{\psi}(\vec{x},t)\right|^2}{\int\limits_{all\ space} d^3x\left|\tilde{\psi}(\vec{x},t)\right|^2}$$
$$= \frac{|Z|^2}{|Z|^2}\frac{|\psi(\vec{x},t)|^2}{\int\limits_{all\ space} d^3x\,|\psi(\vec{x},t)|^2} = \wp(\vec{x},t)$$

8. $\psi(\vec{x},t)$ should be thought of as a *construct of the mind* to facilitate the prediction of probabilities. It is meaningless to ask whether $\psi(\vec{x},t)$ really exists as a physical quantity. $\wp(\vec{x},t)$ is the measurable quantity, and

$\psi(\vec{x},t)$ only helps us to calculate $\wp(\vec{x},t)$. It is analogous to the situation with $\vec{E}$ and $\vec{B}$ fields - $\vec{E}$ and $\vec{B}$ are mental concepts which allow us to calculate the force exerted on one charge by another charge (we think of one charge producing $\vec{E}$ and $\vec{B}$ fields which propagate to another charge and which then give rise to a force on the other charge).

9. One wave function $\psi(\vec{x},t)$ is adequate to describe certain *particles*, called spinless particles (for example, an alpha particle). However, other *particles* (particles with spin, for example, electrons, photons) require a wave function with several components for an accurate description (for example, a photon requires a vector wave function [3 components] to describe it because of its various modes of polarization). For non-relativistic speeds, an electron is approximately described by one wave function [one component]. We shall restrict our attention to one-component wave functions during most of chapters 2 and 3.

Let $f(\vec{x})$ be an arbitrary function of $\vec{x}$. Then the average (or expectation) value of $f(\vec{x})$ is defined by

$$\langle f(\vec{x})\rangle = \int d^3x\, \wp(\vec{x},t) f(\vec{x}) = \frac{\int d^3x\, |\psi(\vec{x},t)|^2 f(\vec{x})}{\int d^3x\, |\psi(\vec{x},t)|^2} \tag{2.3}$$

which may change with time. Therefore,

$$\langle f(\vec{x})\rangle = \frac{\int d^3x\, \psi^*(\vec{x},t) f(\vec{x}) \psi(\vec{x},t)}{\int d^3x\, \psi^*(\vec{x},t)\psi(\vec{x},t)} \tag{2.4}$$

2.1.1.2. Definition

$\psi(\vec{x},t)$ is said to be normalized if

$$\int d^3x\, |\psi(\vec{x},t)|^2 = 1 \tag{2.5}$$

Let $\tilde{\psi}(\vec{x},t)$ be a normalizable wave function. Then

$$\psi(\vec{x},t) = \frac{\tilde{\psi}(\vec{x},t)}{\sqrt{|\tilde{\psi}(\vec{x},t)|^2}} \tag{2.6}$$

is obviously normalized and determines the same $\wp(\vec{x},t)$ as $\tilde{\psi}(\vec{x},t)$.

If $\psi(\vec{x},t)$ is normalized, then

$$\wp(\vec{x},t) = |\psi(\vec{x},t)|^2 \text{ and } \langle f(\vec{x})\rangle = \int d^3x \psi^*(\vec{x},t) f(\vec{x}) \psi(\vec{x},t) \tag{2.7}$$

2.1.1.3. Definition

A function $\phi(\vec{x})$ (may also depend on t) is square-integrable if $\int d^3x\,|\phi(\vec{x})|^2$ is finite.

A normalizable function is square-integrable and satisfies $\int d^3x\,|\phi(\vec{x})|^2 \neq 0$.

2.1.1.4. Theorem

If $\phi_1(\vec{x})$ and $\phi_2(\vec{x})$ are square-integrable, then $\lambda_1\phi_1(\vec{x})+\lambda_2\phi_2(\vec{x})$ is also square-integrable for any complex λ_1 and λ_2.

Proof:

$$\begin{aligned}
&\int d^3x\,|\lambda_1\phi_1(\vec{x})+\lambda_2\phi_2(\vec{x})|^2 \\
&= \int d^3x\left[|\lambda_1|^2|\phi_1(\vec{x})|^2+|\lambda_2|^2|\phi_2(\vec{x})|^2+\lambda_1^*\lambda_2\phi_1^*(\vec{x})\phi_2(\vec{x})+\lambda_1\lambda_2^*\phi_1(\vec{x})\phi_2^*(\vec{x})\right] \\
&= \int d^3x\left[|\lambda_1|^2|\phi_1(\vec{x})|^2+|\lambda_2|^2|\phi_2(\vec{x})|^2+2\mathrm{Re}\left(\lambda_1^*\lambda_2\phi_1^*(\vec{x})\phi_2(\vec{x})\right)\right]
\end{aligned}$$

Now let $u_1^* = \lambda_1^*\phi_1^*(\vec{x})$ and $u_2 = \lambda_2\phi_2(\vec{x})$. Then

$$|u_1^*u_2| = \sqrt{\left[\mathrm{Re}\left(u_1^*u_2\right)\right]^2+\left[\mathrm{Im}\left(u_1^*u_2\right)\right]^2} \geq \mathrm{Re}\left(u_1^*u_2\right)$$

Also,

$$\left[|u_1^*|-|u_2|\right]^2 = |u_1|^2+|u_2|^2-2|u_1^*u_2| \geq 0 \rightarrow |u_1^*u_2| \leq \frac{1}{2}\left[|u_1|^2+|u_2|^2\right]$$

Therefore,

$$\mathrm{Re}\left(u_1^*u_2\right) \leq |u_1^*u_2| \leq \frac{1}{2}\left[|u_1|^2+|u_2|^2\right]$$

and

$$\int d^3x\mathrm{Re}\left(\lambda_1^*\lambda_2\phi_1^*(\vec{x})\phi_2(\vec{x})\right) \leq \int d^3x\left\{|\lambda_1|^2|\phi_1(\vec{x})|^2+|\lambda_2|^2|\phi_2(\vec{x})|^2\right\}$$

so that

$$\int d^3x\,|\lambda_1\phi_1(\vec{x})+\lambda_2\phi_2(\vec{x})|^2 \leq \int d^3x\left\{|\lambda_1|^2|\phi_1(\vec{x})|^2+|\lambda_2|^2|\phi_2(\vec{x})|^2\right\} = \text{ finite}$$

Therefore, $\int d^3x\,|\lambda_1\phi_1(\vec{x})+\lambda_2\phi_2(\vec{x})|^2$ is finite and $\lambda_1\phi_1(\vec{x})+\lambda_2\phi_2(\vec{x})$ is square-integrable.

This theorem implies that the set of all square-integrable functions forms a linear vector space (with the usual addition of functions and the usual multiplication of a function by a complex constant) - this space is designated L^2.

2.1.2. Postulate 1b

Motivation: Linear superposition of classical waves.

If $\psi_1(\vec{x},t)$ and $\psi_2(\vec{x},t)$ are possible wave functions for a particle under the influence of given forces, that is, $\psi_1(\vec{x},t)$ and $\psi_2(\vec{x},t)$ could correspond to different initial conditions), then, for any complex constants λ_1 and λ_2, $\lambda_1\phi_1(\vec{x}) + \lambda_2\phi_2(\vec{x})$, which is necessarily square-integrable by the previous theorem, is a possible wave function for the particle under the influence of the given forces, provided that $\lambda_1\phi_1(\vec{x}) + \lambda_2\phi_2(\vec{x})$ is not identically zero at any time, where a function $f(\vec{x},t)$ is identically zero at time t if $f(\vec{x},t) = 0$ for all $\vec{x}$.

Let $\phi_1(\vec{x})$ and $\phi_2(\vec{x}) \in L^2$, that is, they are square-integrable. Then,

$$\left|\int d^3x\phi_1^*(\vec{x})\phi_2(\vec{x})\right| \leq \int d^3x\,|\phi_1^*(\vec{x})\phi_2(\vec{x})|$$
$$\leq \frac{1}{2}\int d^3x\left[|\phi_1(\vec{x})|^2 + |\phi_2(\vec{x})|^2\right] = finite$$

so that $\int d^3x\ \phi_1^*(\vec{x})\phi_2(\vec{x})$ is finite.

2.1.2.1. Definition

Let $\phi_1(\vec{x})$ and $\phi_2(\vec{x}) \in L^2$. The *scalar product(inner product)* of $\phi_1(\vec{x})$ and $\phi_2(\vec{x})$ is defined to be

$$\langle\phi_1 \mid \phi_2\rangle \equiv \langle\phi_1,\phi_2\rangle = \int d^3x\phi_1^*(\vec{x})\phi_2(\vec{x}) \tag{2.8}$$

where the 2^{nd} expression is the standard scalar product notation, the 1^{st} expression is a different notation (due to Dirac) for the same thing and the 3^{rd} expression is the actual definition. The scalar product is finite for $\phi_1(\vec{x})$ and $\phi_2(\vec{x}) \in L^2$.

2.1.2.2. Properties of this Inner Product

(obvious by inspection)

1. $\langle\phi_1 \mid \phi_2\rangle^* = \langle\phi_2 \mid \phi_1\rangle$
2. $$\langle\phi_1 \mid \lambda_2\phi_2 + \lambda_3\phi_3\rangle = \lambda_2\langle\phi_1 \mid \phi_2\rangle + \lambda_3\langle\phi_1 \mid \phi_3\rangle$$
$$\langle\lambda_2\phi_2 + \lambda_3\phi_3 \mid \phi_1\rangle = \lambda_2^*\langle\phi_2 \mid \phi_1\rangle + \lambda_3^*\langle\phi_3 \mid \phi_1\rangle$$
3. $\langle\phi\,|\,\phi\rangle$ is real with $\langle\phi\,|\,\phi\rangle \geq 0$, where equality occurs if and only if $\phi(\vec{x} = 0$ almost everywhere(a.e.), that is, $\phi(\vec{x}$ at all $\vec{x}$ with the possible exception of some isolated points.

Definition: $\phi(\vec{x}$ is *normalized* if $\langle\phi\,|\,\phi\rangle = 1$

Definition: $\phi_1(\vec{x})$ and $\phi_2(\vec{x})$ are *orthogonal* if $\langle\phi_1\,|\,\phi_2\rangle = 0$

Definition: Let $f(\vec{x})$ be an arbitrary function of $\vec{x}$. The *matrix element* of $f(\vec{x})$ between $\phi_1(\vec{x})$ and $\phi_2(\vec{x})$ is defined to be:

$$\langle\phi_1|\,f(\vec{x})\,|\phi_2\rangle \equiv \langle\phi_1, f(\vec{x})\phi_2\rangle \equiv \int d^3x\phi_1^*(\vec{x})f(\vec{x})\phi_2(\vec{x}) \tag{2.9}$$

where the 2^{nd} expression is the standard scalar product notation, the 1^{st} expression is a different notation (due to Dirac) for the same thing and the 3^{rd} expression is the actual definition.

In the Dirac notation, we have $\langle\phi_1|\,f(\vec{x})\,|\phi_2\rangle$, where

$$\langle\phi_1| = bra\ vector \qquad , \qquad |\phi_2\rangle = ket\ vector \tag{2.10}$$

and

$$\langle\phi_1|\,f(\vec{x})\,|\phi_2\rangle = bracket\ f(\vec{x}) \tag{2.11}$$

In Dirac notation, postulate 1a takes the following form:

1. $\langle\phi\,|\,\phi\rangle$ is finite and non-zero
2. $\wp(\vec{x},t) = \frac{|\psi(\vec{x},t)|^2}{\langle\phi\,|\,\phi\rangle}$

Also

$$\langle f(\vec{x})\rangle = \frac{\langle\psi|\,f(\vec{x})\,|\psi\rangle}{\langle\psi\,|\,\psi\rangle} \tag{2.12}$$

If $\psi(\vec{x},t)$ is normalized, then we have

$$\langle\psi\,|\,\psi\rangle = 1 \quad , \quad \wp(\vec{x},t) = |\psi(\vec{x},t)|^2 \quad , \quad \langle f(\vec{x})\rangle = \langle\psi|\,f(\vec{x})\,|\psi\rangle \tag{2.13}$$

2.1.2.3. Theorem: Schwarz Inequality

Let $\phi_1(\vec{x})$ and $\phi_2(\vec{x}) \in L^2$. Then

$$|\langle\phi_1\,|\,\phi_2\rangle|^2 \leq \langle\phi_1\,|\,\phi_1\rangle\,\langle\phi_2\,|\,\phi_2\rangle \tag{2.14}$$

where the equality occurs if and only if $\phi_2(\vec{x}) = \lambda\phi_1(\vec{x})$ a.e. for λ a complex constant.

Proof

Consider $\phi_2(\vec{x})-\lambda\phi_1(\vec{x})$ with λ arbitrary. Then we must have $\langle\phi_2 - \lambda\phi_1\,|\,\phi_2 - \lambda\phi_1\rangle \geq 0$ for any λ. Again, equality occurs if and only if $\phi_2(\vec{x}) = \lambda\phi_1(\vec{x})$ a.e. We then find

$$\langle\phi_2 - \lambda\phi_1\,|\,\phi_2 - \lambda\phi_1\rangle = \langle\phi_2\,|\,\phi_2\rangle + |\lambda|^2\,\langle\phi_1\,|\,\phi_1\rangle - \lambda\,\langle\phi_2\,|\,\phi_1\rangle - \lambda^*\,\langle\phi_1\,|\,\phi_2\rangle \geq 0$$

This must be true for all λ. In particular, it is true for

$$\lambda = \frac{\langle \phi_1 \mid \phi_2 \rangle}{\langle \phi_1 \mid \phi_1 \rangle} \tag{2.15}$$

Note that if $\langle \phi_1 \mid \phi_1 \rangle = 0$, then the theorem is trivially true since

$$|\langle \phi_1 \mid \phi_2 \rangle|^2 = 0 = \langle \phi_1 \mid \phi_1 \rangle \langle \phi_2 \mid \phi_2 \rangle$$

Using the choice for λ in (2.15) we have

$$\langle \phi_2 \mid \phi_2 \rangle + \left| \frac{\langle \phi_1 \mid \phi_2 \rangle}{\langle \phi_1 \mid \phi_1 \rangle} \right|^2 \langle \phi_1 \mid \phi_1 \rangle - \frac{\langle \phi_1 \mid \phi_2 \rangle}{\langle \phi_1 \mid \phi_1 \rangle} \langle \phi_2 \mid \phi_1 \rangle - \frac{\langle \phi_1 \mid \phi_2 \rangle}{\langle \phi_1 \mid \phi_1 \rangle}^* \langle \phi_1 \mid \phi_2 \rangle \geq 0$$

$$\langle \phi_2 \mid \phi_2 \rangle - \frac{|\langle \phi_1 \mid \phi_2 \rangle|^2}{\langle \phi_1 \mid \phi_1 \rangle} \geq 0 \Rightarrow |\langle \phi_1 \mid \phi_2 \rangle|^2 \leq \langle \phi_1 \mid \phi_1 \rangle \langle \phi_2 \mid \phi_2 \rangle$$

with equality if and only if $\phi_2(\vec{x}) = \lambda \phi_1(\vec{x})$ a.e.

Note: The above inner product, its properties, and the Schwarz inequality can be generalized in an obvious manner to functions of n variables as shown below:

1. $\phi(x_1, ..., x_n)$ is square-integrable if $\int d^n x \, \phi^*(x_1, ..., x_n) \phi(x_1, ..., x_n)$ is finite, where $d^n x = dx_1 dx_2 ..... dx_n$.
2. $\langle \phi_1 \mid \phi_2 \rangle = \int d^n x \, \phi_1^*(x_1, ..., x_n) \phi_2(x_1, ..., x_n)$
3. $\langle \phi_1 | f(x_1, ..., x_n) | \phi_2 \rangle = \int d^n x \, \phi_1^*(x_1, ..., x_n) f(x_1, ..., x_n) \phi_2(x_1, ..., x_n)$

2.1.2.4. Examples

Let $\phi_1(\vec{x}) = e^{-r/2}$ and $\phi_2(\vec{x}) = re^{-r/2}$, then

$$\begin{aligned} \langle \phi_1 \mid \phi_1 \rangle &= \int d^3x \phi_1^*(r, \theta, \varphi) \phi_1(r, \theta, \varphi) \\ &= \int_0^\infty r^2 e^{-r} dr \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\varphi = 4\pi \int_0^\infty r^2 e^{-r} dr = 8\pi \end{aligned}$$

where we have used

$$\int_0^\infty du \, u^n e^{-u} = n! \quad \text{for} \quad n = 0, 1, 2, ... \tag{2.16}$$

Similarly,

$$\begin{aligned} \langle \phi_2 \mid \phi_2 \rangle &= \int d^3x \phi_2^*(r, \theta, \varphi) \phi_2(r, \theta, \varphi) \\ &= \int_0^\infty r^4 e^{-r} dr \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\varphi = 4\pi \int_0^\infty r^4 e^{-r} dr = 96\pi \end{aligned}$$

and

$$\langle \phi_1 \mid \phi_2 \rangle = \int d^3x \phi_1^*(r,\theta,\varphi)\phi_2(r,\theta,\varphi)$$
$$= \int_0^\infty r^3 e^{-r} dr \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\varphi = 4\pi \int_0^\infty r^3 e^{-r} dr = 24\pi$$

We then have

$$|\langle \phi_1 \mid \phi_2 \rangle|^2 = 576\pi^2 \quad , \quad \langle \phi_1 \mid \phi_1 \rangle \langle \phi_2 \mid \phi_2 \rangle = 768\pi^2 \tag{2.17}$$

so that

$$|\langle \phi_1 \mid \phi_2 \rangle|^2 < \langle \phi_1 \mid \phi_1 \rangle \langle \phi_2 \mid \phi_2 \rangle \tag{2.18}$$

as required by the Schwarz inequality.

Now let $\vec{k}$ be some fixed vector. Then we have

$$\langle \phi_2 | \vec{k} \cdot \vec{x} | \phi_1 \rangle = \int d^3x \, \phi_2^*(\vec{x})(\vec{k} \cdot \vec{x})\phi_1(\vec{x}) \tag{2.19}$$

Now we are free to choose our coordinate system for specifying the spherical polar coordinates of $\vec{x}$ so that the $z-$axis is along $\vec{k}$ (remember that $\vec{k}$ is fixed during the integration) as shown in Figure 2.1below.

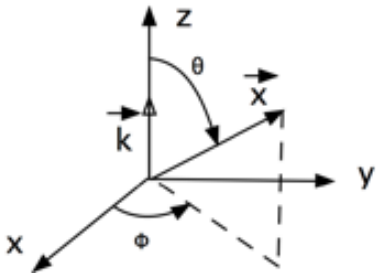


Figure 2.1: Vector Orientations

We then have

$$\vec{k} \cdot \vec{x} = kz = kr\cos\theta \quad , \quad d^3x = r^2 \sin\theta dr d\theta d\varphi$$

and we get

$$\begin{aligned}\langle\phi_2|\,\vec{k}\cdot\vec{x}\,|\phi_1\rangle &= \int d^3x\,\phi_2^*(\vec{x})(\vec{k}\cdot\vec{x})\phi_1(\vec{x})\\ &= \int_0^\infty r^2dr\int_0^\pi \sin\theta d\theta\int_0^{2\pi} d\varphi\,(kr\cos\theta)(re^{-r})\\ &= k\left(\int_0^\infty r^4e^{-r}dr\right)\left(\int_0^\pi \sin\theta\cos\theta d\theta\right)\left(\int_0^{2\pi} d\varphi\right)\\ &= k(4!)(0)(2\pi) = 0\end{aligned}$$

Now let $\phi(\vec{x}) = 1/r$, then we have

$$\begin{aligned}\langle\phi\mid\phi\rangle &= \int d^3x\phi^*(r,\theta,\varphi)\phi(r,\theta,\varphi)\\ &= \int_0^\infty r^2dr\int_0^\pi \sin\theta d\theta\int_0^{2\pi} d\varphi\frac{1}{r^2} = 4\pi\int_0^\infty dr = \infty\end{aligned}$$

The integrand diverges at $r = \infty$. Therefore, $\phi(\vec{x}) = 1/r$ is not in L^2.

Now let $\phi(\vec{x}) = 1/r^2$, then we have

$$\begin{aligned}\langle\phi\mid\phi\rangle &= \int d^3x\phi^*(r,\theta,\varphi)\phi(r,\theta,\varphi)\\ &= \int_0^\infty r^2dr\int_0^\pi \sin\theta d\theta\int_0^{2\pi} d\varphi\frac{1}{r^4} = 4\pi\int_0^\infty \frac{dr}{r^2} = \infty\end{aligned}$$

The integrand diverges at $r = 0$. Therefore, $\phi(\vec{x}) = 1/r^2$ is not in L^2.

Note: Now

$$\langle\phi\mid\phi\rangle = \int_0^\infty r^2dr\int_0^\pi \sin\theta d\theta\int_0^{2\pi} d\varphi\,|\phi(\vec{x})|^2 \tag{2.20}$$

Therefore, for the integration over r to converge, it is clearly necessary for $|\phi(\vec{x})| \to 0$ sufficiently fast as $r \to \infty$. Thus, square-integrable functions must vanish as $r \to \infty$.

If the wave function $\psi(\vec{x},t)$ for a particle is given, we can calculate $\wp(\vec{x},t)$ from postulate 1. Postulate 2 will tell us how to calculate $\tilde{\wp}(\vec{p},t)$ (the momentum probability distribution) from $\psi(\vec{x},t)$. For this, we must introduce the Fourier transform of $\psi(\vec{x},t)$.

2.1.3. Fourier Series and Transforms and Dirac Delta Function

2.1.3.1. Fourier Series

Let $f(\vec{x})$ be a square-integrable function of one variable on the interval $[-a/2, a/2]$, that is,

$$\int_{-a/2}^{a/2} dx\,|f(x)|^2 \quad \text{is finite} \tag{2.21}$$

Then

$$f(x) = \sum_{n=-\infty}^{\infty} c_n \frac{e^{i\frac{2\pi nx}{a}}}{\sqrt{a}} \tag{2.22}$$

with convergence a.e.

Let

$$u_n(x) = \frac{e^{i\frac{2\pi nx}{a}}}{\sqrt{a}} = \frac{1}{\sqrt{a}}\left(\cos\frac{2\pi nx}{a} + i\sin\frac{2\pi nx}{a}\right) \tag{2.23}$$

$$\rightarrow f(x) = \sum_{n=-\infty}^{\infty} c_n u_n(x) \tag{2.24}$$

Now,

$$\begin{aligned}
\langle u_n \mid u_m\rangle &= \int_{-a/2}^{a/2} dx\, u_n^*(x)u_m(x) = \frac{1}{a}\int_{-a/2}^{a/2} dx\, e^{i\frac{2\pi x}{a}(m-n)} \\
&= \frac{1}{ai\frac{2\pi}{a}(m-n)}\left(e^{i\pi(m-n)} - e^{-i\pi(m-n)}\right) \\
&= \frac{1}{2\pi i(m-n)}\left((-1)^{(m-n)} - (-1)^{(m-n)}\right) \\
&= \delta_{nm} = \begin{cases} 1 & \text{for} \quad n = m \\ 0 & \text{for} \quad n \neq m \end{cases} \Rightarrow \text{ Kronecker delta}
\end{aligned}$$

Therefore, multiplying

$$f(x) = \sum_{n=-\infty}^{\infty} c_n u_n(x) \tag{2.25}$$

by $u_m^*(x)$ and integrating over x, we get

$$\int_{-a/2}^{a/2} dx\, u_m^*(x) f(x) = \sum_{n=-\infty}^{\infty} c_n \int_{-a/2}^{a/2} dx\, u_m^*(x) u_n(x)$$

$$= \sum_{n=-\infty}^{\infty} c_n \delta_{nm} = c_m$$

$$c_m = \frac{1}{\sqrt{a}} \int_{-a/2}^{a/2} dx\, f(x) e^{-i\frac{2\pi m x}{a}} \tag{2.26}$$

Note that the Fourier series gives rise to an expansion of $f(x)$ on $[-a/2, a/2]$ in terms of the functions $e^{i2\pi nx/a} = e^{ikx}$ where

$$k = \frac{2\pi n}{a} = \frac{2\pi}{\lambda} \to \lambda = \frac{a}{n} \tag{2.27}$$

We are therefore expanding $f(x)$ in terms of sines and cosines with wavelengths $a, a/2, a/3, ...$

Now we let $a \to \infty$, which will give us a heuristic proof of the Fourier integral theorem. We have

$$f(x) = \sum_{n=-\infty}^{\infty} c_n \frac{e^{i\frac{2\pi nx}{a}}}{\sqrt{a}} \quad , \quad c_n = \frac{1}{\sqrt{a}} \int_{-a/2}^{a/2} dx\, f(x) e^{-i\frac{2\pi nx}{a}} \tag{2.28}$$

Let

$$k = \frac{2\pi n}{a} \to k \tag{2.29}$$

varies from $-\infty$ to $+\infty$ in steps of $\Delta k = 2\pi/a$, $(\Delta n = 1)$. Then $a \to \infty \Rightarrow \Delta k \to 0$. Therefore,

$$f(x) = \sum_{k=-\infty}^{\infty} c_n \frac{e^{ikx}}{\sqrt{a}} \left[\frac{a(\Delta k)}{2\pi}\right] \text{ since } \left[\frac{a(\Delta k)}{2\pi}\right] = 1 \tag{2.30}$$

Now let

$$F(k) = c_n \sqrt{\frac{a}{2\pi}} \tag{2.31}$$

so that

$$f(x) = \sum_{k=-\infty}^{\infty} e^{ikx} F(k) \frac{\Delta k}{\sqrt{2\pi}} \tag{2.32}$$

Then as $a \to \infty \Rightarrow \Delta k \to 0$, we have

$$f(x) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} e^{ikx} F(k) \tag{2.33}$$

and

$$F(k) = c_n\sqrt{\frac{a}{2\pi}} = \int_{-a/2}^{a/2} \frac{dx}{\sqrt{2\pi}} f(x)e^{-ikx} \tag{2.34}$$

which is the Fourier Transform of $f(x)$. Thus, we have the *Fourier Integral Theorem* (heuristically proved):

If $f(x)$ is square-integrable, the Fourier transform

$$F(k) = \int_{-a/2}^{a/2} \frac{dx}{\sqrt{2\pi}} f(x)e^{-ikx} \tag{2.35}$$

exists a.e. and is also square-integrable. Furthermore,

$$f(x) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} e^{ikx}F(k) \tag{2.36}$$

For a more rigorous derivation see Mathematical Methods notes.

2.1.3.2. Example

Let $f(x)$ be a Gaussian $f(x) = Ne^{-(x-x_0)^2/4\sigma^2}$, where x_0, σ and N are real and $\sigma > 0, N > 0$. First we determine N so that $f(x)$ is normalized.

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} dx\, |f(x)|^2 = N^2 \int_{-\infty}^{\infty} dx\, e^{-(x-x_0)^2/2\sigma^2} \\ &= N^2 \int_{-\infty}^{\infty} du\, e^{-u^2/2\sigma^2} = N^2\sigma\sqrt{2} \int_{-\infty}^{\infty} dv\, e^{-v^2} \\ 1 &= N^2\sigma\sqrt{2\pi} \rightarrow N = \sqrt{\frac{1}{\sqrt{2\pi}\sigma}} \end{aligned}$$

so that the normalized $f(x)$ is

$$f(x) = \sqrt{\frac{1}{\sqrt{2\pi}\sigma}} e^{-(x-x_0)^2/4\sigma^2} \tag{2.37}$$

as shown in Figure 2.2 below.

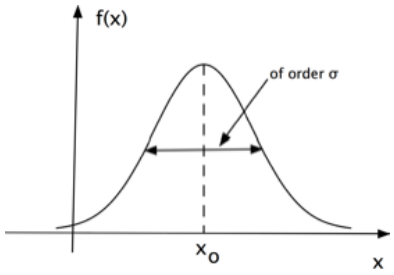


Figure 2.2: Gaussian Function

Now let us calculate the Fourier transform. We have

$$\begin{aligned}
F(k) &= \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} \sqrt{\frac{1}{\sqrt{2\pi}\sigma}} e^{-(x-x_0)^2/4\sigma^2} e^{-ikx} \\
&= \frac{1}{\sqrt{2\pi}} \sqrt{\frac{1}{\sqrt{2\pi}\sigma}} \int_{-\infty}^{\infty} dx\, e^{-(x-x_0)^2/4\sigma^2} e^{-ikx} \\
&= \frac{1}{\sqrt{2\pi}} \sqrt{\frac{1}{\sqrt{2\pi}\sigma}} \int_{-\infty}^{\infty} du\, e^{-u^2/4\sigma^2} e^{-ik(u+x_0)} \\
&= \frac{1}{\sqrt{2\pi}} \sqrt{\frac{1}{\sqrt{2\pi}\sigma}} e^{-ikx_0} \int_{-\infty}^{\infty} du\, e^{-(u+2ik\sigma^2)^2/4\sigma^2} e^{-4\sigma^4 k^2/4\sigma^2} \\
&= \frac{1}{\sqrt{2\pi}} \sqrt{\frac{1}{\sqrt{2\pi}\sigma}} e^{-ikx_0} e^{-\sigma^2 k^2} \int_{-\infty}^{\infty} du\, e^{-(u+2ik\sigma^2)^2/4\sigma^2}
\end{aligned}$$

where the last two steps follow from completing the square. We then have

$$F(k) = \frac{2\sigma}{\sqrt{2\pi}} \sqrt{\frac{1}{\sqrt{2\pi}\sigma}} e^{-ikx_0} e^{-\sigma^2 k^2} \int_{-\infty+i\sigma k}^{\infty+i\sigma k} dZ\, e^{-Z^2} \tag{2.38}$$

This last integral can be done using complex integration methods (again see Mathematical Methods notes), which would show that it does not matter whether we integrate over the path in the complex plane as indicated ($k0$) or along the real axis ($k = 0$).

We will now show this property another way. We define

$$I(k) = \int_{-\infty+i\sigma k}^{\infty+i\sigma k} dZ\, e^{-Z^2} \tag{2.39}$$

We now show that $dI/dk = 0$, so that $I(k)$ is independent of k. Let $Z = v + i\sigma k$.

Then

$$I(k) = \int_{-\infty}^{\infty} dv e^{-(v+i\sigma k)^2} \tag{2.40}$$

so that

$$\begin{aligned}
\frac{dI}{dk} &= \int_{-\infty}^{\infty} dv \frac{d}{dk}\left(e^{-(v+i\sigma k)^2}\right) = i\sigma \int_{-\infty}^{\infty} dv \frac{d}{d(i\sigma k)}\left(e^{-(v+i\sigma k)^2}\right) \\
&= i\sigma \int_{-\infty}^{\infty} dv \frac{d}{dv}\left(e^{-(v+i\sigma k)^2}\right) = i\sigma \int_{-\infty}^{\infty} d\left(e^{-(v+i\sigma k)^2}\right) \\
&= i\sigma \left[e^{-(v+i\sigma k)^2}\right]_{v=-\infty}^{v=+\infty} = 0
\end{aligned}$$

Therefore, $I(k) = \text{constant} = I(0)$ and

$$I(0) = \int_{-\infty}^{\infty} dv e^{-v^2} = \sqrt{\pi} \tag{2.41}$$

Therefore,

$$\begin{aligned}
F(k) &= \frac{2\sigma}{\sqrt{2\pi}} \sqrt{\frac{1}{\sqrt{2\pi}\sigma}} e^{-ikx_0} e^{-\sigma^2 k^2} \sqrt{\pi} \\
&= \sqrt{\sqrt{\frac{2}{\pi}}\sigma} e^{-ikx_0} e^{-\sigma^2 k^2}
\end{aligned} \tag{2.42}$$

as shown in Figure 2.3 below.

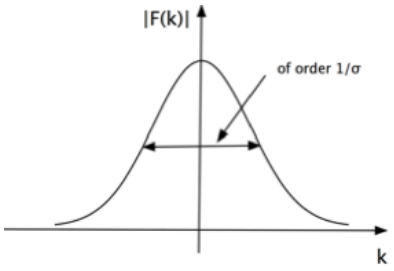


Figure 2.3: Gaussian Fourier Transform

Note that

$$\begin{aligned}
\int_{-\infty}^{\infty} dk\, |F(k)|^2 &= \sqrt{\frac{2}{\pi}}\sigma \int_{-\infty}^{\infty} dk e^{-2\sigma^2 k^2} \\
&= \sqrt{\frac{2}{\pi}}\sigma \sqrt{\frac{\pi}{2}} \frac{1}{\sigma} = 1 = \int_{-\infty}^{\infty} dx\, |f(x)|^2
\end{aligned}$$

This will be seen to be *Parseval's relation*, which we derive shortly.

Now we generalize to 3 dimensions. Let $f(\vec{x}) = f(x, y, z)$ be a square-integrable function of 3 variables. We can Fourier transform in z first, then in y and finally in x.

$$\begin{aligned} F(\vec{k}) &= F(k_x, k_y, k_z) \\ &= \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-ik_x x} \int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi}} e^{-ik_y y} \int_{-\infty}^{\infty} \frac{dz}{\sqrt{2\pi}} e^{-ik_z z} f(x, y, z) \\ &= \int_{-\infty}^{\infty} \frac{d^3x}{(2\pi)^{3/2}} e^{-i\vec{k}\cdot\vec{x}} f(\vec{x}) \end{aligned} \tag{2.43}$$

where $d^3x = dxdydz$ and $\vec{k} \cdot \vec{x} = k_x x + k_y y + k_z z$. Similarly, we have

$$\begin{aligned} f(\vec{x}) &= f(x, y, z) \\ &= \int_{-\infty}^{\infty} \frac{dk_x}{\sqrt{2\pi}} e^{ik_x x} \int_{-\infty}^{\infty} \frac{dk_y}{\sqrt{2\pi}} e^{ik_y y} \int_{-\infty}^{\infty} \frac{dk_z}{\sqrt{2\pi}} e^{ik_z z} F(k_x, k_y, k_z) \\ &= \int_{-\infty}^{\infty} \frac{d^3k}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{x}} F(\vec{k}) \end{aligned} \tag{2.44}$$

which is obtained by Fourier inverting first in x, then in y and finally in z. It is the inverse Fourier transform.

Thus, if $f(\vec{x})$ is square-integrable, the Fourier transform

$$F(\vec{k}) = \int_{-\infty}^{\infty} \frac{d^3x}{(2\pi)^{3/2}} e^{-i\vec{k}\cdot\vec{x}} f(\vec{x}) \tag{2.45}$$

exists a.e. and is also square-integrable. Furthermore

$$f(\vec{x}) = \int_{-\infty}^{\infty} \frac{d^3k}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{x}} F(\vec{k}) \tag{2.46}$$

2.1.3.3. Parseval's Relation

Let $F(\vec{k})$ and $G(\vec{k})$ be the Fourier transforms of $f(\vec{x})$ and $g(\vec{x})$ respectively. Then

$$\langle f \mid g \rangle = \langle F \mid G \rangle \tag{2.47}$$

that is,

$$\int d^3x \, f^*(\vec{x}) g(\vec{x}) = \int d^3k \, F^*(\vec{k}) G(\vec{k}) \tag{2.48}$$

Proof

$$\int d^3x\, f^*(\vec{x})g(\vec{x}) = \int d^3x \left[\int_{-\infty}^{\infty} \frac{d^3k}{(2\pi)^{3/2}} e^{-i\vec{k}\cdot\vec{x}} F^*(\vec{k})\right] g(\vec{x})$$
$$= \int d^3k F^*(\vec{k}) \left[\int_{-\infty}^{\infty} \frac{d^3x}{(2\pi)^{3/2}} e^{-i\vec{k}\cdot\vec{x}} g(\vec{x})\right]$$
$$= \int d^3k\, F^*(\vec{k}) G(\vec{k}) \tag{2.49}$$

Note: For $f = g$ we obtain $\langle f \,|\, f\rangle = \langle F \,|\, F\rangle$, that is,

$$\int d^3x\, |f(\vec{x})|^2 = \int d^3k\, \left|F(\vec{k})\right|^2 \tag{2.50}$$

which will be very useful.

2.1.3.4. The Dirac Delta Function(a generalized function)

We define the function $\delta_\varepsilon(x)$ as shown in Figure 2.4 below.

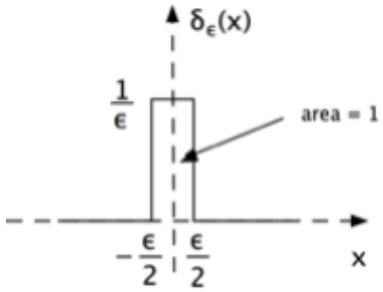


Figure 2.4: Delta Function Definition

by the relation

$$\delta_\varepsilon(x) = \begin{cases} 0 & \text{for } |x| > \varepsilon/2 \\ 1/\varepsilon & \text{for } |x| < \varepsilon/2 \end{cases} \tag{2.51}$$

Taking the limit $\varepsilon \to 0^+$ we get

$$\lim_{\varepsilon\to 0^+} \delta_\varepsilon(x) = \begin{cases} 0 & \text{for } x \neq 0 \\ \infty & \text{for } x = 0 \end{cases} \tag{2.52}$$

such that the area under curve remains = 1.

The problem is that such a limit does *not* exist as an ordinary function. Instead, consider

$$\lim_{\varepsilon\to 0^+} \int_{-\infty}^{\infty} dx\, f(x)\delta_\varepsilon(x - x_0) \tag{2.53}$$

where the function $\delta_\varepsilon(x - x_0)$ is as shown in Figure 2.5 below:

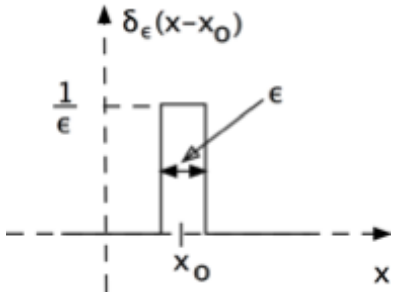


Figure 2.5: Another Delta Function Definition

and $f(x)$ is some arbitrary function continuous at $x = x_0$. One takes the limit *after* the integral has been done. We then have the result (which is the correct defining relation)

$$\begin{aligned}\lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty} dx\, f(x)\delta_\varepsilon(x-x_0) &= \lim_{\varepsilon\to 0^+}\frac{1}{\varepsilon}\int_{-\frac{\varepsilon}{2}+x_0}^{+\frac{\varepsilon}{2}+x_0} dx\, f(x)\\ &= \lim_{\varepsilon\to 0^+}\frac{1}{\varepsilon}f(x_0)\int_{-\frac{\varepsilon}{2}+x_0}^{+\frac{\varepsilon}{2}+x_0} dx\\ &= \lim_{\varepsilon\to 0^+}\frac{1}{\varepsilon}f(x_0)\varepsilon = f(x_0)\end{aligned} \tag{2.54}$$

where we have used the continuity of $f(x)$ at $x = x_0$ to take the term $f(x_0)$ outside the integral.

2.1.3.5. Definition

Let $\delta_\varepsilon(x - x_0)$ be any function of the type described above and depending on some parameter ε. Then, $\lim_{\varepsilon\to 0^+}\delta_\varepsilon(x - x_0) = \delta(x - x_0)$, which is the Dirac delta function, means, for any function $f(x)$ continuous at x_0,

$$\lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty} dx\, f(x)\delta_\varepsilon(x-x_0) = f(x_0) = \int_{-\infty}^{\infty} dx\, f(x)\delta(x-x_0) \tag{2.55}$$

where the last form is just a *notation* because $\lim_{\varepsilon\to 0^+}$ *cannot* be brought inside the integral to give

$$\int_{-\infty}^{\infty} dx\, f(x)\left[\lim_{\varepsilon\to 0^+}\delta_\varepsilon(x-x_0)\right] \tag{2.56}$$

since

$$\left[\lim_{\varepsilon\to 0^+}\delta_\varepsilon(x-x_0)\right] \tag{2.57}$$

does not exist.

Note: Compare the delta function with the Kronecker delta:

$$\sum_j c_j\delta_{ij} = c_i \text{ picks out } j = i$$
$$\int_{-\infty}^{\infty} dx\, f(x)\delta(x-x_0) = f(x_0) \text{ picks out } x = x_0$$

There are many different functions $\delta_\varepsilon(x-x_0)$ such that $\lim_{\varepsilon\to 0^+}\delta_\varepsilon(x-x_0) = \delta(x-x_0)$ in the above sense.

2.1.3.6. Properties of the Delta Function

1. In a non-rigorous way,

$$\lim_{\varepsilon\to 0^+}\delta_\varepsilon(x) = \begin{cases} 0 & \text{for } x \neq 0 \\ \infty & \text{for } x = 0 \end{cases} \tag{2.58}$$

2. For $f(x)$ continuous at $x = 0$

$$\int_{-\infty}^{\infty} dx\, f(x)\delta(x) = f(0) \tag{2.59}$$

3. In particular

$$\int_{-\infty}^{\infty} dx\, \delta(x-x_0) = 1 \tag{2.60}$$

4. Let

$$g(x) = \begin{cases} f(x) & \text{for } x \in (a,b) \\ 0 & \text{for } x \notin [a,b] \end{cases}$$

then

$$\int_a^b dx\, f(x)\delta(x-x_0) = \int_{-\infty}^{\infty} dx\, g(x)\delta(x-x_0)$$
$$= g(x_0) = \begin{cases} f(x) & \text{for } x \in (a,b) \\ 0 & \text{for } x \notin [a,b] \end{cases} \tag{2.61}$$

5. For any real constant $a0$

$$\delta(ax) = \frac{1}{|a|}\delta(x) \tag{2.62}$$

Proof

For $a > 0$

$$\int_{-\infty}^{\infty} dx\, f(x)\delta(ax) = \frac{1}{|a|}\int_{-\infty}^{\infty} du\, f(u/a)\delta(u) = \frac{1}{|a|}f(0)$$

For $a < 0$

$$\begin{aligned}\int_{-\infty}^{\infty} dx\, f(x)\delta(ax) &= \frac{1}{a}\int_{\infty}^{-\infty} du\, f(u/a)\delta(u) \\ &= \frac{1}{|a|}\int_{-\infty}^{\infty} du\, f(u/a)\delta(u) = \frac{1}{|a|}f(0)\end{aligned}$$

But,

$$\int_{-\infty}^{\infty} dx\, f(x)\frac{\delta(x)}{|a|} = \frac{1}{|a|}f(0)$$

Therefore,

$$\delta(ax) = \frac{1}{|a|}\delta(x)$$

6. It follows from (5) that

$$\delta(-x) = \delta(x) \tag{2.63}$$

2.1.3.7. Fourier Transform of a δ-function

Heuristic: Fourier transform(this is well-defined)

$$\Delta(k) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-ikx}\delta(x) = \frac{1}{\sqrt{2\pi}} \tag{2.64}$$

Therefore,

$$\delta(x) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} e^{ikx}\Delta(k) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} \tag{2.65}$$

where this integral is really not defined!

Rigorous: Let

$$\delta_\varepsilon(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{\pm ikx} e^{-\varepsilon k^2} \tag{2.66}$$

where $e^{-\varepsilon k^2}$ is a convergence factor which gives a well-defined integral for $\varepsilon \neq 0$. We ask the question: does $\lim_{\varepsilon\to 0^+} \delta_\varepsilon(x) = \delta(x)$ in the same sense as the earlier definition?

$$\begin{aligned}\lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty} dx\, f(x)\delta_\varepsilon(x) &= \lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty} dx\, f(x)\int_{-\infty}^{\infty}\frac{dk}{2\pi}e^{\pm ikx}e^{-\varepsilon k^2}\\ &= \lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty}\frac{dk}{\sqrt{2\pi}}e^{-\varepsilon k^2}\int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi}}e^{\pm ikx}f(x)\\ &= \lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty}\frac{dk}{\sqrt{2\pi}}e^{-\varepsilon k^2}F(\mp k)\end{aligned}$$

We can now take the limit inside the integral if and only if the resulting integral is well-defined. We have

$$\begin{aligned}\lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty} dx\, f(x)\delta_\varepsilon(x) &= \lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty}\frac{dk}{\sqrt{2\pi}}e^{-\varepsilon k^2}F(\mp k)\\ &= \int_{-\infty}^{\infty}\frac{dk}{\sqrt{2\pi}}F(\mp k) = \int_{-\infty}^{\infty}\frac{dk'}{\sqrt{2\pi}}F(k') = f(0)\end{aligned}$$

Therefore,

$$\delta(x) = \lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty}\frac{dk}{2\pi}e^{\pm ikx}e^{-\varepsilon k^2} \tag{2.67}$$

which we will write as

$$\delta(x) = \int_{-\infty}^{\infty}\frac{dk}{2\pi}e^{\pm ikx} \tag{2.68}$$

with the above limit in mind.

2.1.3.8. Derivatives of a δ-function

Let $\lim_{\varepsilon\to 0^+} \delta_\varepsilon(x) = \delta(x)$. Then

$$\lim_{\varepsilon\to 0^+}\frac{d\delta_\varepsilon(x-x_0)}{dx} = \frac{d\delta(x-x_0)}{dx} \tag{2.69}$$

which means

$$\begin{aligned}\int_{-\infty}^{\infty} dx\, f(x)\frac{d\delta(x-x_0)}{dx} &= \lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty} dx\, f(x)\frac{d\delta_\varepsilon(x-x_0)}{dx}\\ &= \lim_{\varepsilon\to 0^+}\left[f(x)\delta(x-x_0)\right]_{-\infty}^{\infty} - \lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty} dx\,\frac{df(x)}{dx}\delta_\varepsilon(x-x_0)\\ &= -\lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty} dx\,\frac{df(x)}{dx}\delta_\varepsilon(x-x_0) = -\frac{df(x_0)}{dx}\end{aligned}$$

where we have used integration by parts and $\delta_\varepsilon(\pm\infty) = 0$. Therefore,

$$\int_{-\infty}^{\infty} dx\, f(x) \frac{d\delta(x - x_0)}{dx} = -\frac{df(x_0)}{dx} \tag{2.70}$$

when $df(x)/dx$ is continuous at $x = x_0$. Similar results hold for higher derivatives of $\delta(x - x_0)$ (just keep on integrating by parts).

2.1.3.9. Three-Dimensional Delta Function

We will write all integrals with the limiting process understood where appropriate.

$$\int d^3x f(\vec{x})\delta^3(\vec{x} - \vec{x}_0) = f(\vec{x}_0) = \lim_{\varepsilon \to 0^+} \int d^3x f(\vec{x})\delta_\varepsilon^3(\vec{x} - \vec{x}_0) \tag{2.71}$$

for all functions $f(\vec{x})$ continuous at $\vec{x} = \vec{x}_0$. But

$$f(\vec{x}_0) = \int dxdydz\, f(x, y, z)\delta(x - x_0)\delta(y - y_0)\delta(z - z_0) \tag{2.72}$$

or

$$\begin{aligned} \delta^3(\vec{x} - \vec{x}_0) &= \delta(x - x_0)\delta(y - y_0)\delta(z - z_0) \\ &= \int \frac{d^3k}{(2\pi)^3} e^{\pm i\vec{k}\cdot(\vec{x} - \vec{x}_0)} \end{aligned} \tag{2.73}$$

2.1.4. Postulate 2

2.1.4.1. Motivation

$\psi(\vec{x}, t)$ is square-integrable which implies that we can Fourier analyze it in $\vec{x}$ (t fixed)

$$\psi(\vec{x}, t) = \int \frac{d^3k}{(2\pi)^{3/2}} e^{+i\vec{k}\cdot\vec{x}} \phi(\vec{k}, t) \tag{2.74}$$

This is just a superposition of sines and cosines with wavelengths $\lambda = 2\pi/k$. But $\lambda = h/p$ (deBroglie) relates this wave property (λ) to the particle property (p) by

$$k = \frac{2\pi}{\lambda} = \frac{2\pi}{h} p = \frac{p}{\hbar} \tag{2.75}$$

where we have defined $\hbar = h/2\pi$. Then we have $[= \hbar k$. Since the spatial variation of $e^{+i\vec{k}\cdot\vec{x}}$ occurs in the $\vec{k}$ direction, we expect $\vec{p}$ to be along $\vec{k}$'s direction, that is, $\vec{p} = \hbar\vec{k}$, that is, $\psi(\vec{x}, t)$ is a weighted (weighted by something related to probabilities) superposition of states of different momentum. Now, Parseval's relation gives

$$\langle \psi \mid \psi \rangle = \langle \phi \mid \phi \rangle = \int d^3k \left|\phi(\vec{k}, t)\right|^2 \tag{2.76}$$

Therefore,

$$\int d^3k \left|\phi(\vec{k},t)\right|^2 = 1 = \int \frac{d^3p}{\hbar^3} \frac{\left|\phi(\vec{k},t)\right|^2}{\langle\psi \mid \psi\rangle} \tag{2.77}$$

But $\tilde{\wp}(\vec{p},t)$ must satisfy

$$\int d^3p \tilde{\wp}(\vec{p},t) = 1 \tag{2.78}$$

We are therefore led to the conjecture that

$$\tilde{\wp}(\vec{p},t) = \frac{1}{\hbar^3} \frac{\left|\phi(\vec{k},t)\right|^2}{\langle\psi \mid \psi\rangle} \tag{2.79}$$

Let

$$\tilde{\psi}(\vec{p},t) = \frac{1}{\hbar^{3/2}} \phi(\vec{k},t) \tag{2.80}$$

with $\vec{p} = \hbar\vec{k}$. Therefore

$$\tilde{\wp}(\vec{p},t) = \frac{\left|\tilde{\psi}(\vec{p},t)\right|^2}{\langle\psi \mid \psi\rangle} \tag{2.81}$$

where

$$\begin{aligned} \tilde{\psi}(\vec{p},t) &= \frac{1}{\hbar^{3/2}} \int \frac{d^3x}{(2\pi)^{3/2}} e^{-i\vec{k}\cdot\vec{x}} \psi(\vec{x},t) \\ &= \int \frac{d^3x}{(2\pi\hbar)^{3/2}} e^{-i\frac{\vec{p}}{\hbar}\cdot\vec{x}} \psi(\vec{x},t) \end{aligned} \tag{2.82}$$

which is the Fourier transform of $\psi(\vec{x},t)$ in momentum space. We also have

$$\begin{aligned} \psi(\vec{x},t) = \int \frac{d^3k}{(2\pi)^{3/2}} e^{+i\vec{k}\cdot\vec{x}} \phi(\vec{k},t) = \int \frac{d^3p}{(2\pi)^{3/2}\hbar^3} e^{+i\frac{\vec{p}}{\hbar}\cdot\vec{x}} \hbar^{3/2} \tilde{\psi}(\vec{p},t) \\ \tilde{\psi}(\vec{x},t) = \int \frac{d^3p}{(2\pi\hbar)^{3/2}} e^{+i\frac{\vec{p}}{\hbar}\cdot\vec{x}} \tilde{\psi}(\vec{p},t) \end{aligned} \tag{2.83}$$

Note that Parseval's relation becomes:

$$\begin{aligned} \langle\psi_1 \mid \psi_2\rangle &= \langle\psi_1, \psi_2\rangle = \langle v_1, \phi_2\rangle = \langle\phi_1 \mid \phi_2\rangle \\ &= \int d^3k \phi_1^*(\vec{k},t)\phi_2(\vec{k},t) = \int d^3p \tilde{\psi}_1^*(\vec{k},t)\tilde{\psi}_2(\vec{k},t) \\ &= \left\langle\tilde{\psi}_1 \,\middle|\, \tilde{\psi}_2\right\rangle = \left\langle\tilde{\psi}_1, \tilde{\psi}_2\right\rangle \end{aligned}$$

Therefore,

$$\langle\psi_1 \mid \psi_2\rangle = \left\langle\tilde{\psi}_1 \,\middle|\, \tilde{\psi}_2\right\rangle \Rightarrow \langle\psi \mid \psi\rangle = \left\langle\tilde{\psi} \,\middle|\, \tilde{\psi}\right\rangle \tag{2.84}$$

Postulate 2

Let $\psi(\vec{x},t)$ be the wave function for a particle under the influence of given forces. Then,

$$\tilde{\wp}(\vec{p},t) = \frac{\left|\tilde{\psi}(\vec{p},t)\right|^2}{\langle\psi \mid \psi\rangle} \tag{2.85}$$

where $\psi(\vec{x},t)$ and $\tilde{\psi}(\vec{p},t)$ are related as in (2.83).

Recall that postulate 1 says that

$$\wp(\vec{x},t) = \frac{|\psi(\vec{x},t)|^2}{\langle\psi \mid \psi\rangle} \tag{2.86}$$

Thus, the position distribution and the momentum distribution are related!!! The relationship is somewhat complicated because $\psi(\vec{x},t)$ and $\tilde{\psi}(\vec{p},t)$ are related by Fourier transformation in momentum space.

We recall that the average value of $f(\vec{x})$ is given by

$$\begin{aligned}\langle f(\vec{x})\rangle &= \frac{1}{\langle\psi \mid \psi\rangle}\int d^3x\psi^*(\vec{x},t)f(\vec{x})\psi(\vec{x},t)\\ &= \frac{1}{\langle\psi \mid \psi\rangle}\langle\psi|\, f(\vec{x})\,|\psi\rangle\end{aligned} \tag{2.87}$$

Now consider the function $g(\vec{p})$. We have for the average value of $g(\vec{p})$

$$\begin{aligned}\langle g(\vec{p})\rangle &= \int d^3p\tilde{\wp}(\vec{p},t)g(\vec{p}) = \int d^3p\frac{\left|\tilde{\psi}(\vec{p},t)\right|^2}{\langle\psi \mid \psi\rangle}g(\vec{p})\\ &= \frac{1}{\langle\psi \mid \psi\rangle}\int d^3p\tilde{\psi}^*(\vec{p},t)g(\vec{p})\tilde{\psi}(\vec{p},t) = \frac{1}{\langle\psi \mid \psi\rangle}\left\langle\tilde{\psi}\right|g(\vec{p})\left|\tilde{\psi}\right\rangle\end{aligned}$$

It would be somewhat simpler if we could calculate $\langle g(\vec{p})\rangle$ in terms of $\psi(\vec{x},t)$, so that we would not have to Fourier transform $\psi(\vec{x},t)$ explicitly.

Consider $\langle p_i\rangle$ where

$$p_1 = p_x,\ p_2 = p_y,\ p_3 = p_z,\ x_1 = x,\ x_2 = y,\ x_3 = z$$

We have

$$\begin{aligned}\langle p_i\rangle &= \frac{1}{\langle\psi \mid \psi\rangle}\int d^3p\tilde{\psi}^*(\vec{p},t)p_i\tilde{\psi}(\vec{p},t)\\ &= \frac{1}{\langle\psi \mid \psi\rangle}\int d^3p\tilde{\psi}^*(\vec{p},t)[p_i\tilde{\psi}(\vec{p},t)]\end{aligned} \tag{2.88}$$

Using Parseval's relation we have

$$\langle p_i\rangle = \frac{1}{\langle\psi \mid \psi\rangle}\int d^3x\psi^*(\vec{x},t)\left(InverseFourierTransform[p_i\tilde{\psi}(\vec{p},t)]\right) \tag{2.89}$$

Now

$$
\begin{aligned}
[p_i\tilde{\psi}(\vec{p},t)] &= p_i \int \frac{d^3x}{(2\pi\hbar)^{3/2}} e^{-i\frac{\vec{p}}{\hbar}\cdot\vec{x}}\psi(\vec{x},t) \\
&= \int \frac{d^3x}{(2\pi\hbar)^{3/2}} \left\{-\frac{\hbar}{i}\frac{\partial}{\partial x_i}e^{-i\frac{\vec{p}}{\hbar}\cdot\vec{x}}\right\}\psi(\vec{x},t) \\
&= -\frac{\hbar}{i}\left[e^{-i\frac{\vec{p}}{\hbar}\cdot\vec{x}}\psi(\vec{x},t)\right]_{surface\ at\ \infty} + \frac{\hbar}{i}\int \frac{d^3x}{(2\pi\hbar)^{3/2}} e^{-i\frac{\vec{p}}{\hbar}\cdot\vec{x}}\frac{\partial\psi(\vec{x},t)}{\partial x_i} \\
&= \frac{\hbar}{i}\int \frac{d^3x}{(2\pi\hbar)^{3/2}} e^{-i\frac{\vec{p}}{\hbar}\cdot\vec{x}}\frac{\partial\psi(\vec{x},t)}{\partial x_i} \qquad (2.90)
\end{aligned}
$$

where we have integrated by parts in dx_i and used the fact that $\psi(\vec{x},t) = 0$ at $r = \infty$ so that all surface terms vanish. Therefore,

$$\langle p_i\rangle = \frac{1}{\langle\psi\mid\psi\rangle}\int d^3x\psi^*(\vec{x},t)\frac{\hbar}{i}\frac{\partial}{\partial x_i}\psi(\vec{x},t) \qquad (2.91)$$

Consider now

$$
\begin{aligned}
\left\langle p_x^L p_y^M p_z^N\right\rangle &= \frac{1}{\langle\psi\mid\psi\rangle}\int d^3p\tilde{\psi}^*(\vec{p},t)p_x^L p_y^M p_z^N\tilde{\psi}(\vec{p},t) \\
&= \frac{1}{\langle\psi\mid\psi\rangle}\int d^3p\tilde{\psi}^*(\vec{p},t)[p_x^L p_y^M p_z^N\tilde{\psi}(\vec{p},t)] \\
&= \frac{1}{\langle\psi\mid\psi\rangle}\int d^3x\psi^*(\vec{x},t)\left(InverseFourierTransform[p_x^L p_y^M p_z^N\tilde{\psi}(\vec{p},t)]\right)
\end{aligned}
$$

As before

$$p_x^L p_y^M p_z^N\tilde{\psi}(\vec{p},t) = \int \frac{d^3x}{(2\pi\hbar)^{3/2}}\left\{\left(-\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^L\left(-\frac{\hbar}{i}\frac{\partial}{\partial y}\right)^M\left(-\frac{\hbar}{i}\frac{\partial}{\partial z}\right)^N e^{-i\frac{\vec{p}}{\hbar}\cdot\vec{x}}\right\}\psi(\vec{x},t)$$

Integrating by parts $L+M+N$ times where all surface terms vanish, we get

$$p_x^L p_y^M p_z^N\tilde{\psi}(\vec{p},t) = \int \frac{d^3x}{(2\pi\hbar)^{3/2}}e^{-i\frac{\vec{p}}{\hbar}\cdot\vec{x}}\left\{\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^L\left(\frac{\hbar}{i}\frac{\partial}{\partial y}\right)^M\left(\frac{\hbar}{i}\frac{\partial}{\partial z}\right)^N\psi(\vec{x},t)\right\}$$

Therefore $InverseFourierTransform[p_x^L p_y^M p_z^N\tilde{\psi}(\vec{p},t)]$ is

$$\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^L\left(\frac{\hbar}{i}\frac{\partial}{\partial y}\right)^M\left(\frac{\hbar}{i}\frac{\partial}{\partial z}\right)^N\psi(\vec{x},t)$$

and we obtain

$$\left\langle p_x^L p_y^M p_z^N\right\rangle = \frac{1}{\langle\psi\mid\psi\rangle}\int d^3x\psi^*(\vec{x},t)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^L\left(\frac{\hbar}{i}\frac{\partial}{\partial y}\right)^M\left(\frac{\hbar}{i}\frac{\partial}{\partial z}\right)^N\psi(\vec{x},t)$$

Thus, if $g(\vec{p})$ has a Taylor expansion about $\vec{p} = 0$, $g(\vec{p})$ = a sum of terms of the form $p_x^L p_y^M p_z^N$. Since the average of a sum is the sum of the averages, we have

$$\langle g(\vec{p})\rangle = \frac{1}{\langle\psi\mid\psi\rangle}\int d^3x\psi^*(\vec{x},t)g\left(\frac{\hbar}{i}\frac{\partial}{\partial x},\frac{\hbar}{i}\frac{\partial}{\partial y},\frac{\hbar}{i}\frac{\partial}{\partial z}\right)\psi(\vec{x},t) \qquad (2.92)$$

where

$$g\left(\frac{\hbar}{i}\frac{\partial}{\partial x}, \frac{\hbar}{i}\frac{\partial}{\partial y}, \frac{\hbar}{i}\frac{\partial}{\partial z}\right) \tag{2.93}$$

acts on $\psi(\vec{x}, t)$. If we use

$$\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right) \tag{2.94}$$

we have

$$\begin{aligned}\langle g(\vec{p})\rangle &= \frac{1}{\langle\psi \mid \psi\rangle}\int d^3x\psi^*(\vec{x}, t)g\left(\frac{\hbar}{i}\nabla\right)\psi(\vec{x}, t)\\ &= \frac{1}{\langle\psi \mid \psi\rangle}\langle\psi| g\left(\frac{\hbar}{i}\nabla\right)|\psi\rangle\end{aligned} \tag{2.95}$$

We now define the momentum operator

$$\vec{p}_{op} = \frac{\hbar}{i}\nabla \tag{2.96}$$

that is,

$$p_{j,op} = \frac{\hbar}{i}\frac{\partial}{\partial x_i} \tag{2.97}$$

Then

$$\langle g(\vec{p})\rangle = \frac{1}{\langle\psi \mid \psi\rangle}\langle\psi| g(\vec{p}_{op})|\psi\rangle \tag{2.98}$$

and

$$\langle f(\vec{x})\rangle = \frac{1}{\langle\psi \mid \psi\rangle}\langle\psi| f(\vec{x})|\psi\rangle \tag{2.99}$$

and we are able to do everything using $\psi(\vec{x}, t)$.

Example: Kinetic Energy

$$\begin{aligned}kinetic\, energy &= \frac{1}{2}m\left(v_x^2 + v_y^2 + v_z^2\right)\\ &= \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2\right) = \frac{1}{2m}\left(\vec{p}\cdot\vec{p}\right)\end{aligned} \tag{2.100}$$

Therefore, the operator for the non-relativistic kinetic energy is

$$\begin{aligned}(KE)_{op} &= \frac{1}{2m}\left(-\hbar^2\frac{\partial^2}{\partial x^2} - \hbar^2\frac{\partial^2}{\partial y^2} - \hbar^2\frac{\partial^2}{\partial z^2}\right)\\ &= -\frac{\hbar^2}{2m}\nabla^2\end{aligned} \tag{2.101}$$

and

$$\begin{aligned}\langle KE\rangle &= \frac{1}{\langle\psi \mid \psi\rangle}\langle\psi| - \frac{\hbar^2}{2m}\nabla^2|\psi\rangle\\ &= -\frac{1}{\langle\psi \mid \psi\rangle}\frac{\hbar^2}{2m}\int d^3x\psi^*(\vec{x}, t)\nabla^2\psi(\vec{x}, t)\end{aligned} \tag{2.102}$$

Operators will play a fundamental role in our development of quantum theory.

2.1.5. Operator Formalism

An operator maps functions into functions. Consider an operator $\hat{A}$ ($\hat{}$ signifies an operator). We have

$$\hat{A}\phi_1(\vec{x}) = \phi_2(\vec{x}) \Rightarrow \hat{A}\phi_1 = \phi_2 \tag{2.103}$$

where the last form is standard and the variable(position)dependence is understood.

In words, the operator $\hat{A}$ acts on the function $\phi_1(\vec{x})$ to produce the function $\phi_2(\vec{x})$.

2.1.5.1. Examples

1. $\hat{A}\phi = x_j\phi$ = multiplication by x_j
2. $\hat{A}\phi = \frac{\hbar}{i}\frac{\partial}{\partial x_j}\phi$ = momentum operator
3. $\hat{A}\phi = x_j\phi + \frac{\hbar}{i}\frac{\partial}{\partial x_j}\phi$ or $\hat{A} = x_j + \frac{\hbar}{i}\frac{\partial}{\partial x_j}$
4. $\hat{A}\phi(\vec{x}) = \int d^3y\, K(\vec{x},\vec{y})\phi(\vec{y})$ or $\hat{A}$ = an integral operator
5. $\hat{A}\phi = \phi\frac{\partial\phi}{\partial x_j}$

Definition: An operator is *linear* if $\hat{A}(\lambda_1\phi_1 + \lambda_2\phi_2) = \lambda_1\hat{A}\phi_1 + \lambda_2\hat{A}\phi_2$ for all complex constants λ_1 and λ_2 and for all ϕ_1 and ϕ_2.

In the examples above (1), (2), (3) and (4) are linear operators and (5) is not linear. From now on, all our operators will be linear.

The momentum operator and the kinetic energy operator are both linear!

2.1.5.2. Example

Consider

$$\hat{A} = \frac{\partial}{\partial x} \quad , \quad \hat{B} = x$$

First

$$\hat{A}\hat{B} \neq \frac{\partial}{\partial x}x = 1 \tag{2.104}$$

To calculate $\hat{A}\hat{B}$ correctly, we must compute $(\hat{A}\hat{B})\phi = \hat{A}(\hat{B}\phi)$ with an arbitrary ϕ. We have

$$\begin{aligned}(\hat{A}\hat{B})\phi = \hat{A}(\hat{B}\phi) &= \frac{\partial}{\partial x}(x\phi) \\ &= \phi + x\frac{\partial\phi}{\partial x} = \left(1 + x\frac{\partial}{\partial x}\right)\phi = \hat{A}(\hat{B}\phi)\end{aligned} \tag{2.105}$$

so that

$$\hat{A}\hat{B} = 1 + x\frac{\partial}{\partial x} \tag{2.106}$$

Definition: The commutator of 2 linear operators $\hat{A}$ and $\hat{B}$ is defined to be $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ (unlike numbers, operators do not necessarily commute).

2.1.5.3. Example

$$\begin{aligned}
&[x_i, p_{j,op}]\,\phi \\
&\quad = \frac{\hbar}{i} x_i \frac{\partial \phi}{\partial x_j} - \frac{\hbar}{i}\frac{\partial (x_i \phi)}{\partial x_j} \\
&\quad = -\frac{\hbar}{i}\frac{\partial x_i}{\partial x_j}\phi = -\frac{\hbar}{i}\delta_{ij}\phi
\end{aligned}$$

so that

$$[x_i, p_{j,op}] = i\hbar\delta_{ij} \tag{2.107}$$

Using similar algebra, we find

$$[x_i, x_j] = 0 \;\;,\;\; [p_{i,op}, p_{j,op}] = 0 \quad \text{using} \quad \frac{\partial^2}{\partial x_i \partial x_j} = \frac{\partial^2}{\partial x_j \partial x_i} \tag{2.108}$$

These commutators will be of fundamental importance in our development of quantum theory.

Now, recall the definition of the inner product

$$\langle \phi_1 \mid \phi_2 \rangle = \int d^3x\, \phi_1^*(\vec{x})\phi_2(\vec{x}) \tag{2.109}$$

Thus,

$$\left\langle \phi_1 \,\middle|\, \hat{A}\phi_2 \right\rangle = \langle \phi_1 \mid \psi \rangle = \int d^3x \phi_1^*(\vec{x})\psi(\vec{x}) = \int d^3x \phi_1^*(\vec{x})\hat{A}\phi_2(\vec{x}) \tag{2.110}$$

$$\left\langle \hat{A}\phi_1 \,\middle|\, \phi_2 \right\rangle = \langle \varsigma \mid \phi_2 \rangle = \int d^3x \varsigma^*(\vec{x})\phi_2(\vec{x}) = \int d^3x \left[\hat{A}\phi_1\right]^* \phi_2(\vec{x}) \tag{2.111}$$

where $\left[\hat{A}\phi_1\right]^*$ means that the operator $\hat{A}$ acts on ϕ_1 to produce ξ and then it is complex-conjugated.

Definition: A linear operator is *hermitian* if

$$\left\langle \phi \,\middle|\, \hat{A}\phi \right\rangle = \left\langle \hat{A}\phi \,\middle|\, \phi \right\rangle \tag{2.112}$$

for all $\phi(\vec{x})$ on which $\hat{A}$ is defined. Note that

$$\left\langle \phi \,\middle|\, \hat{A}\phi \right\rangle = \left\langle \hat{A}\phi \,\middle|\, \phi \right\rangle^* \tag{2.113}$$

implies that an operator $\hat{A}$ is hermitian if $\left\langle \phi \middle| \hat{A}\phi \right\rangle$ is real for all $\phi(\vec{x})$. x_j and $p_{i,op} = -i\hbar\partial/\partial x_j$ are hermitian. If $\hat{A}\hat{B}$ is hermitian, then $\hat{B}\hat{A}$ is hermitian only if $[\hat{A}, \hat{B}] = 0$.

2.1.6. Heisenberg's Uncertainty Principle

We have seen that the probability distribution in $\vec{x}$ (position) and the probability distribution in $\vec{p}$ (momentum) are related, The relationship involves the Fourier transform. For $\vec{p} = \hbar\vec{k}$ we found earlier that

$$\psi(\vec{x},t) = \int \frac{d^3k}{(2\pi)^{3/2}} e^{+i\vec{k}\cdot\vec{x}} \phi(\vec{k},t) \leftrightarrow \phi(\vec{k},t) = \int \frac{d^3x}{(2\pi)^{3/2}} e^{-i\vec{k}\cdot\vec{x}} \psi(\vec{x},t)$$

$$\psi(\vec{x},t) = \int \frac{d^3p}{(2\pi\hbar)^{3/2}} e^{+i\frac{\vec{p}}{\hbar}\cdot\vec{x}} \tilde{\psi}(\vec{p},t) \leftrightarrow \tilde{\psi}(\vec{p},t) = \int \frac{d^3x}{(2\pi\hbar)^{3/2}} e^{-i\frac{\vec{p}}{\hbar}\cdot\vec{x}} \psi(\vec{x},t)$$

$$\wp(\vec{x},t) = \frac{|\psi(\vec{x},t)|^2}{\langle\psi \mid \psi\rangle} \leftrightarrow \tilde{\wp}(\vec{p},t) = \frac{\left|\tilde{\psi}(\vec{p},t)\right|^2}{\langle\psi \mid \psi\rangle} = \frac{1}{\hbar^3} \frac{\left|\phi(\vec{k},t)\right|^2}{\langle\psi \mid \psi\rangle}$$

In wave mechanics, Heisenberg's Uncertainty Principle relates the rms deviation of the position distribution to the rms deviation of the momentum distribution. Such a relationship follows from the above Fourier transform relationship.

Heuristic Argument: We have

$$\psi(\vec{x},t) = \int \frac{d^3k}{(2\pi)^{3/2}} e^{+i\vec{k}\cdot\vec{x}} \phi(\vec{k},t) \tag{2.114}$$

Let $y = z = 0$ and consider the dependence on the $x-$coordinate. Let $\phi(\vec{k},t)$ be real for simplicity and consider $Real(\psi(\vec{x},t))$. Therefore,

$$\mathrm{Re}(\psi(\vec{x},t)) = \int \frac{d^3k}{(2\pi)^{3/2}} \cos(k_x x)\phi(\vec{k},t) \tag{2.115}$$

that is, $Real(\psi(\vec{x},t))$ = sum of cosine terms, each with a different wavelength $\lambda_x = 2\pi/k_x$. As shown in Figure 2.6 below for two such cosine terms with different wavelengths, we have regions where the waves are in phase and regions where the waves are out of phase.

waves in phase → constructive interference

waves out of phase → destructive interference

$Real(\psi(\vec{x},t))$ will be negligible in the regions where the cosine terms interfere destructively. In the $x-$region where the cosine terms interfere constructively, $Real(\psi(\vec{x},t))$ will be non-negligible (similarly for $Imag(\psi(\vec{x},t))$).

Now consider the more general case: $\phi(\vec{k},t)$ is complex and x, y, and z are arbitrary. Let Δx be the $x-$region in which $\psi(\vec{x},t)$ is non-negligible (t fixed, y and z fixed). Let Δk_x be the k_x integration region over which $\phi(\vec{k},t)$ is non-negligible. $\psi(\vec{x},t)$ is a superposition of terms $e^{ik_x x}$ of wavelength $\lambda_x = 2\pi/k_x$. For $\psi(\vec{x},t)$ to a certain region Δx, there must be constructive interference of the $e^{ik_x x}$ terms in this region and destructive interference everywhere else. Let

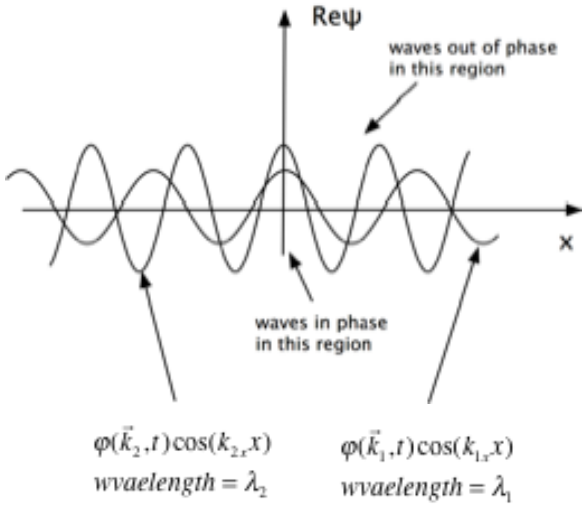


Figure 2.6: Wave Interference

$\phi(\vec{k},t)$ be non-negligible only when $k_a < k_x < k_b$ (t, k_y, k_z $fixed$) so that $\Delta k_x = k_b - k_a$. There are

$$\frac{\Delta x}{\lambda_a} = \frac{k_a \Delta x}{2\pi} \tag{2.116}$$

number of wavelengths in the region Δx when $k_x = k_a$ and

$$\frac{\Delta x}{\lambda_b} = \frac{k_b \Delta x}{2\pi} \tag{2.117}$$

number of wavelengths in the region Δx when $k_x = k_b$. For the $e^{ik_x x}$ terms ($k_a < k_x < k_b$) to interfere destructively at the limits of (and beyond) the interval Δx

$$\frac{k_b \Delta x}{2\pi} - \frac{k_a \Delta x}{2\pi} \tag{2.118}$$

must be at least one, that is,

$$\frac{\Delta k_x \Delta x}{2\pi} \geq 1 \tag{2.119}$$

(similar arguments hold for the localization in the y and z directions). Therefore we have

$$\Delta k_x \Delta x \geq 2\pi \quad , \quad \Delta k_y \Delta y \geq 2\pi \quad , \quad \Delta k_z \Delta z \geq 2\pi \tag{2.120}$$

or using $\vec{k} = \vec{p}/\hbar$, $\hbar = h/2\pi$ we have

$$\Delta p_x \Delta x \geq h \quad , \quad \Delta p_y \Delta y \geq h \quad , \quad \Delta p_z \Delta z \geq h \tag{2.121}$$

These are the so-called *Heisenberg Uncertainty Relations. If a particle has non-negligible probability to be found in a region $(\Delta x, \Delta y, \Delta z)$ of $\vec{x}$, that is, the particle is said to be localized within this region, then the probability of measuring*

the particle's linear momentum is non-negligible in the range $(\Delta p_x, \Delta p_y, \Delta p_z)$ *of* $\vec{p}$ *with the Heisenberg Uncertainty Relations a necessary constraint on the position spread and the momentum range.* For example, if we prepare a particle at t_0 so that it has non-negligible probability to be found with x-coordinate in the interval $(x_0, x_0 + \Delta x)$ and negligible probability to be found elsewhere, then any measurement of p_x at t_0 will yield a value somewhere in the range $(p_{x0}, p_{x0} + \Delta p_x)$ where $\Delta p_x \geq h/\Delta x$ (x_0 and p_0 are arbitrary).

Classically, one specifies the precise position *and* momentum (or velocity) of a particle at some initial time. One then finds the position of the particle as a function of time by solving the classical equations of motion with the above initial conditions. We now see that this formulation of a particle's time development is impossible *quantum mechanically*: the Uncertainty Principle prohibits the precise specification of both the particle's position and its momentum at some initial time.

Indeed, $\Delta x = 0$ (particle localized at a point) $\rightarrow \Delta p_x = \infty$, in some sense, (particle's momentum is completely uncertain).

The spread in momentum necessitated by a spatial localization can be illustrated in an electron diffraction experiment as shown Figure 2.7 below.

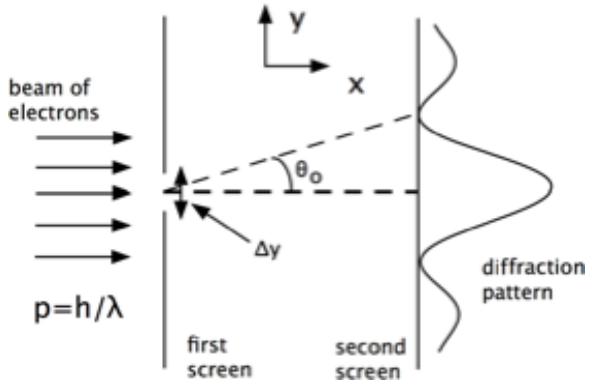


Figure 2.7: Electron Diffraction

Electrons which pass through the slit have a $y-$localization Δy at the first screen. Most of these electrons arrive at the second screen with $\theta < \theta_0$ where θ_0 locates the first diffraction minimum

$$d \sin\theta_0 = (\Delta y) \sin\theta_0 = \lambda = \frac{h}{p} \Rightarrow (\Delta y)(p \sin\theta_0) = h \tag{2.122}$$

But $p \sin\theta_0 = y-$component of momentum of an electron (with total momentum of magnitude p) arriving very near the first diffraction minimum. Of course,

no electrons arrive exactly at θ_0. Thus, most of the electrons(in first or central bump) arriving at the second screen have a $y-$component of momentum in the range $[-p\sin\theta_0, +p\sin\theta_0]$ so that $\Delta p_y \approx p\sin\theta_0$ and thus $\Delta p_y \Delta y \geq h$ in agreement with the *Uncertainty Principle*.

2.1.6.1. Discussion

When electrons are to the left of the first screen, $(\Delta p_y)_{incident} = 0$. Therefore, $(\Delta y)_{incident} = \infty$ (so that $\Delta p_y \Delta y \approx h$) and the incident beam is uniformly distributed over all y. Thus, the wave function $\psi_{incident}(\vec{x}, t)$ for an electron to the left of the first screen is independent of y (so that $\wp_{incident}(\vec{x}, t)$ is independent of y). That is the meaning of an *infinite plane wave*. An electron which passes through the slit (and eventually reaches the second screen) necessarily has a new Δy = linear dimension of the slit. The electron's passage through the slit constitutes a measurement of the electron's coordinate to an accuracy Δy. This measurement has necessarily changed the electron's wave function because $(\Delta y)_{incident} \neq (\Delta y)_{slit}$. *In general, a measurement made on a particle will change the particle's wave function.* In this example, $\psi_{incident}(\vec{x}, t)$ is independent of y. Right after the electron passes through the slit (corresponding to a measurement of the electron's $y-$coordinate), the electron has a new wave function $\psi_{new}(\vec{x}, t)$ which is non-negligible only in a δy range (the slit's width). Detection of the electron at the second screen allows us to determine p_y of the electron which passed through the slit. As we have seen, the spread in such p_y values is $\Delta p_y \approx h/\Delta y$. It seems at this point that The HUP is implied by the fundamental properties of the x and p bases and also the Fourier transform. This latter dependence is deceiving and only appears to be true when using the x and p bases.

2.1.6.2. Rigorous Argument

Let $\hat{A}$ and $\hat{B}$ be two hermitian operators. For example, $\hat{A}$ and $\hat{B}$ can be chosen from the operators x, y, z, $p_{x,op}$, $p_{y,op}$, $p_{z,op}$. Let $\psi(\vec{x}, t)$ be the wave function at time t and let ΔA and ΔB be the rms deviations of measurements of $\hat{A}$ and $\hat{B}$ at time t, defined by

$$(\Delta A)^2 = \left\langle \left(\hat{A} - \left\langle \hat{A} \right\rangle\right)^2 \right\rangle = \left\langle \hat{A}^2 \right\rangle - \left\langle \hat{A} \right\rangle^2 \tag{2.123}$$

$$(\Delta B)^2 = \left\langle \left(\hat{B} - \left\langle \hat{B} \right\rangle\right)^2 \right\rangle = \left\langle \hat{B}^2 \right\rangle - \left\langle \hat{B} \right\rangle^2 \tag{2.124}$$

Now let $\hat{C} = \hat{A} - \langle \hat{A} \rangle$ and $\hat{D} = \hat{B} - \langle \hat{B} \rangle$. Because $\langle \hat{A} \rangle$ and $\langle \hat{B} \rangle$ are real (hermiticity), $\hat{C}$ and $\hat{D}$ are also hermitian. Now we assume that $\psi(\vec{x}, t)$ is normalized so that $\langle \psi \,|\, \psi \rangle = 1$. Then

$$\begin{aligned}(\Delta A)^2 (\Delta B)^2 &= \left\langle \hat{C}^2 \right\rangle \left\langle \hat{D}^2 \right\rangle \\ &= \left\langle \psi \,\middle|\, \hat{C}\hat{C}\psi \right\rangle \left\langle \psi \,\middle|\, \hat{D}\hat{D}\psi \right\rangle = \left\langle \hat{C}\psi \,\middle|\, \hat{C}\psi \right\rangle \left\langle \hat{D}\psi \,\middle|\, \hat{D}\psi \right\rangle\end{aligned}$$

where we have used hermiticity in the last step. Then using the Schwarz inequality we have

$$(\Delta A)^2(\Delta B)^2 \geq \left|\left\langle \hat{C}\psi \mid \hat{D}\psi \right\rangle\right|^2 = \left|\left\langle \psi \mid \hat{C}\hat{D}\psi \right\rangle\right|^2 \tag{2.125}$$

where equality holds if and only if $(\hat{C}\psi) = \lambda(\hat{D}\psi)$ where λ = some constant.

Now we can always write

$$\hat{C}\hat{D} = \frac{1}{2}\left(\hat{C}\hat{D} + \hat{D}\hat{C}\right) + \frac{1}{2}\left(\hat{C}\hat{D} - \hat{D}\hat{C}\right) \tag{2.126}$$

and since $\hat{C}$ and $\hat{D}$ are hermitian, we have

$$\frac{1}{2}\left(\hat{C}\hat{D} + \hat{D}\hat{C}\right) \Rightarrow hermitian \tag{2.127}$$

$$\frac{1}{2}\left(\hat{C}\hat{D} - \hat{D}\hat{C}\right) \Rightarrow anti-hermitian \tag{2.128}$$

so that

$$\left\langle \psi \,\middle|\, \frac{1}{2}\left(\hat{C}\hat{D} + \hat{D}\hat{C}\right)\psi \right\rangle \Rightarrow pure\ real \tag{2.129}$$

$$\left\langle \psi \,\middle|\, \frac{1}{2}\left(\hat{C}\hat{D} - \hat{D}\hat{C}\right)\psi \right\rangle \Rightarrow pure\ imaginary \tag{2.130}$$

Proof

$$\begin{aligned}
\left\langle \psi \,\middle|\, \frac{1}{2}\left(\hat{C}\hat{D} \pm \hat{D}\hat{C}\right)\psi \right\rangle &= \frac{1}{2}\left\langle \psi \mid \hat{C}\hat{D}\psi \right\rangle \pm \frac{1}{2}\left\langle \psi \mid \hat{D}\hat{C}\psi \right\rangle \\
&= \frac{1}{2}\left\langle \hat{C}\psi \mid \hat{D}\psi \right\rangle \pm \frac{1}{2}\left\langle \hat{D}\psi \mid \hat{C}\psi \right\rangle \\
&= \frac{1}{2}\left\langle \hat{D}\hat{C}\psi \mid \psi \right\rangle \pm \frac{1}{2}\left\langle \hat{C}\hat{D}\psi \mid \psi \right\rangle \\
&= \frac{1}{2}\left\langle \psi \mid \hat{D}\hat{C}\psi \right\rangle^* \pm \frac{1}{2}\left\langle \psi \mid \hat{C}\hat{D}\psi \right\rangle^* \\
&= \pm\left\langle \psi \,\middle|\, \frac{1}{2}\left(\hat{C}\hat{D} \pm \hat{D}\hat{C}\right)\psi \right\rangle^*
\end{aligned}$$

Continuing, we then have

$$\begin{aligned}
(\Delta A)^2(\Delta B)^2 &\geq \left| \underbrace{\left\langle \psi \,\middle|\, \frac{1}{2}\left(\hat{C}\hat{D} + \hat{D}\hat{C}\right)\psi \right\rangle}_{pure\ real} + \underbrace{\left\langle \psi \,\middle|\, \frac{1}{2}\left(\hat{C}\hat{D} - \hat{D}\hat{C}\right)\psi \right\rangle}_{pure\ imaginary} \right|^2 \\
&\geq \left|\left\langle \psi \,\middle|\, \frac{1}{2}\left(\hat{C}\hat{D} + \hat{D}\hat{C}\right)\psi \right\rangle\right|^2 + \left|\left\langle \psi \,\middle|\, \frac{1}{2}\left(\hat{C}\hat{D} - \hat{D}\hat{C}\right)\psi \right\rangle\right|^2 \\
&\geq \left|\left\langle \psi \,\middle|\, \frac{1}{2}\left(\hat{C}\hat{D} - \hat{D}\hat{C}\right)\psi \right\rangle\right|^2
\end{aligned}$$

where equality holds if

$$\left\langle \psi \,\middle|\, \frac{1}{2}\left(\hat{C}\hat{D}+\hat{D}\hat{C}\right)\psi \right\rangle = 0 \tag{2.131}$$

Finally, we have

$$(\Delta A)^2(\Delta B)^2 \geq \frac{1}{4}\left|\left\langle \psi \,\middle|\, \left[\hat{C},\hat{D}\right]\psi\right\rangle\right|^2 \tag{2.132}$$

However,

$$\begin{aligned}\left[\hat{C},\hat{D}\right] &= \left(\hat{A}-\left\langle\hat{A}\right\rangle\right)\left(\hat{B}-\left\langle\hat{B}\right\rangle\right)-\left(\hat{B}-\left\langle\hat{B}\right\rangle\right)\left(\hat{A}-\left\langle\hat{A}\right\rangle\right)\\ &= \hat{A}\hat{B}-\hat{B}\hat{A} = \left[\hat{A},\hat{B}\right]\end{aligned}$$

so that

$$(\Delta A)^2(\Delta B)^2 \geq \frac{1}{4}\left|\left\langle \psi \,\middle|\, \left[\hat{A},\hat{B}\right]\psi\right\rangle\right|^2 \tag{2.133}$$

or our final result is

$$(\Delta A)(\Delta B) \geq \frac{1}{2}\left|\left\langle \psi \,\middle|\, \left[\hat{A},\hat{B}\right]\psi\right\rangle\right| \tag{2.134}$$

where equality holds if 2 conditions are simultaneously satisfied:

1. $(\hat{C}\psi) = \lambda(\hat{D}\psi)$ for some constant λ
2. $\left\langle \psi \,\middle|\, \frac{1}{2}\left(\hat{C}\hat{D}+\hat{D}\hat{C}\right)\psi\right\rangle = 0$

This result is the *Uncertainty Principle*. It is a necessary constraint on the rms deviations of measurements of $\hat{A}$ and $\hat{B}$ when a particle has the wave function $\psi(\vec{x},t)$.

This result holds for any hermitian operators $\hat{A}$ and $\hat{B}$. $\hat{A}$ and $\hat{B}$ may be chosen from the operators x, y, z, $p_{x,op}$, $p_{y,op}$, $p_{z,op}$; however, in later applications we will use other operators.

We note that ΔA, ΔB and $\langle\psi|[\hat{A},\hat{B}]|\psi\rangle$ refer to quantities evaluated at the same time t because each has been expressed in terms of $\psi(\vec{x},t)$ evaluated at one fixed time t.

2.1.6.3. Examples

Using $[x_i,p_{j,op}] = i\hbar\delta_{ij}$, $[x_i,x_j] = 0$ and $[p_{i,op},p_{j,op}] = 0$ we have

$$(\Delta x_i)(\Delta x_j) \geq 0 \quad , \quad (\Delta p_i)(\Delta p_j) \geq 0 \tag{2.135}$$

and

$$(\Delta x_i)(\Delta p_j) \geq \frac{\hbar}{2}\delta_{ij} \tag{2.136}$$

which agree with the results of our heuristic arguments.

Let us find $\psi(\vec{x},t)$ such that the equalities hold in the equations

$$\Delta x \Delta p_x \geq \frac{\hbar}{2} \quad , \quad \Delta y \Delta p_y \geq \frac{\hbar}{2} \quad , \quad \Delta z \Delta p_z \geq \frac{\hbar}{2} \tag{2.137}$$

For simplicity we work with the x equation. Similar results follow for the other equations. Now

$$\Delta x \Delta p_x = \frac{\hbar}{2} \tag{2.138}$$

If

1. $(\hat{C}\psi) = \lambda(\hat{D}\psi)$ for some constant λ
2. $\left\langle \psi \mid \frac{1}{2}\left(\hat{C}\hat{D} + \hat{D}\hat{C}\right)\psi \right\rangle = 0$

where $\hat{C} = \hat{A} - \langle \hat{A} \rangle = p_{x,op} - \langle p_{x,op} \rangle$ and $\hat{D} = \hat{B} - \langle \hat{B} \rangle = x - \langle x \rangle$. Substituting condition (1) into condition (2) we get

$$\begin{aligned}
\left\langle \psi \left| \frac{1}{2}\left(\hat{C}\hat{D} + \hat{D}\hat{C}\right)\psi \right. \right\rangle = 0 &= \left\langle \psi \mid \hat{C}\hat{D}\psi \right\rangle + \left\langle \psi \mid \hat{D}\hat{C}\psi \right\rangle \\
&= \left\langle \hat{C}\psi \mid \hat{D}\psi \right\rangle + \left\langle \psi \mid \hat{D}(\hat{C}\psi) \right\rangle \\
&= \left\langle \lambda\hat{D}\psi \mid \hat{D}\psi \right\rangle + \left\langle \psi \mid \lambda\hat{D}\hat{D}\psi \right\rangle \\
&= \lambda^* \left\langle \psi \mid \hat{D}\psi \right\rangle + \lambda \left\langle \psi \mid \lambda\hat{D}\hat{D}\psi \right\rangle \\
&\Rightarrow 0 = (\lambda^* + \lambda) \left\langle \psi \mid \hat{D}\hat{D}\psi \right\rangle
\end{aligned}$$

Since $\left\langle \psi \left| \hat{D}\hat{D}\psi \right. \right\rangle ne 0$, we have $\lambda^* + \lambda = 0 \rightarrow \lambda^* = -\lambda \rightarrow \lambda = i\alpha$ is pure imaginary; α real. The case $\left\langle \psi \left| \hat{D}\hat{D}\psi \right. \right\rangle = 0$, which implies that $\left\langle (x - \langle x \rangle)^2 \right\rangle = 0 = \Delta x$, is not considered here because $\Delta x = 0 \rightarrow \Delta p_x = \infty$. Now

$$\begin{aligned}
&(\hat{C}\psi) = \lambda(\hat{D}\psi) \Rightarrow (p_{x,op} - \langle p_x \rangle)\psi = i\alpha (x - \langle x \rangle)\psi \\
&\left(\frac{\hbar}{i}\frac{\partial}{\partial x} - \langle p_x \rangle\right)\psi = i\alpha (x - \langle x \rangle)\psi \\
&\frac{\partial \psi}{\partial x} = \frac{i}{\hbar}\langle p_x \rangle \psi - \frac{\alpha}{\hbar}(x - \langle x \rangle)\psi
\end{aligned}$$

This has solution

$$\psi(\vec{x},t) = F(y,z,t) e^{\frac{i}{\hbar}\langle p_x \rangle x} e^{-\frac{\alpha}{2\hbar}(x - \langle x \rangle)^2} \tag{2.139}$$

Note that α must be positive for $\psi(\vec{x},t)$ to be normalizable. To see the significance of α, let us calculate

$$(\Delta x)^2 = \frac{\left\langle \psi \left| (x - \langle x \rangle)^2 \psi \right. \right\rangle}{\langle \psi \mid \psi \rangle} \tag{2.140}$$

We have

$$(\Delta x)^2 = \frac{\int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz\, |F(y,z,t)|^2 \int_{-\infty}^{\infty} dx e^{-\frac{\alpha}{\hbar}(x-\langle x\rangle)^2} (x-\langle x\rangle)^2}{\int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz\, |F(y,z,t)|^2 \int_{-\infty}^{\infty} dx e^{-\frac{\alpha}{\hbar}(x-\langle x\rangle)^2}}$$

$$= \frac{\int_{-\infty}^{\infty} dx e^{-\frac{\alpha}{\hbar}(x-\langle x\rangle)^2} (x-\langle x\rangle)^2}{\int_{-\infty}^{\infty} dx e^{-\frac{\alpha}{\hbar}(x-\langle x\rangle)^2}}$$

$$= \frac{\int_{-\infty}^{\infty} du e^{-\frac{\alpha}{\hbar}u^2} u^2}{\int_{-\infty}^{\infty} du x e^{-\frac{\alpha}{\hbar}u^2}} = \frac{\frac{\sqrt{\pi}}{2}\left(\frac{\hbar}{\alpha}\right)^{3/2}}{\frac{\sqrt{\pi}}{2}\left(\frac{\hbar}{\alpha}\right)^{1/2}} \frac{\hbar}{2\alpha}$$

so that

$$\psi(\vec{x},t) = F(y,z,t) e^{\frac{i}{\hbar}\langle p_x\rangle x} e^{-\frac{(x-\langle x\rangle)^2}{4(\Delta x)^2}} \tag{2.141}$$

$F(y,z,t)$ is determined similarly from $\Delta y \Delta p_y = \hbar/2$ and $\Delta z \Delta p_z = \hbar/2$. Therefore,

$$\psi(\vec{x},t) = N(t) e^{\frac{i}{\hbar}[\langle p_x\rangle x + \langle p_y\rangle y + \langle p_z\rangle z]} e^{-\left[\frac{(x-\langle x\rangle)^2}{4(\Delta x)^2} + \frac{(y-\langle y\rangle)^2}{4(\Delta y)^2} + \frac{(z-\langle z\rangle)^2}{4(\Delta z)^2}\right]} \tag{2.142}$$

if

$$\Delta x \Delta p_x = \frac{\hbar}{2} \quad , \quad \Delta y \Delta p_y = \frac{\hbar}{2} \quad , \quad \Delta z \Delta p_z = \frac{\hbar}{2} \tag{2.143}$$

In the above expression $\langle x\rangle, \langle y\rangle, \langle z\rangle, \langle p_x\rangle, \langle p_y\rangle, \langle p_x\rangle, \Delta x, \Delta y, \Delta z$ are arbitrary real numbers. The above expression gives a *Gaussian distribution* for

$$\wp(x,t) = \frac{|\psi(\vec{x},t)|^2}{\langle \psi \mid \psi\rangle} \tag{2.144}$$

For any *arbitrary(non-Gaussian)* wave function $\psi(\vec{x},t)$, we must have

$$(\Delta x_i)(\Delta p_i) \geq \frac{\hbar}{2} \tag{2.145}$$

2.1.6.4. Application of the Uncertainty Principle

Consider a particle constrained to move on the $x-$axis (idealized one-dimensional problem). $F_x = F_x(x)$ is the $x-$component of the force acting on the particle. This force depends on the position of the particle. Let $x = 0$ be an equilibrium point, that is, $F_x(x=0) = 0$. Taylor expanding $F_x(x)$ about $x = 0$ we have

$$F_x(x) = \underbrace{F_x(0)}_{=0} + \left[\frac{dF_x}{dx}\right]_{x=0} x + \frac{1}{2!}\left[\frac{d^2F_x}{dx^2}\right]_{x=0} x^2 + \ldots\ldots\ldots \tag{2.146}$$

For sufficiently small x, we can use

$$F_x(x) \approx \left[\frac{dF_x}{dx}\right]_{x=0} x \tag{2.147}$$

For

$$\left[\frac{dF_x}{dx}\right]_{x=0} > 0 \tag{2.148}$$

we have unstable equilibrium (F_x is directed away from the origin when the particle is slightly displaced from the equilibrium position).

For

$$\left[\frac{dF_x}{dx}\right]_{x=0} < 0 \tag{2.149}$$

we have stable equilibrium (F_x is directed toward the origin when the particle is slightly displaced from the equilibrium position).

Considering *small displacements from a stable equilibrium point* at $x = 0$:

$$F_x(x) = -kx \quad , \quad k > 0 \tag{2.150}$$

Classically, we have

$$m\frac{d^2x}{dt^2} = F_x = -kx \rightarrow \frac{d^2x}{dt^2} + \frac{k}{m}x = 0 \tag{2.151}$$

so that

$$x = A\cos\omega t + B\sin\omega t \quad , \quad \omega = \sqrt{\frac{k}{m}} \tag{2.152}$$

The total energy of such a particle is given by

$$E = \frac{1}{2}mv_x^2 + \frac{1}{2}kx^2 = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2x^2 \tag{2.153}$$

Quantum mechanically,

$$\langle E\rangle = \frac{1}{2m}\left\langle p_x^2\right\rangle + \frac{1}{2}m\omega^2\left\langle x^2\right\rangle \tag{2.154}$$

when the particle is described by the wave function $\psi(\vec{x}, t)$.

Note that this is really an *assumption* because, up to now, we have only considered $\langle f(\vec{x})\rangle$ and $\langle g(\vec{p})\rangle$. We have not yet discussed the quantum mechanical computation of $\langle f(\vec{x}) + g(\vec{p})\rangle$. This is not obvious since x and p cannot be simultaneously measured and will be discussed in detail later.

Now

$$(\Delta p_x)^2 = \left\langle p_x^2\right\rangle - \langle p_x\rangle^2 \quad , \quad (\Delta x)^2 = \left\langle x^2\right\rangle - \langle x\rangle^2 \tag{2.155}$$

Therefore,

$$\langle E\rangle = \frac{1}{2m}\left\langle p_x^2\right\rangle + \frac{1}{2}m\omega^2\left\langle x^2\right\rangle \geq \frac{(\Delta p_x)^2}{2m} + \frac{1}{2}m\omega^2(\Delta x)^2 \tag{2.156}$$

But,

$$\Delta p_x \geq \frac{\hbar}{2}\frac{1}{\Delta x} \tag{2.157}$$

from the uncertainty principle. Therefore,

$$\langle E\rangle \geq \frac{\hbar^2}{8m}\frac{1}{(\Delta x)^2} + \frac{1}{2}m\omega^2(\Delta x)^2 = G((\Delta x)^2) \tag{2.158}$$

This result holds for any wave function $\psi(\vec{x},t)$ since $\psi(\vec{x},t)$ determines both $\langle E\rangle$ and Δx. Therefore, $\langle E\rangle$ for any $\psi(\vec{x},t)$ is $\geq$ the minimum value of $G((\Delta x)^2)$. A sketch of $G((\Delta x)^2)$ is shown in Figure 2.8 below.

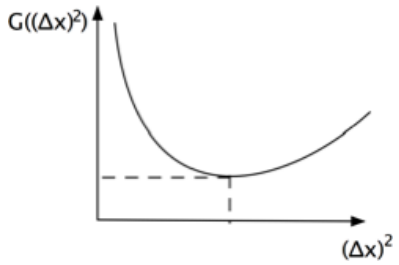


Figure 2.8: G$((\Delta x)^2)$ versus $(\Delta x)^2$

We find the minimum using

$$\frac{dG}{d((\Delta x)^2)} = 0 = -\frac{\hbar^2}{8m}\frac{1}{[(\Delta x)^2]^2} + \frac{1}{2}m\omega^2 \rightarrow (\Delta x)^4 = \frac{\hbar^2}{4m^2\omega^2} \tag{2.159}$$

at the minimum. Therefore,

$$\langle E\rangle \geq G_{\min}((\Delta x)^2) = \frac{\hbar\omega}{2} \tag{2.160}$$

for any wave function $\psi(\vec{x},t)$.

$\hbar\omega/2$ is called the *zero-point energy* of the particle. Classically, the particle could be located at $x = 0$ with zero velocity so that its energy would be zero.

Quantum mechanically, the uncertainty principle prohibits the particle from having a precise position at $x = 0$ and, at the same time a precise momentum of $p_x = 0$. The required spreads Δx and Δp_x satisfying $\Delta x \Delta p_x \geq \hbar/2$ imply

that the average energy of the particle can never be zero. This has striking consequences when the particle happens to be *charged*. Classically, an oscillating charge would radiate energy and thereby lose energy until it had no remaining energy. Quantum mechanically, the particle can radiate energy, but its (average) energy can never go below $\hbar\omega/2$. Thus, *if the particle has* $\langle E\rangle = \hbar\omega/2$ *it cannot radiate any energy* (even though the particle will, in some sense, be oscillating about $x = 0$). Clearly, the classical Maxwell equations must be modified and reinterpreted so that an oscillating charge in its *ground state* (which necessarily has $\langle E\rangle > 0$ for a harmonic oscillator) will not radiate!

I should also like to mention that this zero-point energy phenomenon is responsible for the stability of matter. One may think of the hydrogen atom, for example, as a proton with an electron circling about it. Classically, this accelerating electron would spiral into the proton as it continually radiated away its energy. The hydrogen atom would collapse! Such a fate is prevented by the uncertainty principle, which implies that the electron will have a ground-state energy where the electron and the proton have a non-zero separation - the electron cannot be precisely at the proton's position with precisely zero momentum.

In this case, we have

$$E = \frac{\vec{p}\cdot\vec{p}}{2m} + V(r) \quad , \quad V(r) = -\frac{e^2}{r} \tag{2.161}$$

and e = electron charge, r = distance between electron and proton. Classically, $E_{lowest} = -\infty (r = 0, \vec{p} = 0)$. We can obtain a rough estimate of E_{min} quantum mechanically. We have

$$\langle E\rangle = \frac{1}{2m}\langle \vec{p}\cdot\vec{p}\rangle - e^2\left\langle\frac{1}{r}\right\rangle \tag{2.162}$$

where m = electron mass. As a rough order of magnitude estimate we use

$$\langle \vec{p}\cdot\vec{p}\rangle \approx \left\langle p_{radial}^2\right\rangle \approx (\Delta p_{radial})^2$$
$$\left\langle\frac{1}{r}\right\rangle \approx \frac{1}{\langle r\rangle} \approx \frac{1}{\Delta r}$$

so that

$$\langle E\rangle \approx \frac{(\Delta p_{radial})^2}{2m} - \frac{e^2}{\Delta r} \quad , \quad (\Delta p_{radial})\,\Delta r \geq \frac{\hbar}{2} \approx \hbar \tag{2.163}$$

Therefore,

$$\langle E\rangle \geq \frac{\hbar^2}{2m}\frac{1}{(\Delta r)^2} - \frac{e^2}{\Delta r} = G(\Delta r) \rightarrow \langle E\rangle \geq G_{mimimum} \tag{2.164}$$

Minimizing G we have

$$\frac{dG}{d(\Delta r)} = 0 = -\frac{\hbar^2}{m}\frac{1}{(\Delta r)^3} + \frac{e^2}{(\Delta r)^2} \rightarrow \Delta r = \frac{\hbar^2}{me^2} \tag{2.165}$$

at the minimum. We get

$$\langle E \rangle \geq G_{\min imum} = -\frac{1}{2}\frac{me^4}{\hbar^2} \tag{2.166}$$

and

$$\langle r \rangle \approx \Delta r = \frac{\hbar^2}{me^2} \tag{2.167}$$

as a rough estimate of the hydrogen atom size.

Some numbers are:

$$\langle r \rangle \approx \Delta r = \frac{\hbar^2}{me^2} \approx 10^{-8} cm = 1 \tag{2.168}$$

or the uncertainty principle tells us that the hydrogen atom has a radius of roughly 1 Angstrom!!! (verified experimentally). We also have

$$E_{\min} = -\frac{1}{2}\frac{me^4}{\hbar^2} \approx 10^{-11} erg \approx 6\, eV \tag{2.169}$$

which is very different from the classical $E_{lowest} = -\infty$!!

We now return to our development of the quantum theory.

So far, we have considered the average values of functions of position

$$\langle f(\vec{x}) \rangle = \frac{\langle \psi \mid f(\vec{x})\psi \rangle}{\langle \psi \mid \psi \rangle} \tag{2.170}$$

and the average values of functions of momentum,

$$\langle g(\vec{p}) \rangle = \frac{\langle \psi \mid g(\vec{p}_{op})\psi \rangle}{\langle \psi \mid \psi \rangle} \quad , \quad \vec{p}_{op} = \frac{\hbar}{i}\vec{\nabla} \tag{2.171}$$

Of course, there are other kinds of functions where the average values are physically important, namely, functions of both position and momentum $A(\vec{x}, \vec{p})$. For example, the angular momentum of a particle is given by $\vec{L} = \vec{r} \times \vec{p}$ and the total energy of a particle with potential energy $V(\vec{x})$ is given by

$$E = \frac{\vec{p} \cdot \vec{p}}{2m} + V(\vec{x}) \tag{2.172}$$

Postulate 3 is an *obvious generalization* of the above expressions for $\langle f(\vec{x}) \rangle$ and $\langle g(\vec{p}) \rangle$ to functions $A(\vec{x}, \vec{p})$.

2.1.7. Postulate 3a

For every physical quantity $A(\vec{x}, \vec{p})$ [$A(\vec{x}, \vec{p})$ is a real function of $\vec{x}$ and $\vec{p}$], there exists a linear operator

$$A_{op} = A(\vec{x}, \vec{p}_{op}) \quad , \quad \vec{p}_{op} = \frac{\hbar}{i}\vec{\nabla} \tag{2.173}$$

such that for a particle with wave function $\psi(\vec{x},t)$

$$\langle A(\vec{x},\vec{p})\rangle = \frac{\langle\psi \mid A_{op}\psi\rangle}{\langle\psi \mid \psi\rangle} \tag{2.174}$$

is the average value of $A(\vec{x},\vec{p})$ at time t and

$$\langle f(A(\vec{x},\vec{p}))\rangle = \frac{\langle\psi \mid f(A_{op})\psi\rangle}{\langle\psi \mid \psi\rangle} \tag{2.175}$$

is the average value of $f(A(\vec{x},\vec{p}))$ at time t, where $f(A(\vec{x},\vec{p}))$ is an arbitrary function of $A(\vec{x},\vec{p})$.

2.1.7.1. Comments

1. Postulate 3a agrees with our previous results for $\langle f(\vec{x})\rangle$ and $\langle g(\vec{p})\rangle$ expressed in terms of the operators $f(\vec{x})$ and $g(\vec{p}_{op})$.

2. Consider $A(\vec{x},\vec{p}) = f(\vec{x}) + g(\vec{p})$. Then $\langle A(\vec{x},\vec{p})\rangle$ is given by

$$\begin{aligned}\langle A(\vec{x},\vec{p})\rangle &= \frac{\langle\psi \mid (f(\vec{x}) + g(\vec{p}_{op}))\psi\rangle}{\langle\psi \mid \psi\rangle} \\ &= \frac{\langle\psi \mid f(\vec{x})\psi\rangle + \langle\psi \mid g(\vec{p}_{op})\psi\rangle}{\langle\psi \mid \psi\rangle} \\ &= \langle f(\vec{x})\rangle + \langle g(\vec{p})\rangle\end{aligned} \tag{2.176}$$

   which we assumed to be true earlier. This result

$$\langle f(\vec{x}) + g(\vec{p}_{op})\rangle = \langle f(\vec{x})\rangle + \langle g(\vec{p}_{op})\rangle \tag{2.177}$$

   is *not* a trivial result. Consider an ensemble of identically-prepared particles. $\langle f(\vec{x})\rangle$ is the average value of the measurements of $f(\vec{x})$ performed on many of these particles, while $\langle g(\vec{p}_{op})\rangle$ is the average value of measurements of $g(\vec{p}_{op})$ performed on many of the particles. To measure $\langle f(\vec{x}) + g(\vec{p}_{op})\rangle$ we must do repeated measurements of the one physical quantity $f(\vec{x}) + g(\vec{p}_{op})$, that is, for each particle in the ensemble we must somehow perform a *single measurement* of the physical quantity $f(\vec{x}) + g(\vec{p}_{op})$ and then we must find the average value of such measurements. We *cannot* perform 2 measurements on each particle, the first to measure $f(\vec{x})$ and the second to measure $g(\vec{p}_{op})$, because the first measurement of $f(\vec{x})$ involves a position measurement which, according to the Uncertainty Principle, will change the particle's momentum distribution

$$(\Delta p_i)_{\substack{after\ first \\ measurement}} \geq \frac{\hbar}{2}\frac{1}{\Delta x_i} \tag{2.178}$$

   where Δx_i is the accuracy of the first position measurement, so that the second measurement of $g(\vec{p}_{op})$ does not measure $g(\vec{p}_{op})$ for the particle in

its original state.

Thus, it is not *a priori* obvious that $\langle f(\vec{x}) + g(\vec{p}_{op})\rangle$, calculated from repeated measurements of the single physical quantity $f(\vec{x}) + g(\vec{p}_{op})$ will equal $\langle f(\vec{x})\rangle + \langle g(\vec{p}_{op})\rangle$. While postulate 3a, however, asserts that this equality does hold - the above discussion implies that this is not a trivial result.

3. Postulate 3a as it stands, is ambiguous. For example, consider the physical quantities $A_1(\vec{x},\vec{p}) = xp_x$ and $A_2(\vec{x},\vec{p}) = p_x x$. Classically, $A_1(\vec{x},\vec{p}) = xp_x = p_x x = A_2(\vec{x},\vec{p})$ because x and p_x are just measured numbers. However, the quantum operators A_1 and A_2 differ:

$$A_{1op} = xp_{xop} \quad , \quad A_{2op} = p_{xop}x \tag{2.179}$$

where

$$A_{1op} - A_{2op} = [x, p_{xop}] = i\hbar \neq 0 \tag{2.180}$$

We, therefore, do not know what operator is associated with the classical quantity $xp_x = p_x x$. However, we must require that $\langle xp_x\rangle$ be real (because each of the repeated measurements of xp_x will be real). Thus, the operator A_{op} corresponding to xp_x must be such that

$$\langle xp_x\rangle = \frac{\langle\psi \mid A_{op}\psi\rangle}{\langle\psi \mid \psi\rangle} \tag{2.181}$$

is real for any $\psi(\vec{x},t)$. This means that $\langle\psi\,|\,A_{op}\psi\rangle$ must be real for all $\psi(\vec{x},t)$. This requires that A_{op} be *hermitian*. Neither A_{1op} nor A_{2op} is hermitian, that is, we have

$$\langle\psi \mid xp_x\psi\rangle = \langle x\psi \mid p_x\psi\rangle = \langle p_x x\psi \mid \psi\rangle$$
$$\rightarrow \langle\psi \mid A_{1op}\psi\rangle = \langle A_{2op}\psi \mid \psi\rangle \quad A_{1op} \neq A_{2op}$$

However, we can write

$$A(\vec{x},\vec{p}) = xp_x = p_x x = \frac{xp_x + p_x x}{2} \tag{2.182}$$

for the classical physical quantity. The operator

$$A_{op} = \frac{xp_{xop} + p_{xop}x}{2} \tag{2.183}$$

is hermitian and is therefore an acceptable operator to be associated with $A(\vec{x},\vec{p})$. $A_{1op} = xp_{xop}$ and $A_{2op} = p_{xop}x$ are not hermitian and are therefore not acceptable. In general, we must require that the operator A_{op} corresponding to some physical quantity $A(\vec{x},\vec{p})$ be hermitian so that

$$\langle A\rangle = \frac{\langle\psi \mid A_{op}\psi\rangle}{\langle\psi \mid \psi\rangle} \tag{2.184}$$

is real for any $\psi(\vec{x},t)$.

2.1.8. Postulate 3b

Let $A(\vec{x},\vec{p})$ be some physical quantity (a real function of $\vec{x}$ and $\vec{p}$). The order of the classical variables x_i and p_j in $A(\vec{x},\vec{p})$ is immaterial. The corresponding quantum operator $A_{op} = A(\vec{x},\vec{p}_{op})$, however, depends on the ordering of the non-commuting factors of x_i and $p_{j\,op}$. This ambiguity in ordering is (partially) removed by requiring A_{op} to be *hermitian* (so that $\langle A\rangle$ is real).

Note: The hermiticity requirement does not completely remove the ambiguity. Indeed, *hermitian* operators differing only by the ordering of x_i and $p_{j\,op}$ in a term correspond to the same classical quantity $A(\vec{x},\vec{p})$ but represent different quantum mechanical quantities. For example, let $A(\vec{x},\vec{p}) = x^2p_x^2$ classically. Then

$$A_{1op} = \frac{1}{2}\left(x^2p_{xop}^2 + p_{xop}^2x^2\right) \quad \text{and} \quad A_{2op} = xp_{xop}^2x \tag{2.185}$$

are two possible hermitian operators. However, they represent different quantum mechanical quantities even though they correspond to the same classical quantity. *Only experiment can determine which ordering of non-commuting factors yields the hermitian operator A_{op} that corresponds to a physical quantity $A(\vec{x},\vec{p})$ measured in a specified way.* We will not have to worry about such problems at this level since there will be no ordering ambiguity in the operators we will use.

2.1.8.1. Examples

1. **Energy of a particle in a conservative force field**

   Definition: The force on a particle is conservative if there exists a function $V(\vec{x})$, called the particle's potential energy, such that $\vec{F} = -\nabla V$.

   Let $W^{1\to2}$ be the work done on the particle by $\vec{F}$ as the particle moves from $\vec{x}_1$ to $\vec{x}_2$ along some path

   $$W^{1\to2} = \int_{\vec{x}_1}^{\vec{x}_2} \vec{F}\cdot d\vec{s} \quad , \quad d\vec{s} = dx\hat{x} + dy\hat{y} + dz\hat{z} \tag{2.186}$$

   Therefore,

   $$\begin{aligned} W^{1\to2} &= -\int_{\vec{x}_1}^{\vec{x}_2} \nabla V\cdot d\vec{s} = -\int_{\vec{x}_1}^{\vec{x}_2}\left(\frac{\partial V}{\partial x}dx + \frac{\partial V}{\partial y}dy + \frac{\partial V}{\partial z}dz\right) \\ &= -\int_{\vec{x}_1}^{\vec{x}_2} dV = -\left[V(\vec{x}_2) - V(\vec{x}_1)\right] \end{aligned} \tag{2.187}$$

which is *independent of the particular path connecting* $\vec{x}_1$ and $\vec{x}_2$. We can calculate $W^{1\to 2}$ in another way:

$$\begin{aligned} W^{1\to 2} &= \int_1^2 \vec{F}\cdot d\vec{s} = \int_1^2 m\frac{d\vec{v}}{dt}\cdot d\vec{s} \\ &= m\int_1^2 \frac{d\vec{s}}{dt}\cdot d\vec{v} = m\int_1^2 \vec{v}\cdot d\vec{v} \\ &= \frac{1}{2}m\int_1^2 d(\vec{v}\cdot\vec{v}) = \frac{1}{2}m\vec{v}_2^2 - \frac{1}{2}m\vec{v}_1^2 \end{aligned} \tag{2.188}$$

Therefore,

$$\frac{1}{2}m\vec{v}_2^2 - \frac{1}{2}m\vec{v}_1^2 = -\left[V(\vec{x}_2) - V(\vec{x}_1)\right] \tag{2.189}$$

$$\frac{1}{2}m\vec{v}_2^2 + V(\vec{x}_2) = \frac{1}{2}m\vec{v}_1^2 + V(\vec{x}_1) \tag{2.190}$$

The total energy of the particle is then defined to be

$$E = \frac{1}{2}m\vec{v}^2 + V(\vec{x}) \tag{2.191}$$

and the previous argument shows that $E_2 = E_1$ (conservation of energy).

Since $\vec{p} = m\vec{v}$, we have

$$E = \frac{\vec{p}^2}{2m} + V(\vec{x}) = H(\vec{x},\vec{p}) = \text{ Hamiltonian} \tag{2.192}$$

Therefore,

$$H_{op} = \frac{\vec{p}_{op}\cdot\vec{p}_{op}}{2m} + V(\vec{x}) = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x}) \tag{2.193}$$

Clearly, in this case, there is no ambiguity in the ordering of factors.

2. **Angular momentum of a particle**

We have

$$\vec{L} = \vec{r}\times\vec{p} \Rightarrow \begin{cases} L_x = yp_z - zp_y \\ L_y = zp_x - xp_z \\ L_z = xp_y - yp_x \end{cases} \tag{2.194}$$

Therefore,

$$L_{xop} = yp_{zop} - zp_{yop} = \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \tag{2.195}$$

$$L_{yop} = zp_x - xp_z = \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \tag{2.196}$$

$$L_{zop} = xp_y - yp_x = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \tag{2.197}$$

Again, there is no ambiguity in the ordering of factors because $[x_i, p_{jop}] = i\hbar\delta_{ij} = 0 \;\; for\; i \neq j$.

Note: The uncertainty principle

$$(\Delta A)(\Delta B) \geq \frac{1}{2}\left|\langle [A_{op}, B_{op}]\rangle\right| \tag{2.198}$$

holds for any hermitian operators A_{op} and B_{op}. We may therefore apply it to any physical quantities $A(\vec{x}, \vec{p})$ and $B(\vec{x}, \vec{p})$ (ΔA and ΔB represent rms deviations in the measurements of $\hat{A}$ and $\hat{B}$).

The evaluation of commutators $[A_{op}, B_{op}]$ will be very important throughout our discussions.

2.1.8.2. Some general rules for commutators

1. $[A, A] = 0$
2. $[A, B] = -[B, A]$
3. $[A, B + C] = [A, B] + [A, C]$
4. $[A + B, C] = [A, C] + [B, C]$
5. $[A, BC] = [A, B]C + B[A, C]$
6. $[AB, C] = [A, C]B + A[B, C]$
7. $[A, [B, C]] = [B, [C, A]] + [C, [A, B]]$ – Jacobi Identity

2.1.9. Important Question

Can we find a wave function $\psi(\vec{x}, t)$ for a particle such that a measurement of the quantity $A(\vec{x}, \vec{p})$ performed at time t_0 on identically-prepared particles (each particle is described by the same wave function) will always yield the value will yield the value "a".

Let $\psi(\vec{x}, t_0) = \psi_0(\vec{x})$. A measurement of A at time t_0 will yield the value "a" with certainty if $\Delta A = 0 \Rightarrow \left\langle A^2 \right\rangle = \langle A \rangle^2$ at t_0. Now

$$\begin{aligned}\left\langle A^2 \right\rangle &= \frac{\left\langle \psi_0 \mid A^2\psi_0 \right\rangle}{\langle \psi_0 \mid \psi_0 \rangle} = \frac{\langle A\psi_0 \mid A\psi_0 \rangle}{\langle \psi_0 \mid \psi_0 \rangle} \quad (hermiticity) \\ &= \frac{\langle A\psi_0 \mid A\psi_0 \rangle \langle \psi_0 \mid \psi_0 \rangle}{\langle \psi_0 \mid \psi_0 \rangle^2} \geq \frac{\left|\langle \psi_0 \mid A\psi_0 \rangle\right|^2}{\langle \psi_0 \mid \psi_0 \rangle^2} \quad (Schwarz\; inequality)\end{aligned}$$

Therefore,

$$\left\langle A^2 \right\rangle \geq \frac{\left|\langle \psi_0 \mid A\psi_0 \rangle\right|^2}{\langle \psi_0 \mid \psi_0 \rangle^2} = \langle A \rangle^2 \tag{2.199}$$

with $\langle \psi_0 \mid A\psi_0 \rangle$ real. The equality occurs when $A_{op}\psi_0(\vec{x}) = \lambda\psi_0(\vec{x})$ a.e. with λ = a constant. Therefore, $(\Delta A)^2 = \left\langle A^2 \right\rangle - \langle A \rangle^2 = 0$ if $A_{op}\psi_0(\vec{x}) = \lambda\psi_0(\vec{x})$ where

$$a = \langle A \rangle = \frac{\langle \psi_0 \mid A\psi_0 \rangle}{\langle \psi_0 \mid \psi_0 \rangle} = \lambda \frac{\langle \psi_0 \mid \psi_0 \rangle}{\langle \psi_0 \mid \psi_0 \rangle} = \lambda \tag{2.200}$$

2.1.9.1. Important Result

A measurement of $A(\vec{x}, \vec{p})$ performed at time t_0 yields the value "a" *with certainty* ($\langle A \rangle = a$ and $\Delta A = 0$) if $\psi(\vec{x}, t_0) = \psi_0(\vec{x})$ is a normalizable wave function such that $A_{op}\psi_0(\vec{x}) = \lambda\psi_0(\vec{x})$ for all $\vec{x}$ (a.e.).

This is an *eigenvalue equation* for the operator A_{op}. The constant a is an *eigenvalue* and $\psi_0(\vec{x})$ is an *eigenfunction* belonging to the eigenvalue a.

2.1.9.2. Comments

1. The eigenvalue equation possesses solutions $\psi_0(\vec{x})$ that are normalizable (square-integrable and not identically zero) only for certain values of a.
2. $\psi_0(\vec{x}) = 0$ satisfies the eigenvalue equation for any a; however, this $\psi_0(\vec{x})$ is not normalizable.
3. $A_{op}\psi_0(\vec{x}) = \lambda\psi_0(\vec{x}) \Rightarrow NA_{op}\psi_0(\vec{x}) = N\lambda\psi_0(\vec{x})$, N = constant. Therefore, by linearity,
$$A_{op}(N\psi_0(\vec{x})) = \lambda(N\psi_0(\vec{x})) \tag{2.201}$$
Therefore, any non-zero constant multiple of an eigenfunction belonging to eigenvalue a is also an eigenfunction belonging to eigenvalue a.
4. We have $A_{op}^2\psi_0(\vec{x}) = A_{op}A_{op}\psi_0(\vec{x}) = aA_{op}\psi_0(\vec{x}) = a^2\psi_0(\vec{x})$ explicitly. In general, we have $A_{op}^N\psi_0(\vec{x}) = a^N\psi_0(\vec{x})$.
5. The wave function for a particle will develop in time according to the forces present (we will discuss the exact time dependence later). In general, if $\psi(\vec{x}, t)$ is an eigenfunction of A_{op} with eigenvalue a at time t_0, it will not be an eigenfunction of A_{op} at some other time t_1.

2.1.9.3. Theorem

The eigenvalues of a hermitian operator are real.

Proof: We have

$A_{op}\psi_0 = \lambda\psi_0$
$\Rightarrow \langle \psi_0 \mid A\psi_0 \rangle = \langle \psi_0 \mid a\psi_0 \rangle = a \langle \psi_0 \mid \psi_0 \rangle = \langle A\psi_0 \mid \psi_0 \rangle = \langle a\psi_0 \mid \psi_0 \rangle = a^* \langle \psi_0 \mid \psi_0 \rangle$

so that $a = a^*$ or a is real.

2.1.10. Time-Independent Schrodinger Equation

Assume A_{op} = Hamiltonian operator is given by

$$H_{op} = \frac{\vec{p}_{op} \cdot \vec{p}_{op}}{2m} + V(\vec{x}) = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x}) \tag{2.202}$$

for a particle in a conservative force field. The eigenvalue equation for the energy is

$$H_{op}\psi_0(\vec{x}) = E\psi_0(\vec{x}) \tag{2.203}$$

with E the eigenvalue. This corresponds to the partial differential equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi_0(\vec{x}) + V(\vec{x})\psi_0(\vec{x}) = E\psi_0(\vec{x}) \tag{2.204}$$

which is the *time-independent Schrodinger equation.*

A normalizable wave function satisfying this equation at time t_0 ($\psi(\vec{x}, t_0) = \psi_0(\vec{x})$) describes a particle whose energy at time t_0 is *precisely* the eigenvalue E ($\Delta E = 0$ - there is no spread in the possible energy values). This equation can be solved once the potential energy $V(\vec{x})$ is specified, that is, once the force $\vec{F} = -\nabla V$ acting on the particle is specified.

We postpone solving this equation for various possible forces at the moment and, instead, consider the eigenvalue equations for linear momentum, position, and angular momentum.

2.1.11. Some Operator Eigenvalue/Eigenfunction Equations

2.1.11.1. Linear Momentum

Consider

$$p_x \to p_{xop} = \frac{\hbar}{i}\frac{\partial}{\partial x} \tag{2.205}$$

The eigenvalue equation is

$$\frac{\hbar}{i}\frac{\partial\psi_0(\vec{x})}{\partial x} = p_x\psi_0(\vec{x}) \tag{2.206}$$

where p_x = eigenvalue. Therefore,

$$\frac{\partial\psi_0(\vec{x})}{\partial x} = \frac{ip_x}{\hbar}\psi_0(\vec{x}) \tag{2.207}$$

with p_x a constant to be determined. The solution is obviously

$$\psi_0(\vec{x}) = N(y, z)e^{\frac{ip_x x}{\hbar}} \tag{2.208}$$

This is the solution for any complex p_x. However, we must find only those values of p_x for which $\psi_0(\vec{x})$ is normalizable (this condition should, at least, restrict p_x to real values according to our earlier results).

Let $p_x = \alpha + i\beta$, α, β *real*. Then

$$\langle \psi_0 \mid \psi_0 \rangle = \int d^3x \, |N(y,z)|^2 \left| e^{\frac{ip_x x}{\hbar}} \right|^2 = \int d^3x \, |N(y,z)|^2 \, e^{-\frac{2\beta x}{\hbar}} \tag{2.209}$$

Therefore,

$$\langle \psi_0 \mid \psi_0 \rangle = \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \, |N(y,z)|^2 \int_{-\infty}^{\infty} dx e^{-\frac{2\beta x}{\hbar}} = \infty \tag{2.210}$$

that is, there exists *no* real β for which this integral is finite. Thus, there are no physical (normalizable) solutions(in L^2) to the eigenvalue equations for p_x (and similary for p_y and p_z). A measurement of p_i on a physical system will *never* yield a specified value with certainty. Measurements of linear momentum performed on identically-prepared particles will always yield a spread in results. Recall that $\Delta x \Delta p_x \geq \hbar/2$. If $\Delta p_x = 0$, then $\Delta x = \infty$, which is a rather unphysical situation. However, we can make $\Delta p_x \neq 0$ as small as we want, but we cannot make Δp_x exactly zero in any physical system.

2.1.11.2. Position

Consider $x_3 = z$, ($\vec{x} = (x, y, z)$). Here $x_3 = z$ is the operator which multiplies functions by z. The eigenvalue equation is

$$z\psi_0(\vec{x}) = Z\psi_0(\vec{x}) \tag{2.211}$$

where Z = eigenvalue(constant). Therefore,

$$(z - Z)\psi_0(\vec{x}) = 0 \rightarrow \psi_0(\vec{x}) = 0 \tag{2.212}$$

for all $z \neq Z$. We claim that $\psi_0(\vec{x}) = N(x,y)\delta(z - Z)$?. To prove this we must show that $(z - Z)\delta(z - Z) = 0$.

Let $f(z)$ be a function continuous at $z = Z$. Then

$$\int_{-\infty}^{\infty} dz f(z)(z - Z)\delta(z - Z) = \left[f(z)(z - Z) \right]_{z=Z} = 0 \tag{2.213}$$

for *all* $f(z)$ continuous at $z = Z$. This says that $(z - Z)\delta(z - Z) = 0$.

Is $\psi_0(\vec{x}) = N(x,y)\delta(z - Z)$ normalizable?

$$\begin{aligned} \langle \psi_0 \mid \psi_0 \rangle &= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \, |N(x,y)|^2 \int_{-\infty}^{\infty} dx \delta(z - Z)\delta(z - Z) \\ &= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \, |N(x,y)|^2 \left[\delta(z - Z) \right]_{z=Z} = \infty \end{aligned}$$

since $\delta(0) = \infty$.

Thus, there are no physical (normalizable) solutions (in L^2) to the eigenvalue equation for z (and similarly for x and y). This says that measurements of the position of identically-prepared particles will always yield a spread in results.

2.1.11.3. Angular Momentum

Consider

$$L_z \to L_{zop} = xp_y - yp_x = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \tag{2.214}$$

The eigenvalue equations is

$$\frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\psi_0(\vec{x}) = a\psi_0(\vec{x}) \tag{2.215}$$

where a = the eigenvalue.

Consider now a switch to spherical-polar coordinates as shown in Figure 2.9 below.

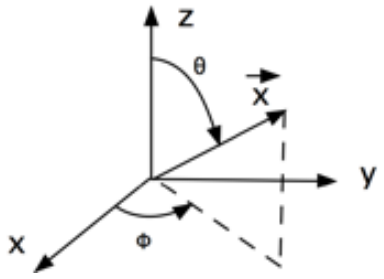


Figure 2.9: Spherical Polar Coordinates

We express $\psi_0(\vec{x}) = \psi_0(r, \theta, \phi)$ and use the chain rule to find

$$\frac{\partial\psi_0}{\partial x} \quad , \quad \frac{\partial\psi_0}{\partial y}$$

$$x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} = x\left(\frac{\partial r}{\partial y}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial y}\frac{\partial}{\partial\theta} + \frac{\partial\phi}{\partial y}\frac{\partial}{\partial\phi}\right) - y\left(\frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial x}\frac{\partial}{\partial\theta} + \frac{\partial\phi}{\partial x}\frac{\partial}{\partial\phi}\right)$$

Now

$$r = \sqrt{x^2 + y^2 + z^2} \Rightarrow \frac{\partial r}{\partial y} = \frac{y}{r} \quad , \quad \frac{\partial r}{\partial x} = \frac{x}{r} \tag{2.216}$$

and

$$\cos\theta = \frac{z}{r} = \frac{z}{\sqrt{x^2 + y^2 + z^2}} \tag{2.217}$$

so that

$$-\sin\theta\frac{\partial\theta}{\partial y}=-\frac{z}{r^2}\frac{\partial r}{\partial y}=-\frac{zy}{r^3}\Rightarrow\frac{\partial\theta}{\partial y}=\frac{zy}{r^3\sin\theta}$$
$$-\sin\theta\frac{\partial\theta}{\partial x}=-\frac{z}{r^2}\frac{\partial r}{\partial x}=-\frac{zx}{r^3}\Rightarrow\frac{\partial\theta}{\partial x}=\frac{zx}{r^3\sin\theta}$$

and

$$\tan\phi=\frac{y}{x}$$

so that

$$\sec^2\phi\frac{\partial\phi}{\partial y}=\frac{1}{x}\Rightarrow\frac{\partial\phi}{\partial y}=\frac{1}{x}\cos^2\phi$$
$$\sec^2\phi\frac{\partial\phi}{\partial x}=-\frac{y}{x^2}\Rightarrow\frac{\partial\phi}{\partial y}=-\frac{y}{x^2}\cos^2\phi$$

Thus,

$$\begin{aligned}x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}&=\left(\frac{xy}{r}\frac{\partial}{\partial r}+\frac{xyz}{r^3\sin\theta}\frac{\partial}{\partial\theta}+\cos^2\phi\frac{\partial}{\partial\phi}\right)\\&\quad-\left(\frac{xy}{r}\frac{\partial}{\partial r}+\frac{xyz}{r^3\sin\theta}\frac{\partial}{\partial\theta}-\frac{y^2}{x^2}\cos^2\phi\frac{\partial}{\partial\phi}\right)\\&=\cos^2\phi\frac{\partial}{\partial\phi}+\frac{y^2}{x^2}\cos^2\phi\frac{\partial}{\partial\phi}=\cos^2\phi\frac{\partial}{\partial\phi}+\tan^2\phi\cos^2\phi\frac{\partial}{\partial\phi}\\&=\cos^2\phi\frac{\partial}{\partial\phi}+\sin^2\phi\frac{\partial}{\partial\phi}=\frac{\partial}{\partial\phi}\end{aligned}$$

Therefore,

$$L_z=\frac{\hbar}{i}\frac{\partial}{\partial\phi}\tag{2.218}$$

and the eigenvalue equation is

$$\frac{\hbar}{i}\frac{\partial\psi_0(\vec{x})}{\partial\phi}=a\psi_0(\vec{x})\rightarrow\frac{\partial\psi_0(\vec{x})}{\partial\phi}=\frac{ia}{\hbar}\psi_0(\vec{x})\tag{2.219}$$

The solution is

$$\psi_0(\vec{x})=f(r,\theta)e^{i\frac{a}{\hbar}\phi}\tag{2.220}$$

for any complex value of the eigenvalue a.

2.1.11.4. Important observation

$\phi=0$ and $\phi=2\pi$ for the same r and θ correspond to the same point in space. If $\psi_0(r,\theta,\phi=0)\neq\psi_0(r,\theta,\phi=2\pi)$ then $\psi_0(\vec{x})$ will be discontinuous at this point and

$$L_{zop}=\frac{\hbar}{i}\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)\tag{2.221}$$

would not be defined on $\psi_0(\vec{x})$. We must, therefore, require that

$$\psi_0(r,\theta,\phi=0)=\psi_0(r,\theta,\phi=2\pi) \tag{2.222}$$

This is often called the *single-valuedness* assumption.

This means that

$$f(r,\theta)e^0=f(r,\theta)e^{i2\pi\frac{a}{\hbar}}\rightarrow e^{i2\pi\frac{a}{\hbar}}=1$$
$$\frac{2\pi a}{\hbar}=2\pi\ell \quad , \quad \ell=0,\pm1,\pm2,.....$$

Therefore, $a=\ell\hbar$, that is, the eigenvalues of L_{zop} can take on only certain discrete values!

$$L_{zop}\psi_0(\vec{x})=\ell\hbar\psi_0(\vec{x}) \quad , \quad \psi_0(\vec{x})=f(r,\theta)e^{i\ell\phi} \quad , \quad \ell=0,\pm1,\pm2,..... \tag{2.223}$$

Is $\psi_0(\vec{x})$ normalizable? We have

$$\begin{aligned}\langle\psi_0\mid\psi_0\rangle&=\int_0^\infty r^2dr\int_0^\pi\sin\theta d\theta\left|f(r,\theta)\right|^2\int_0^{2\pi}d\phi\left|e^{i\ell\phi}\right|^2\\&=2\pi\int_0^\infty r^2dr\int_0^\pi\sin\theta d\theta\left|f(r,\theta)\right|^2\end{aligned}$$

Clearly, this can be made to be finite and non-zero with a suitable $f(r,\theta)$. Thus, there are physical (normalizable) wave functions such that a measurement of L_z will yield the value "a" *with certainty*. Furthermore, the measured value of L_z in such a system must be *one* of the values $0,\pm\hbar,\pm2\hbar,.....$ L_z is said to be *quantized*. Classically, we expect L_z to be capable of taking on *any* definite value. However, we now see that L_z can only have the precise values $0,\pm\hbar,\pm2\hbar,.....$ when this particle has a definite angular momentum ($\Delta L_z=0$). *Macroscopically, this discreteness cannot be observed because $\hbar\approx10^{-27}\,erg-sec$ is so small that L_z appears continuous with macroscopic measurements.*

2.1.11.5. Notes

1. Let $\psi(\vec{x},t_0)$ be an eigenfunction of L_z with eigenvalue $\ell\hbar$. What is the probability of finding the particle in a region of space at time t_0?

$$\wp(\vec{x},t_0)=\frac{\left|\psi(\vec{x},t_0)\right|^2}{\langle\psi_0\mid\psi_0\rangle}=\frac{\left|f(r,\theta)e^{i\frac{a}{\hbar}\phi}\right|^2}{\langle\psi_0\mid\psi_0\rangle}=\frac{\left|f(r,\theta)\right|^2}{\langle\psi_0\mid\psi_0\rangle} \tag{2.224}$$

which is *independent* of ϕ?. Thus, the particle is equally likely to be found at any ϕ.

2. Let $\psi(\vec{x}, t_0)$ be an eigenfunction of L_z with eigenvalue $\ell\hbar$. ($\langle L_z \rangle = \ell\hbar$, $\Delta L_z = 0$). What are $\langle L_x \rangle$ and $\langle L_y \rangle$? Since

$$\begin{aligned} L_y L_z - L_z L_y &= (zp_x - xp_z)(xp_y - yp_x) - (xp_y - yp_x)(zp_x - xp_z) \\ &= zp_y p_x x - zp_x y p_x - xp_z x p_y + p_z y x p_x \\ &\qquad - p_y z x p_x + x p_y x p_z + y p_x z p_x - y p_z p_x x \\ &= (zp_y - yp_z)p_x x + (p_z y - p_y z)xp_x = L_x[x, p_x] = i\hbar L_x \end{aligned}$$

we have

$$\begin{aligned} i\hbar \langle \psi_0 \mid L_x \psi_0 \rangle &= \langle \psi_0 \mid L_y L_z \psi_0 \rangle - \langle \psi_0 \mid L_z L_y \psi_0 \rangle \\ &= \langle \psi_0 \mid L_y \ell\hbar \psi_0 \rangle - \langle L_z \psi_0 \mid L_y \psi_0 \rangle \\ &= \ell\hbar \langle \psi_0 \mid L_y \psi_0 \rangle - \langle \ell\hbar \psi_0 \mid L_y \psi_0 \rangle \\ &= \ell\hbar \left(\langle \psi_0 \mid L_y \psi_0 \rangle - \langle \psi_0 \mid L_y \psi_0 \rangle \right) = 0 \end{aligned}$$

so that $\langle \psi_0 \mid L_x \psi_0 \rangle = \langle L_x \rangle = 0$ and similarly $\langle L_x \rangle = 0$.

Our basic result was the following:

> A measurement of the physical quantity $A(\vec{x}, \vec{p})$ performed at the time t_0 yields the value "a" with certainty if, and only if, $\psi(\vec{x}, t_0) = \psi_0(\vec{x})$ is a normalizable wave function such that
>
> $$A_{op} \psi_0(\vec{x}) = a \psi_0(\vec{x})$$

Suppose that $\psi(\vec{x}, t_0)$ is not an eigenfunction of A_{op}. Then, a measurement of $A(\vec{x}, \vec{p})$ at time t_0 will necessarily have $\Delta A \neq 0$, that is, there will be a non-zero spread in the possible results of the measurement. Two important questions must then be answered:

1. If a measurement of $A(\vec{x}, \vec{p})$ is performed at t_0 on such a particle, what are the possible results of such a measurement?

2. What is the probability of obtaining each of these possible results?

To answer these questions, it is necessary to develop some more operator concepts. The functions used in the following discussion will be square-integrable (they $\in L^2$).

Consider the linear operator $A = A(\vec{x}, \vec{p})$. It need not be hermitian for this discussion.

A = sum of terms of the form

$$x^n y^m z^\ell \frac{\partial^N}{\partial x^N} \frac{\partial^M}{\partial x^M} \frac{\partial^L}{\partial x^L} \tag{2.225}$$

with other possible orderings of the non-commuting operators

$$x_i \; and \; \frac{\partial}{\partial x_i} \tag{2.226}$$

also present, for example

$$\frac{\partial}{\partial x} x^n \frac{\partial^{N-1}}{\partial x^{N-1}} ..... \tag{2.227}$$

A usually cannot be defined on all square-integrable functions. For example, $\partial/\partial x_j$ cannot be defined on discontinuous functions.

In the following, $A\phi$ signifies that A can be defined on this ϕ. For a typical operator term

$$A = x^n y^m z^\ell \frac{\partial^N}{\partial x^N} \frac{\partial^M}{\partial x^M} \frac{\partial^L}{\partial x^L} \tag{2.228}$$

we can write

$$\begin{aligned} \langle \phi_1 \mid A\phi_2 \rangle &= \int d^3x \phi_1^* x^n y^m z^\ell \frac{\partial^N}{\partial x^N} \frac{\partial^M}{\partial x^M} \frac{\partial^L}{\partial x^L} \phi_2 \\ &= \int d^3x \left[x^n y^m z^\ell \phi_1^* \right] \frac{\partial^N}{\partial x^N} \frac{\partial^M}{\partial x^M} \frac{\partial^L}{\partial x^L} \phi_2 \\ &= (-1)^{N+M+L} \int d^3x \left\{ \frac{\partial^N}{\partial x^N} \frac{\partial^M}{\partial x^M} \frac{\partial^L}{\partial x^L} \left[x^n y^m z^\ell \phi_1 \right] \right\}^* \phi_2 \end{aligned} \tag{2.229}$$

which *defines* the operator $A^\dagger$.

Note that a typical surface term occurring in one of the integrations by parts is of the form

$$\left[\int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \left[x^n y^m z^\ell \phi_1^* \right] \frac{\partial^{N-1}}{\partial x^{N-1}} \frac{\partial^M}{\partial x^M} \frac{\partial^L}{\partial x^L} \phi_2 \right]_{x=-\infty}^{x=+\infty} \tag{2.230}$$

Even though the square-integrable $\phi_1 \to 0$ and $\phi_2 \to 0$ as $x \to \infty$, this surface term need not be zero because $x^n \phi_1$ need not go to zero as $x \to \infty$. Thus, the above derivation holds for many but not all ϕ_1 and ϕ_2. We shall ignore such difficulties in the following discussions.

Thus, if A is a linear operator, there exists an operator $A^\dagger$ (is read *A-dagger*) called the *adjoint operator* of A, such that

$$\langle \phi_1 \mid A\phi_2 \rangle = \langle A^+ \phi_1 \mid \phi_2 \rangle \tag{2.231}$$

2.1.11.6. Notes

1. $\langle A\phi_1 \mid \phi_2 \rangle = \langle \phi_1 \mid A\phi_2 \rangle^* = \langle A^+ \phi_1 \mid \phi_2 \rangle^* = \langle \phi_1 \mid A^+ \phi_2 \rangle$

2. The operator $A^\dagger$ is unique, that is, there exists only one operator $A^\dagger$ satisfying $\langle \phi_1 \mid A\phi_2 \rangle = \langle A^+\phi_1 \mid \phi_2 \rangle$.

   Proof: Suppose the operator B also satisfies $\langle \phi_1 \mid A\phi_2 \rangle = \langle B\phi_1 \mid \phi_2 \rangle$. Then

$$\begin{aligned}
&\langle A^+\phi_1 \mid \phi_2 \rangle = \langle B\phi_1 \mid \phi_2 \rangle \\
&\langle (B - A^+)\phi_1 \mid \phi_2 \rangle = 0 \quad for\ all \quad \phi_2 \\
&Let \quad \phi_2 = B\phi_1 - A^+\phi_1, \quad then \\
&\langle (B - A^+)\phi_1 \mid (B - A^+)\phi_1 \rangle = 0 \rightarrow (B - A^+)\phi_1 = 0 \\
&B\phi_1 = A^+\phi_1 \quad for\ all \quad \phi_1 \Rightarrow B = A^+
\end{aligned}$$

3. $A^\dagger$ is linear.
4. $(A^+)^+ = A$
5. $(A + B)^+ = A^+ + B^+$
6. $(\lambda A)^+ = \lambda^* A^+$
7. $(AB)^+ = B^+A^+$

2.1.11.7. Definition

A is *hermitian* if $\langle \phi_1 \mid A\phi_2 \rangle = \langle A\phi_1 \mid \phi_2 \rangle$ for ϕ_1 and ϕ_2 on which A is defined. This means that A is hermitian if $A^\dagger = A$.

2.1.11.8. Definition

The N functions $\phi_1, \phi_2, \phi_3, ..., \phi_N$ are *linearly independent* if

$$\sum_{i=1}^{N} \lambda_i \phi_i = 0 \tag{2.232}$$

a.e. implies that $\lambda_i = 0$ for $i = 1, 2, ..., N$, that is,

$$\sum_{i=1}^{N} \lambda_i \phi_i = 0 \tag{2.233}$$

a.e. can be satisfied only if $\lambda_1 = \lambda_2 = ... = \lambda_N = 0$.

2.1.11.9. Notes

1. The functions $\phi_1, \phi_2, \phi_3, ..., \phi_N$ are linearly dependent if one of the functions $\phi_j(\vec{x}) = 0$ a.e. because

$$\sum_{i=1}^{N} \lambda_i \phi_i = 0 \tag{2.234}$$

can have $\lambda_j \phi_j = 0$ with λ_j arbitrary.

2. If $\phi_1, \phi_2, \phi_3, ..., \phi_N$ are linearly dependent, then one of these functions can be expressed as a linear superposition of the others. **Proof**:

$$\sum_{i=1}^{N} \lambda_i \phi_i = 0 \text{withsome} \lambda_j \neq 0$$
$$\Rightarrow \lambda_j \phi_j + \sum_{i \neq j} \lambda_i \phi_i = 0 \Rightarrow \phi_j = -\frac{1}{\lambda_j} \sum_{i \neq j} \lambda_i \phi_i$$

3. If $\phi_1, \phi_2, \phi_3, ..., \phi_N$ are mutually orthogonal ($\langle \phi_i \mid \phi_j \rangle = 0 \text{for} i \neq j$) and if no ϕ_i is identically zero, then these N functions are linearly independent. **Proof**: Let

$$\sum_{i=1}^{N} \lambda_i \phi_i = 0 \tag{2.235}$$

Therefore,

$$0 = \left\langle \phi_j \;\middle|\; \sum_{i=1}^{N} \lambda_i \phi_i \right\rangle = \sum_{i=1}^{N} \lambda_i \langle \phi_j \mid \phi_i \rangle$$
$$= \lambda_j \langle \phi_j \mid \phi_j \rangle \Rightarrow \lambda_j = 0$$

since ϕ_i is not identically zero.

2.1.11.10. Definition

$\phi_1, \phi_2, \phi_3, ..., \phi_N$ are orthonormal (ON) if they are mutually orthogonal and normalized: $\langle \phi_i \mid \phi_j \rangle = \delta_{ji}$.

2.1.11.11. Theorem

We now define the so-called *Gram-Schmidt Orthogonalization Procedure.*

Given the *linearly independent* functions $\phi_1, \phi_2, ...$ (finite or infinite number of functions), one can construct an orthogonal set of non-zero (not identically zero) functions $v_1, v_2, ...$ where v_N is a linear superposition of $\phi_1, \phi_2, ..., \phi_N$ (v_N does *not* depend on $\phi_{N+1}, \phi_{N+2}, ...$).

Furthermore,

$$u_n = \frac{v_n}{\langle v_n \mid v_n \rangle} \tag{2.236}$$

gives an ON set of $u_1, u_2, ...$

2.1.11.12. Construction

1. $v_1 = \phi_1$ (ϕ_1 is not identically zero).
2. Let $v_2 = \phi_2 + \alpha_{21}\phi_1$ where α_{21} is determined by requiring that

$$\langle v_1 \mid v_2 \rangle = 0 = \langle v_1 \mid \phi_2 + \alpha_{21}\phi_1 \rangle = \langle v_1 \mid \phi_2 \rangle + \alpha_{21} \langle v_1 \mid \phi_1 \rangle$$
$$\alpha_{21} = -\frac{\langle v_1 \mid \phi_2 \rangle}{\langle v_1 \mid \phi_1 \rangle} \tag{2.237}$$

   (v_2 is not identically zero because $0 = \phi_2 + \alpha_{21}v_1$ is impossible when ϕ_2 and $v_1 = \phi_1$ are linearly independent).

3. Let $v_3 = \phi_3 + \alpha_{32}v_2 + \alpha_{31}v_1$ where α_{32} and α_{31} are determined by requiring that

$$\begin{aligned}\langle v_1 \mid v_3 \rangle = 0 &= \langle v_1 \mid \phi_3 + \alpha_{32}v_2 + \alpha_{31}v_1 \rangle \\ &= \langle v_1 \mid \phi_3 \rangle + \alpha_{32} \underbrace{\langle v_1 \mid v_2 \rangle}_{=0} + \alpha_{31} \underbrace{\langle v_1 \mid v_1 \rangle}_{\neq 0}\end{aligned}$$

   so that

$$0 = \langle v_1 \mid \phi_3 \rangle + \alpha_{31} \langle v_1 \mid v_1 \rangle \Rightarrow \alpha_{31} = -\frac{\langle v_1 \mid \phi_3 \rangle}{\langle v_1 \mid v_1 \rangle} \tag{2.238}$$

   and

$$\begin{aligned}\langle v_2 \mid v_3 \rangle = 0 &= \langle v_2 \mid \phi_3 + \alpha_{32}v_2 + \alpha_{31}v_1 \rangle \\ &= \langle v_2 \mid \phi_3 \rangle + \alpha_{32} \underbrace{\langle v_2 \mid v_2 \rangle}_{\neq 0} + \alpha_{31} \underbrace{\langle v_2 \mid v_1 \rangle}_{=0}\end{aligned}$$

   so that

$$0 = \langle v_2 \mid \phi_3 \rangle + \alpha_{32} \langle v_2 \mid v_2 \rangle \Rightarrow \alpha_{32} = -\frac{\langle v_2 \mid \phi_3 \rangle}{\langle v_2 \mid v_2 \rangle} \tag{2.239}$$

4. The construction of $v_4, v_5, \ldots..$ proceeds in a similar manner.

2.1.11.13. Note

$$a_n u_n = \frac{v_n}{\langle v_n \mid v_n \rangle} \Rightarrow \langle u_n \mid u_n \rangle = \frac{\langle v_n \mid v_n \rangle}{\langle v_n \mid v_n \rangle} = 1 \tag{2.240}$$

implies that u_n is normalized.

2.1.11.14. Example

Consider functions of one variable $\phi_n(x) = x^n$, $n = 0, 1, 2, \ldots..$ defined on $[-1, 1]$ so that

$$\langle \phi_1 \mid \phi_2 \rangle = \int_{-1}^{1} dx\, \phi_1^*(x)\phi_2(x) \tag{2.241}$$

These functions are linearly independent by the properties of a power series, that is,

$$\sum_n a_n \phi_n(x) = \sum_n a_n x^n = 0 \tag{2.242}$$

implies that all a_n are zero. If we designate the orthogonal polynomials that result from the Gram-Schmidt process, applied to $\phi_n(x) = x^n$, $n = 0, 1, 2, ...$ by $P_0(x), P_1(x), P_2(x), ...$ and require that $P_n(x = +1) = +1$ *instead of* the standard normalization given by

$$\langle P_n \mid P_n \rangle = \int_{-1}^{1} dx P_n(x) P_n(x) = 1 \tag{2.243}$$

then the resulting functions are the standard Legendre polynomials

$$P_0(x) = 1 \ , \ P_1(x) = x \ , \ P_2(x) = \frac{1}{2}(3x^2 - 1) \ , \ etc \tag{2.244}$$

with

$$\langle P_n \mid P_n \rangle = \int_{-1}^{1} dx P_n(x) P_n(x) = \frac{2}{2n+1} \tag{2.245}$$

2.1.11.15. Definition

$\phi_1, \phi_2, ...$ is a complete orthonormal (CON) set in L^2 if it is an ON set ($\langle \phi_i \mid \phi_j \rangle = \delta_{ij}$) and any $\phi \in L^2$ can be expanded in terms of the ϕ_i:

$$\phi(\vec{x}) = \sum_{i=1}^{\infty} \lambda_i \phi_i(\vec{x}) \tag{2.246}$$

with convergence a.e.

The λ_i's can be found explicitly:

$$\begin{aligned} \langle \phi_j \mid \phi \rangle &= \left\langle \phi_j \;\middle|\; \sum_{i=1}^{\infty} \lambda_i \phi_i(\vec{x}) \right\rangle \\ &= \sum_{i=1}^{\infty} \lambda_i \langle \phi_j \mid \phi_i \rangle = \sum_{i=1}^{\infty} \lambda_i \delta_{ij} = \lambda_j \quad , \quad j = 1, 2, 3, ... \end{aligned}$$

2.1.11.16. Theorem

Let $\phi_\lambda \in L^2$ and $\phi_\mu \in L^2$ so that we can write

$$\phi_\lambda = \sum_{i=1}^{\infty} \lambda_i \phi_i \quad , \quad \phi_\mu = \sum_{i=1}^{\infty} \mu_i \phi_i \tag{2.247}$$

with $\phi_1, \phi_2, ...$ a CON set. Then,

$$\langle \phi_\lambda \mid \phi_\mu \rangle = \sum_i \lambda_i^* \mu_i \tag{2.248}$$

Proof:

$$\langle \phi_\lambda \mid \phi_\mu \rangle = \left\langle \sum_{i=1}^{\infty} \lambda_i \phi_i \;\middle|\; \sum_{j=1}^{\infty} \mu_j \phi_j \right\rangle = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \lambda_i^* \mu_j \langle \phi_i \mid \phi_j \rangle$$
$$= \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \lambda_i^* \mu_j \delta_{ij} = \sum_i \lambda_i^* \mu_i$$

2.1.11.17. Note

If $\phi \in {}^2$ with $\phi = \sum_{i=1}^{\infty} \lambda_i \phi_i$ where $\{\phi_i\}$ is a CON set, then an immediate consequence of the previous theorem is

$$\langle \phi \mid \phi \rangle = \sum_{i=1}^{\infty} \lambda_i^* \lambda_i = \sum_{i=1}^{\infty} |\lambda_i|^2 \tag{2.249}$$

Now let A be a linear operator (acting on functions in L^2). The *eigenvalue equation* for A in L^2 is $A\phi(\vec{x}) = a\phi(\vec{x})$ for all $\vec{x}$, where the *eigenfunction* $\phi(\vec{x})$ is normalizable (square-integrable and not identically zero) and where the eigenvalue a is a constant. Since $\phi(\vec{x})$ is normalizable, the equation can be satisfied for only certain values of a.

2.1.11.18. Theorem

The eigenvalues of a hermitian operator are real.

Proof: Let $A\phi = a\phi$. Therefore,

$$\langle \phi \mid A\phi \rangle = \langle \phi \mid a\phi \rangle = a \langle \phi \mid \phi \rangle$$
$$= \langle A\phi \mid \phi \rangle = \langle a\phi \mid \phi \rangle$$
$$= a^* \langle \phi \mid \phi \rangle \Rightarrow a = a^* \Rightarrow a \quad is\ real$$

where we have used $A = A^\dagger$ and $\langle \phi \mid \phi \rangle \neq 0$.

For a given eigenvalue a, there may exist several linearly independent eigenfunctions: $A\phi_1 = a\phi_1$, $A\phi_2 = a\phi_2$, ... with $\phi_1, \phi_2, ...$ linearly independent but having the same eigenvalue a.

2.1.11.19. Definition

The eigenvalue a is g–fold degenerate if there exist g linearly independent eigenfunctions belonging to the eigenvalue a and any $(g+1)$ eigenfunctions belonging to a are linearly dependent. The eigenvalue a is non-degenerate if there exists only one linearly independent eigenfunction belonging to a.

Some of the eigenvalues of A may be non-degenerate while other eigenvalues of

A may have differing orders of degeneracy.

Note that $A\phi = a\phi \Rightarrow A(N\phi) = a(N\phi)$ for any constant N. However, ϕ and $N\phi$ are linearly dependent and therefore, the eigenfunction $N\phi$ does not add to the degeneracy of the eigenvalue a.

2.1.11.20. Theorem

Let $\phi_1, \phi_2, \phi_3, ..., \phi_N$ be eigenfunctions of A belonging to the same eigenvalue a. These eigenfunctions need not be linearly independent. Then, any linear superposition

$$\sum_{i=1}^{n} c_i \phi_i \tag{2.250}$$

which is not identically zero is also an eigenfunction belonging to the eigenvalue a.

Proof:

$$A\phi_i = a\phi_i \quad , \quad i = 1, 2, 3, ..., n$$
$$A\left(\sum_{i=1}^{n} c_i \phi_i\right) = \sum_{i=1}^{n} c_i A\phi_i = \sum_{i=1}^{n} c_i a\phi_i = a\left(\sum_{i=1}^{n} c_i \phi_i\right)$$

where we have used the linearity of A.

2.1.11.21. Theorem

Let the eigenvalue a be g–fold degenerate. Then, there exists g orthonormal eigenfunctions $(u_1, u_2, ..., u_g)$ all belonging to the eigenvalue a such that *any* eigenfunction ϕ belonging to the eigenvalue a can be written

$$\phi = \sum_{i=1}^{g} c_i u_i \quad , \quad \langle u_i \mid u_j \rangle = \delta_{ij} \tag{2.251}$$

that is, $\{u_1, u_2, ..., u_g\}$ forms a CON set of eigenfunctions for the eigenvalue a.

Proof: g–fold degeneracy implies there exists linearly independent eigenfunctions $\phi_1, \phi_2, \phi_3, ..., \phi_g$ all belonging to the eigenvalue a. One can perform the Gram-Schmidt procedure on these eigenfunctions to obtain $\{u_1, u_2, ..., u_g\}$, an ON set of (non-zero) eigenfunctions belonging to the eigenvalue a (since u_n is a linear superposition of $\phi_1, \phi_2, \phi_3, ..., \phi_g$, u_n must be an eigenfunction belonging to the eigenvalue a). To show completeness for the eigenfunctions belonging to a, let ϕ be an arbitrary eigenfunction belonging to a. g–fold degeneracy implies

$$\overbrace{u_1, u_2, ..., u_g, \phi}^{(g+1)\ eigenfunctions}$$

must be linearly dependent. Therefore,

$$\sum_{i=1}^{g} d_i u_i + d\phi = 0 \tag{2.252}$$

with a non-zero d is possible. If d is zero, the all $d_i = 0$ by the linear independence of $\{u_1, u_2, ..., u_g\}$. Therefore,

$$\phi = -\frac{1}{d} \sum_{i=1}^{g} d_i u_i \tag{2.253}$$

2.1.11.22. Theorem

Let A be hermitian. The eigenfunctions of A belonging to different eigenvalues are orthogonal.

Proof: Let $A\phi_1 = a_1\phi_1 \quad , \quad A\phi_2 = a_2\phi_2 \quad , \quad a_1 \neq a_2$. Then

$$\begin{aligned} \langle \phi_2 \mid A\phi_1 \rangle &= \langle \phi_2 \mid a_1\phi_1 \rangle = a_1 \langle \phi_2 \mid \phi_1 \rangle \\ &= \langle A\phi_2 \mid \phi_1 \rangle = \langle a_2\phi_2 \mid \phi_1 \rangle \\ &= a_2^* \langle \phi_2 \mid \phi_1 \rangle = a_2 \langle \phi_2 \mid \phi_1 \rangle \end{aligned}$$

$$\begin{aligned} &(a_1 - a_2) \langle \phi_2 \mid \phi_1 \rangle = 0 \quad , \quad a_1 - a_2 \neq 0 \\ &\langle \phi_2 \mid \phi_1 \rangle = 0 \end{aligned}$$

Let A be a hermitian operator with eigenvalues $a_1, a_2, a_3, ...a_n, ...$

Let the eigenvalue a_n be g_n–fold degenerate ($g_n = 1$ if a_n is non-degenerate).

Let $\left\{u_n^{(1)}, u_n^{(2)}, ..., u_n^{(g_n)}\right\}$ be a CON set of eigenfunctions for the eigenvalue a_n. Note that the eigenvalues a_n are *countable*, that is, they do not take on a continuum of values. This property (called separability) will be discussed further later. Now we have

$$Au_n^{(\alpha)} = a_n u_n^{(\alpha)} \quad , \quad \alpha = 1, 2, ..., g_n \tag{2.254}$$

so α labels each member of the set of degenerate functions which belong to the eigenvalue a_n and n labels the eigenvalue a_n.

Since eigenfunctions belonging to different eigenvalues are necessarily orthogonal, we have

$$\left\langle u_n^{(\alpha)} \mid u_m^{(\beta)} \right\rangle = \delta_{nm}\delta_{\alpha\beta} \tag{2.255}$$

Let $\left\{u_n^{(\alpha)}\right\}$ be an ON set of eigenfunctions of A with n *taking on all possible values*, that is, with a_n going through *all* eigenvalues of A, and with α going through a CON set of eigenfunctions for each eigenvalue a_n, that is, any

eigenfunction belonging to a_n can be expressed as a linear superposition of $\left\{u_n^{(1)}, u_n^{(2)}, ..., u_n^{(g_n)}\right\}$. We will call such a set $\left\{u_n^{(\alpha)}\right\}$ a *maximal* ON set of eigenfunctions of A.

$\left\{u_n^{(\alpha)}\right\}$ contains the following eigenfunctions:

$u_1^{(1)}, u_1^{(2)}, ..., u_1^{(g_1)}$ = CON set for eigenvalue a_1 (g_1−fold degenerate)

$u_2^{(1)}, u_2^{(2)}, ..., u_2^{(g_2)}$ = CON set for eigenvalue a_2 (g_2−fold degenerate)

.....

.....

(going through *all* eigenvalues of A)

The set $\left\{u_n^{(\alpha)}\right\}$ *may or may not* be a complete orthonormal set for all square-integrable functions, that is, an arbitrary square-integrable function $\phi(\vec{x})$ may or may not be expressible in the form

$$\phi(\vec{x}) = \sum_n \sum_{\alpha=1}^{g_n} c_n^{(\alpha)} u_n^{(\alpha)}(\vec{x}) \tag{2.256}$$

2.1.11.23. Example

Consider

$$A = p_{xop} = \frac{\hbar}{i}\frac{\partial}{\partial x_i} \tag{2.257}$$

As we showed earlier, there are no normalizable eigenfunctions of p_{xop}. Thus, $\left\{u_n^{(\alpha)}\right\}$ contains *no* functions - it is not a CON set in L^2.

2.1.11.24. Example

Consider

$$A = L_{zop} = \frac{\hbar}{i}\frac{\partial}{\partial \phi} \tag{2.258}$$

As we showed earlier, the eigenfunctions of L_{zop} are $f(r,\theta)e^{i\ell\phi}$ with $\ell = 0, \pm 1, \pm 2, ...$ and

$$\int_0^\infty r^2 dr \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi \left| f(r,\theta)e^{i\ell\phi}\right|^2 \tag{2.259}$$

is finite and non-zero. Let $\{f_\alpha(r,\theta)\}_{\alpha=1,2,....}$ be any CON set for square-integrable functions of r and θ so that

$$\int_0^\infty r^2 dr \int_0^\pi \sin\theta d\theta \, f_\alpha^\star(r,\theta) f_\beta(r,\theta) = \delta_{\alpha\beta} \tag{2.260}$$

and

$$f(r,\theta) = \sum_{\alpha} d_\alpha f_\alpha(r,\theta) \tag{2.261}$$

for any square-integrable function $f(r,\theta)$. Now

$$u_\ell^{(\alpha)}(\vec{x}) = \frac{1}{\sqrt{2\pi}} f_\alpha(r,\theta) e^{i\ell\phi} \tag{2.262}$$

is an eigenfunction of L_{zop} with eigenvalue $\ell\hbar$ for any α.

Since $u_\ell^{(1)}, u_\ell^{(2)}, \ldots\ldots\ldots$ are linearly independent, the eigenvalues $\ell\hbar$ have infinite order (all r and θ values) of degeneracy. We also have

$$\left\langle u_\ell^{(\alpha)} \,\middle|\, u_{\ell'}^{(\alpha')} \right\rangle = \int_0^\infty r^2 dr \int_0^\pi \sin\theta d\theta \, f_\alpha^*(r,\theta) f_\beta(r,\theta) \int_0^{2\pi} \frac{d\phi}{2\pi} e^{i\phi(\ell-\ell')} = \delta_{\alpha\alpha'}\delta_{\ell\ell'} \tag{2.263}$$

Let $\Phi(\vec{x})$ be an arbitrary square-integrable function. The we have

$$\Phi(r,\theta,\phi) = \sum_{\ell=-\infty}^{\infty} b_\ell(r,\theta) \frac{e^{i\ell\phi}}{\sqrt{2\pi}} \tag{2.264}$$

which is just the Fourier series expansion of a function of $\Phi(r,\theta fixed)$ in the interval $[0,2\pi]$. But, we can always write

$$b_\ell(r,\theta) = \sum_{\alpha} c_\ell^{(\alpha)} f_\alpha(r,\theta) \tag{2.265}$$

since $\{f_\alpha(r,\theta)\}_{\alpha=1,2,\ldots}$ is a CON set. Therefore,

$$\Phi(r,\theta,\phi) = \sum_{\ell=-\infty}^{\infty} \sum_{\alpha} c_\ell^{(\alpha)} f_\alpha(r,\theta) \frac{e^{i\ell\phi}}{\sqrt{2\pi}} = \sum_{\ell=-\infty}^{\infty} \sum_{\alpha} c_\ell^{(\alpha)} u_\ell^{(\alpha)}(\vec{x}) \tag{2.266}$$

that is, $\left\{u_\ell^{(\alpha)}(\vec{x})\right\}$ is a CON set in L^2.

Let $A_{op} = A(\vec{x},\vec{p}_{op})$ be the hermitian operator corresponding to some physical quantity $A = A(\vec{x},\vec{p})$. Then, as we have stated earlier, a measurement of A performed at time t_0 will yield the value a with certainty if $\psi(\vec{x},t_0) = \psi_0(\vec{x})$ is a (normalizable) eigenfunction of A_{op} with eigenvalue a.

Suppose $\psi(\vec{x},t_0) = \psi_0(\vec{x})$ is normalizable but it is not an eigenfunction of A. Then, as we stated earlier, a measurement of A at time t_0 will necessarily have $\Delta A \neq 0$.

We first consider physical quantities A such that the maximal set of ON eigenfunctions $\left\{u_n^{(\alpha)}\right\}$ *of* A_{op} *is complete in* L^2.

Therefore,

$$\psi_0(\vec{x}) = \sum_n \sum_\alpha c_n^{(\alpha)} u_n^{(\alpha)}(\vec{x}) \tag{2.267}$$

a.e. We then have

$$\begin{aligned}\left\langle u_m^{(\beta)} \mid \psi_0 \right\rangle &= \left\langle u_m^{(\beta)} \,\middle|\, \sum_n \sum_\alpha c_n^{(\alpha)} u_n^{(\alpha)} \right\rangle = \sum_n \sum_\alpha c_n^{(\alpha)} \left\langle u_m^{(\beta)} \mid u_n^{(\alpha)} \right\rangle \\ &= \sum_n \sum_\alpha c_n^{(\alpha)} \delta_{\alpha\beta} \delta_{nm} = c_m^{(\beta)}\end{aligned}$$

or

$$c_n^{(\alpha)} = \left\langle u_n^{(\alpha)} \,\middle|\, \psi_0 \right\rangle = \text{ expansion coefficients} \tag{2.268}$$

Also,

$$\begin{aligned}\langle \psi_0 \mid \psi_0 \rangle &= \left\langle \sum_m \sum_\beta c_m^{(\beta)} u_m^{(\beta)} \,\middle|\, \sum_n \sum_\alpha c_n^{(\alpha)} u_n^{(\alpha)} \right\rangle \\ &= \sum_m \sum_\beta \sum_n \sum_\alpha c_n^{(\alpha)} c_m^{(\beta)*} \left\langle u_m^{(\beta)} \mid u_n^{(\alpha)} \right\rangle \\ &= \sum_m \sum_\beta \sum_n \sum_\alpha c_n^{(\alpha)} c_m^{(\beta)*} \delta_{\alpha\beta} \delta_{nm} = \sum_n \sum_\alpha \left| c_n^{(\alpha)} \right|^2\end{aligned} \tag{2.269}$$

Let us now calculate $\langle A^N \rangle$, the so-called N^{th} moment of the probability distribution of measurements of A ($N = 01, 2, ...$). We have

$$\begin{aligned}\left\langle A^N \right\rangle &= \frac{\left\langle \psi_0 \mid A_{op}^N \psi_0 \right\rangle}{\langle \psi_0 \mid \psi_0 \rangle} = \frac{1}{\langle \psi_0 \mid \psi_0 \rangle} \left\langle \sum_m \sum_\beta c_m^{(\beta)} u_m^{(\beta)} \,\middle|\, A_{op}^N \sum_n \sum_\alpha c_n^{(\alpha)} u_n^{(\alpha)} \right\rangle \\ &= \frac{1}{\langle \psi_0 \mid \psi_0 \rangle} \left\langle \sum_m \sum_\beta c_m^{(\beta)} u_m^{(\beta)} \,\middle|\, \sum_n \sum_\alpha c_n^{(\alpha)} A_{op}^N u_n^{(\alpha)} \right\rangle \\ &= \frac{1}{\langle \psi_0 \mid \psi_0 \rangle} \left\langle \sum_m \sum_\beta c_m^{(\beta)} u_m^{(\beta)} \,\middle|\, \sum_n \sum_\alpha c_n^{(\alpha)} (a_n)^N u_n^{(\alpha)} \right\rangle \\ &= \frac{1}{\langle \psi_0 \mid \psi_0 \rangle} \sum_m \sum_\beta \sum_n \sum_\alpha c_m^{(\beta)*} c_n^{(\alpha)} (a_n)^N \left\langle u_m^{(\beta)} \mid u_n^{(\alpha)} \right\rangle = \sum_n \sum_\alpha \left| c_n^{(\alpha)} \right|^2 (a_n)^N\end{aligned}$$

Therefore, the N^{th} moment of the probability distribution of measurements of A is

$$\left\langle A^N \right\rangle = \frac{1}{\langle \psi_0 \mid \psi_0 \rangle} \sum_n \sum_\alpha \left| c_n^{(\alpha)} \right|^2 (a_n)^N = \sum_n (a_n)^N \left\{ \sum_{\alpha=1}^{g_n} \frac{\left| c_n^{(\alpha)} \right|^2}{\langle \psi_0 \mid \psi_0 \rangle} \right\} \tag{2.270}$$

Let $\wp(a, t_0)$ be the probability that a measurement of A will yield the value a at time t_0. Therefore, from our earlier definition,

$$\left\langle A^N \right\rangle = \sum_{\substack{all\ measured \\ values\ of\ a}} a^N \wp(a, t_0) \tag{2.271}$$

As we showed earlier, the $\left\langle A^N \right\rangle$ for $N = 0, 1, 2, ...$ uniquely determine the probability distribution of measurements of A. Therefore, comparing (calculation versus definition) the above expressions for $\left\langle A^N \right\rangle$ we have a most important result

$$\wp(a, t_0) = \begin{cases} \sum_{\alpha=1}^{g_n} \frac{|c_n^{(\alpha)}|^2}{\langle \psi_0 \mid \psi_0 \rangle} & \text{for } a = a_n \text{ [an eigenvalue of } A_{op}] \\ 0 & \text{for } a \text{ not an eigenvalue of } A_{op} \end{cases} \tag{2.272}$$

Any measurement of A will yield a value which *must be an eigenvalue* of A_{op}. The probability of observing a given eigenvalue is given by the above expression (2.272).

Now

$$c_n^{(\alpha)} = \left\langle u_n^{(\alpha)} \,\middle|\, \psi_0 \right\rangle \quad , \quad c_n^{(\alpha)*} = \left\langle \psi_0 \,\middle|\, u_n^{(\alpha)} \right\rangle \tag{2.273}$$

Therefore,

$$\wp(a, t_0) = \begin{cases} \sum_{\alpha=1}^{g_n} \frac{\left\langle \psi_0 \middle| u_n^{(\alpha)} \right\rangle \left\langle u_n^{(\alpha)} \middle| \psi_0 \right\rangle}{\langle \psi_0 \mid \psi_0 \rangle} & \text{for } a = a_n \text{ [an eigenvalue of } A_{op}] \\ 0 & \text{for } a \text{ not an eigenvalue of } A_{op} \end{cases} \tag{2.274}$$

Thus, the only possible results of a measurement of some operator are its eigenvalues!

2.1.11.25. Notes

1. Let $\psi(\vec{x}, t_0) = \psi_0(\vec{x})$ be an eigenfunction of A_{op} with eigenvalue a_r so that $A_{op}\psi_0(\vec{x}) = a_r\psi_0(\vec{x})$. We should find that a measurement of A will yield the result a_r with certainty. Let us check this. $\left\{u_r^{(1)}, u_r^{(2)}, ..., u_r^{(g_r)}\right\}$ is a CON set of eigenfunctions for the eigenvalue a_r. Therefore,

   $$\psi_0(\vec{x}) = \sum_{\alpha=1}^{g_r} d_\alpha u_r^{(\alpha)} \tag{2.275}$$

   that is, only eigenfunctions for a_r occur in the expansion. Therefore,

   $$\langle \psi_0 \mid \psi_0 \rangle = \sum_{\alpha=1}^{g_r} |d_\alpha|^2 \tag{2.276}$$

   and

   $$\wp(a, t_0) = \begin{cases} \sum_{\alpha=1}^{g_n} \frac{|d_\alpha|^2}{\langle \psi_0 \mid \psi_0 \rangle} = 1 & \text{for } a = a_r \\ 0 & \text{for } a \neq a_r \end{cases} \tag{2.277}$$

2. If the eigenvalues are *non-degenerate*, then $\alpha = 1$ is the only value and we need not write α at all

   $$\psi_0(\vec{x}) = \sum_n c_n u_n(\vec{x}) \quad , \quad A_{op}u_n(\vec{x}) = a_n u_n(\vec{x})$$
   $$c_n = \langle u_n \mid \psi_0 \rangle \quad , \quad \langle u_n \mid u_m \rangle = \delta_{nm}$$
   $$\langle \psi_0 \mid \psi_0 \rangle = \sum_n |c_n|^2$$

$$\wp(a,t_0) = \begin{cases} \frac{|c_n|^2}{\langle\psi_0 \mid \psi_0\rangle} & \text{for } a = a_r \\ 0 & \text{for } a \neq \text{eigenvalue of } A_{op} \end{cases} \tag{2.278}$$

3. A required condition on $\wp(a,t_0)$ is

$$\sum_{\substack{\text{all values} \\ \text{of } a}} \wp(a,t_0) = 1 \tag{2.279}$$

Let us check this. Recall that

$$\langle\psi_0 \mid \psi_0\rangle = \sum_{n,\alpha} \left|c_n^{(\alpha)}\right|^2 \tag{2.280}$$

so that

$$\begin{aligned} \sum_{\substack{\text{all values} \\ \text{of } a}} \wp(a,t_0) &= \sum_n \frac{1}{\langle\psi_0 \mid \psi_0\rangle} \sum_{\alpha=1}^{g_n} \left|c_n^{(\alpha)}\right|^2 \\ &= \frac{1}{\langle\psi_0 \mid \psi_0\rangle} \sum_{n,\alpha} \left|c_n^{(\alpha)}\right|^2 = 1 \end{aligned}$$

as required.

2.1.11.26. Example

Let $A_{op} = L_{zop}$. We have shown that the eigenvalues are $\ell\hbar$ ($\ell = 0, \pm 1, ...$) and that the maximal ON set of eigenfunctions $\left\{u_\ell^{(\alpha)}(\vec{x})\right\}$ is complete in L^2. Thus, a measurement of L_z at any time will yield a value which must be $0, \pm\hbar, \pm 2\hbar, ...$ L_z is said to be *quantized*. If $\psi(\vec{x},t_0)$ is not an eigenfunction, then there will be a spread in possible values of L_z and the previous discussion tells us how to calculate $\wp(\ell\hbar, t_0)$.

2.2. Energy Measurements

Let us now turn our attention to *energy measurements*. We must therefore consider the eigenvalue equation for energy (called the *time-independent Schrodinger equation*). Assume that the particle has conservative forces acting on it so that $\vec{F} = -\nabla V(\vec{x})$ where $V(\vec{x})$ is the potential energy. Then

$$H = Hamiltonian(energy) = \frac{\vec{p}\cdot\vec{p}}{2m} + V(\vec{x}) \tag{2.281}$$

and

$$H_{op} = \frac{\vec{p}_{op}\cdot\vec{p}_{op}}{2m} + V(\vec{x}) = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x}) \tag{2.282}$$

We must solve the eigenvalue equation

$$H_{op}\phi(\vec{x}) = E\phi(\vec{x}) \Rightarrow -\frac{\hbar^2}{2m}\nabla^2\phi(\vec{x}) + V(\vec{x})\phi(\vec{x}) = E\phi(\vec{x}) \tag{2.283}$$

The eigenvalue E is a constant (independent of $\vec{x}$). Only for certain values of E will the equation have a solution $\phi(\vec{x})$ which is normalizable.

These normalizable eigenfunctions of H_{op} are said to represent bound states. If $\psi(\vec{x}, t_0)$ is a normalizable eigenfunction of H_{op} then it has a precise energy ($\Delta E = 0$) and

$$\wp(\vec{x}, t_0) = \frac{1}{\langle \psi \mid \psi \rangle} |\psi(\vec{x}, t_0)|^2 \to 0 \ \ as \ \ r \to \infty \tag{2.284}$$

which is required for normalizability. Thus, the probability of observing the particle at a certain position is confined (non-negligible probability) to some finite (bounded) region of space - the particle has definite energy and is *bound* in this region.

As an example, consider the classical motion of a charge $(-q)$ about a fixed charge $(+q)$ as shown in Figure 2.10 below.

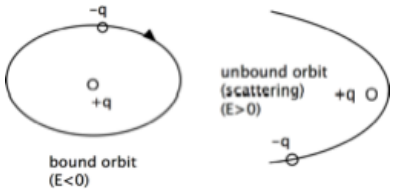


Figure 2.10: Classical Orbits

Quantum mechanically, the orbit trajectories are not well-defined (even though the energies are precise). However, one would expect the classical bound orbit to correspond to a normalizable quantum eigenfunction ($\wp(\vec{x}, t_0)$ non-zero for $r \to \infty$). The non-normalizable eigenfunctions are therefore physically interesting and should play a role in the theory. Indeed, we expect that the normalizable eigenfunctions of H_{op} for the above charge will not be complete in L^2 because unbound motion is also possible. We will postpone discussing non-normalizable eigenfunctions of H_{op} and concentrate on the normalizable eigenfunctions. Remember only normalizable wave functions have been incorporated in our theory so far. *We expect that the normalizable eigenfunctions of H_{op} will be complete in L^2 if there are no unbound orbits possible for the classical H.*

2.2.0.1. Note

For the differential equation

$$-\frac{\hbar^2}{2m}\nabla^2\phi(\vec{x}) + V(\vec{x})\phi(\vec{x}) = E\phi(\vec{x}) \tag{2.285}$$

if $V(\vec{x})$ is finite in some region ($V(\vec{x})$ may, however, contain discontinuities in this region), *then $\phi(\vec{x})$ and $\partial\phi(\vec{x})/\partial x_i$ must be continuous in this region* (so that $\nabla^2\phi(\vec{x})$ is finite, as required by the above equation for finite $V(\vec{x})$.

2.2.0.2. Example

We consider a particle (mass m) constrained to move along a frictionless horizontal wire (dashed line in top part of Figure 2.11 below) between two rigid (impenetrable) walls. This is one-dimensional motion. We then have

$$H = \frac{p^2}{2m} + V(x) \quad , \quad F_x = -\frac{dV}{dx} \tag{2.286}$$

with

$$V(x) = 0 \text{ for } x \in (0, L) \text{ so that } F_x = 0 \text{ for } x \in (0, L)$$

and

$$V(x) = V_0 \to \infty \text{ for } x < 0 \text{ and for } x > L$$

as shown in the lower part of Figure 2.11 below.

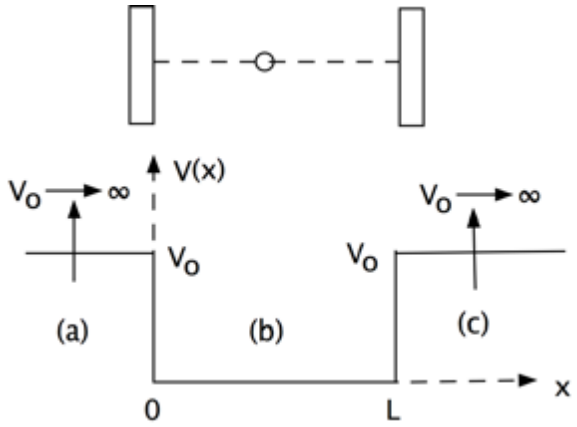


Figure 2.11: Particle in a Rigid Box

We have $F_x = -\infty$ at $x = L$ and $F_x = +\infty$ at $x = 0$. Therefore, the (classical) particle cannot get into the regions $x < 0$ and $x > L$ no matter how energetic it is (the kinetic energy $p^2/2m$ would have to be negative to obtain a finite total energy).

Classical Motion: The particle moves back and forth between the two walls with constant speed. The reflections at each wall just reverses the particle's direction of motion. $E_{classical} = mv^2/2$ can take on any value from 0 to ∞. All motion is bound between 0 and L.

The eigenvalue equation for energy(time-independent Schrodinger equation) is

$$H_{op}\phi(x) = E\phi(x) \Rightarrow -\frac{\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2} + V(x)\phi(x) = E\phi(x) \tag{2.287}$$

with E = constant and $\phi(\vec{x})$ normalizable.

Note: Because $V_0 \to \infty$, it is not clear whether or not $\phi(\vec{x})$ and $d\phi(\vec{x})/dx$ are continuous at $x = 0, L$ ($\phi(\vec{x})$ and $d\phi(\vec{x})/dx$ must be continuous in regions where $V(\vec{x})$ is finite).

Let us look at this issue of boundary conditions in two ways, first for this specific problem and then in general using the Schrodinger equation (this last approach will then apply to all potential energy functions)

2.2.0.3. Boundary Condition for this Particular System

Claims:

1. $\phi(\vec{x}) = 0$ for $x < 0$ (region (a)) and for $x > L$ (region (c)).
2. $\phi(\vec{x}$ in region (b) $(0 < x < L)$ goes to zero as $x \to 0$ and as $x \to L$ so that $\phi(\vec{x}$ is continuous for *all* x.

Conditions (1) and (2) will determine $\phi(\vec{x}$ and we will then see that $d\phi(\vec{x})/dx$ is discontinuous at $x = 0$ and at $x = L$.

2.2.0.4. Proof of conditions (1) and (2)

Let V_0 be finite. Then $\phi(\vec{x}$ and $d\phi(\vec{x})/dx$ are are necessarily continuous everywhere - in particular at $x = 0$ and $x = L$. After obtaining the conditions on $\phi(\vec{x}$ for finite V_0 we now let $V_0 \to \infty$.

Let $E < V_0$ (this is no restriction since $V_0 \to \infty$).

Region (a):

$$-\frac{\hbar^2}{2m}\frac{d^2\phi^a}{dx^2} + V_0\phi^a = E\phi^a \tag{2.288}$$

Region (b):

$$-\frac{\hbar^2}{2m}\frac{d^2\phi^b}{dx^2} = E\phi^b \tag{2.289}$$

Region (c):

$$-\frac{\hbar^2}{2m}\frac{d^2\phi^c}{dx^2} + V_0\phi^c = E\phi^c \tag{2.290}$$

where E is the same in regions (a), (b), and (c) because the eigenvalue is independent of x.

Now, let

$$k = \frac{\sqrt{2mE}}{\hbar} \quad , \quad K = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \tag{2.291}$$

Note that K is a positive real number for $E < V_0$. Therefore,

Region (a):

$$\frac{d^2\phi^a}{dx^2} - K^2\phi^a = 0 \rightarrow \phi^a = \alpha e^{Kx} + \beta e^{-Kx} \tag{2.292}$$

Since $x < 0$ the term e^{-Kx} diverges as $x \rightarrow -\infty$.

Thus, ϕ is normalizable only if $\beta = 0$.

Therefore, $\phi^a = \alpha e^{Kx}$.

Region (b):

$$\frac{d^2\phi^b}{dx^2} = -k^2\phi^b \rightarrow \phi^b = A\sin kx + B\cos kx \tag{2.293}$$

Region (c):

$$\frac{d^2\phi^c}{dx^2} - K^2\phi^c = 0 \rightarrow \phi^c = \gamma e^{Kx} + \delta e^{-Kx} \tag{2.294}$$

Since $x > L$ the term e^{-Kx} diverges as $x \rightarrow +\infty$.

Thus, ϕ is normalizable only if $\gamma = 0$.

Therefore, $\phi^c = \delta e^{-Kx}$.

We note that α, A, B, δ may depend on V_0.

For finite V_0, $\phi(\vec{x}$ and $d\phi(\vec{x})/dx$ are continuous at $x = 0$ and $x = L$.

$x = 0$:

$$\phi^a(0) = \phi^b(0) \Rightarrow \alpha = \beta$$
$$\frac{d\phi^a(0)}{dx} = \frac{d\phi^b(0)}{dx} \Rightarrow \alpha K = Ak$$

$x = L$:

$$\phi^c(L) = \phi^b(L) \Rightarrow A\sin kL + B\cos kL = \delta e^{-KL}$$
$$\frac{d\phi^a(0)}{dx} = \frac{d\phi^b(0)}{dx} \Rightarrow Ak\cos kL - Bk\sin kL = -K\delta e^{-KL}$$

The two conditions at $x = 0$ give

$$K = k\frac{A}{B} \tag{2.295}$$

The two conditions at $x = L$ give

$$-K = \frac{k(A\cos kL - B\sin kL)}{A\sin kL + B\cos kL} \tag{2.296}$$

Now let $V_0 \rightarrow \infty$. This corresponds to $K \rightarrow \infty$ while k, A and B stay finite. Note also that $\phi^b = A\sin kx + B\cos kx$ must stay continuous with a continuous

derivative as $V_0 \to \infty$ because

$$-\frac{\hbar^2}{2m}\frac{d^2\phi^b}{dx^2} = E\phi^b \tag{2.297}$$

in region (b) for any V_0. Now

$$\begin{aligned} K = k\frac{A}{B} = \infty \text{ with } kA \text{ finite } &\Rightarrow B \to 0 \\ -K = \frac{k(A\cos kL - B\sin kL)}{A\sin kL + B\cos kL} & \\ = -\infty = \frac{k\cos kL}{\sin kL} \text{ with } B = 0 &\Rightarrow \sin kL \to 0 \end{aligned}$$

Therefore,

$$\phi^b = A\sin kx \text{ with } \sin kL \to 0 \tag{2.298}$$

so that at $\phi^a \to 0$ $x = 0$ and $x = L$ when $V_0 \to \infty$.

Furthermore, $\phi^a = \alpha e^{Kx} \to 0$ as $K \to \infty$ $(x > L)$ because $A\sin kL + B\cos kL = \delta e^{-KL} \to 0$ requires $\delta e^{-KL} \to 0$ for $x > L$.

This completes the proof of claims (1) and (2). *Notice that* $\phi^b(0) = \phi^b(L) = 0$ *with* $\phi^a(x) = \phi^c(x) = 0$ *means that* $\phi(x)$ *is continuous at* $x = 0$ *and at* $x = L$ *as* $V_0 \to \infty$.

2.2.0.5. General Discussion of Boundary Conditions

The Schrodinger equation in 1–dimension is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_E(x)}{dx^2} + V(x)\psi_E(x) = E\psi_E(x) \tag{2.299}$$

The solutions $\psi_E(x)$ are the energy eigenstates (eigenfunctions). We are thus faced with solving an ordinary differential equation with boundary conditions.

Since $\psi_E(x)$ is physically related to a probability amplitude and hence to a measurable probability, we assume that $\psi_E(x)$ is continuous since a measurable probability should not be discontinuous. This is the way physics is supposed to interact with the mathematics.

Using this fact, we can determine the general continuity properties of $d\psi_E(x)/dx$. The continuity property at a particular point, say $x = x_0$, is derived as follows. Integrating the equation across the point $x = x_0$ we get

$$\begin{aligned} \int_{x_0-\varepsilon}^{x_0+\varepsilon} \frac{d^2\psi_E(x)}{dx^2}dx &= \int_{x_0-\varepsilon}^{x_0+\varepsilon} d\left(\frac{d\psi_E(x)}{dx}\right) \\ &= -\frac{2m}{\hbar^2}\left[E\int_{x_0-\varepsilon}^{x_0+\varepsilon}\psi_E(x)dx - \int_{x_0-\varepsilon}^{x_0+\varepsilon} V(x)\psi_E(x)dx\right] \end{aligned}$$

Taking the limit as $\varepsilon \to 0$ we have

$$\lim_{\varepsilon\to 0}\left(\left.\frac{d\psi_E(x)}{dx}\right|_{x=x_0+\varepsilon} - \left.\frac{d\psi_E(x)}{dx}\right|_{x=x_0-\varepsilon}\right)$$
$$= -\frac{2m}{\hbar^2}\left[E\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon}\psi_E(x)dx - \lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon}V(x)\psi_E(x)dx\right]$$

or the discontinuity in the derivative is given by

$$\Delta\left(\frac{d\psi_E(x)}{dx}\right) = \frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon}V(x)\psi_E(x)dx \tag{2.300}$$

where we have used the continuity of $\psi_E(x)$ to set

$$\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon}\psi_E(x)dx = 0 \tag{2.301}$$

This makes it clear that whether or not $d\psi_E(x)/dx$ has a discontinuity at some point depends directly on the potential energy function at that point.

If $V(x)$ is continuous at $x = x_0$ (harmonic oscillator example), i.e., if

$$\lim_{\varepsilon\to 0}[V(x_0+\varepsilon) - V(x_0-\varepsilon)] = 0 \tag{2.302}$$

then

$$\Delta\left(\frac{d\psi_E(x)}{dx}\right) = \frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon}V(x)\psi_E(x)dx = 0 \tag{2.303}$$

and $d\psi_E(x)/dx$ is continuous.

Finally, if $V(x)$ has an infinite jump at $x = x_0$(infinite square well and delta-function examples), then we have two choices

1. if the potential is infinite over an extended range of x (the infinite well), then we must force $\psi_E(x) = 0$ in that region and use only the continuity of $\psi_E(x)$ as a boundary condition at the edge of the region.

2. if the potential is infinite at a single point, i.e., $V(x) = \delta(x - x_0)$ then

$$\Delta\left(\frac{d\psi_E(x)}{dx}\right) = \frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon}V(x)\psi_E(x)dx$$
$$= \frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon}\delta(x-x_0)\psi_E(x)dx$$
$$= \frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\psi_E(x_0) = \frac{2m}{\hbar^2}\psi_E(x_0) \tag{2.304}$$

and thus $d\psi_E(x)/dx$ is discontinuous by an amount proportional to the value of the wave function at that point.

These general results work for all potential energy functions, as we shall see.

2.2.0.6. One-Dimensional Infinite Square Well

Now let us start from the beginning and solve the Schrodinger equation for $V_0 = \infty$, the so-called *one-dimensional infinite square well*, with the following given:

1. for $0 < x < L$
$$-\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} = E\phi$$
2. for $x \geq L$ and $x \leq 0$
$$\phi = 0$$
3. ϕ is continuous for all x; $d\phi(x)/dx$ need not be continuous for $V_0 = \infty$.

(2) and (3) are the conditions we just proved to be required when $V_0 = \infty$.

For $0 < x < L$, we have

$$\frac{d^2\phi}{dx^2} = -k^2\phi \quad , \quad k^2 = \frac{2mE}{\hbar^2} \tag{2.305}$$

so that

$$\phi = A\sin kx + B\cos kx \tag{2.306}$$

Then

$$\phi(0) = 0 \Rightarrow B = 0 \Rightarrow \phi = A\sin kx$$
$$\phi(L) = 0 \Rightarrow A\sin kL = 0$$

Assuming that $A \neq 0$ (or the solution would be identically zero everywhere) we have the condition

$$\sin kL = 0 \Rightarrow k_n L = n\pi \quad , \quad n = 1, 2, 3, ... \tag{2.307}$$

Note that the case $n = 0 \Rightarrow k = 0 \Rightarrow \phi = 0$ and is not normalizable and the case n negative implies k negative. With $\phi = A\sin kx$, positive and negative k do not lead to independent solutions. Therefore, we need only consider positive k.

We have

$$k_n^2 = \frac{2mE_n}{\hbar^2} = \frac{n^2\pi^2}{L^2} \Rightarrow E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \quad , \; n = 1, 2, 3, ... \tag{2.308}$$

These are the energy eigenvalues. The corresponding energy eigenfunctions are

$$\phi_n(x) = A_n \sin k_n x = A_n \sin\frac{n\pi}{L}x \tag{2.309}$$

Notice that each energy eigenvalue is non-degenerate

$$\sin\frac{n\pi}{L}x \quad and \quad \sin\frac{n'\pi}{L}x \tag{2.310}$$

are linearly independent for $n \neq n'$).

The energy levels are quantized, that is, they take on only certain discrete values. This is to be contrasted with the classical situation, in which the particle can have any energy in the range $[0, \infty)$.

The ground-state energy

$$E_1 = \frac{\pi^2\hbar^2}{2mL^2} \neq 0 \tag{2.311}$$

This is consistent with the uncertainty principle. The localization of the particle within a range

$$L \Rightarrow \Delta p_x \geq \frac{\hbar}{L} \Rightarrow E \approx \frac{(\Delta p_x)^2}{2m} \geq \frac{\hbar^2}{2mL^2} \Rightarrow E_{\min} = \frac{\hbar^2}{2mL^2} \tag{2.312}$$

The spacing between low-lying energy levels is of the order $\hbar^2/mL^2$.

1. Macroscopic object

$$m \approx 1\,gm\ ,\ L \approx 10\,cm \text{ or } \frac{\hbar^2}{mL^2} \approx 10^{-56} erg \tag{2.313}$$

2. Electron confined to an atomic distance

$$m \approx 10^{-27}\,gm\ ,\ L \approx 1\ Angstrom = 10^{-8}\,cm \text{ or } \frac{\hbar^2}{mL^2} \approx 10^{-11} erg \approx 10\,eV \tag{2.314}$$

3. Proton confined to an nuclear distance

$$m \approx 10^{-24}\,gm\ ,\ L \approx 10^{-12}\,or\ 10^{-13} cm \text{ or } \frac{\hbar^2}{mL^2} \approx 10^{-6} erg \approx 1\,MeV \tag{2.315}$$

Note: An electron-volt (eV) is the energy obtained by an electron when it is accelerated through a potential difference of one volt:

$$1\,eV = (1.60 \times 10^{-19} coul)(1\,volt) = 1.60 \times 10^{-19} joule = .60 \times 10^{-12} erg \tag{2.316}$$

and

$$1\,MeV = 10^6 eV \tag{2.317}$$

Also, visible light typically has $\nu \approx 10^{15}\,\text{sec}^{-1}$ so that

$$E_{1\,photon} = h\nu \approx 10^{-12} erg \approx 1\,eV \tag{2.318}$$

Let us check that the eigenfunctions corresponding to different eigenvalues are orthogonal. We have

$$\begin{aligned}
\langle \phi_n \mid \phi_\ell \rangle &= \int_0^L dx A_n^* \sin\frac{n\pi x}{L} A_\ell \sin\frac{\ell\pi x}{L} \\
&= \frac{A_n^* A_\ell}{(2i)^2} \int_0^L dx \left(e^{i\frac{n\pi x}{L}} - e^{-i\frac{n\pi x}{L}} \right) \left(e^{i\frac{\ell\pi x}{L}} - e^{-i\frac{\ell\pi x}{L}} \right) \\
&= \frac{A_n^* A_\ell}{-4} \int_0^L dx \left(e^{i\frac{(n+\ell)\pi x}{L}} + e^{-i\frac{(n+\ell)\pi x}{L}} - e^{i\frac{(n-\ell)\pi x}{L}} - e^{-i\frac{(n-\ell)\pi x}{L}} \right) \\
&= -\frac{A_n^* A_\ell}{2} \int_0^L dx \left(\cos\left(\frac{(n+\ell)\pi x}{L} \right) - \cos\left(\frac{(n-\ell)\pi x}{L} \right) \right)
\end{aligned}$$

so that

$$\begin{aligned}
-\frac{A_n^* A_n}{2} \int_0^L dx \left(\cos\left(\frac{2n\pi x}{L} \right) - 1 \right) &= -\frac{A_n^* A_n}{2} \left(\left[\frac{L}{2n\pi} \sin\left(\frac{2n\pi x}{L} \right) - L \right]_0^L - L \right) \\
&= -L \quad , \quad n = \ell
\end{aligned} \tag{2.319}$$

and

$$\begin{aligned}
&-\frac{A_n^* A_\ell}{2} \int_0^L dx \left(\cos\left(\frac{(n+\ell)\pi x}{L} \right) - \cos\left(\frac{(n-\ell)\pi x}{L} \right) \right) \\
&\qquad = -\frac{A_n^* A_\ell}{2} \left(\left[\frac{L}{(n+\ell)\pi} \sin\left(\frac{(n+\ell)\pi x}{L} \right) \right]_0^L - \left[\frac{L}{(n-\ell)\pi} \sin\left(\frac{(n-\ell)\pi x}{L} \right) \right]_0^L \right) \\
&\qquad = 0 \quad , \quad n \neq \ell
\end{aligned} \tag{2.320}$$

or

$$\langle \phi_n \mid \phi_\ell \rangle = \frac{L}{2} |A_n|^2 \delta_{n\ell} \tag{2.321}$$

Letting

$$A_n = \sqrt{\frac{2}{L}} \quad , \quad \phi_n = u_n \tag{2.322}$$

where $\{u_n\}$ is an ON set of eigenfunctions, we have

$$u_n(x) = \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L} \quad , \quad \langle u_n \mid u_m \rangle = \delta_{nm} \tag{2.323}$$

We note that du_n/dx is discontinuous at $x = 0$ and $x = L$. Some plots of the first three wave functions ($n = 1, 2, 3$) are shown in Figure 2.12 below:

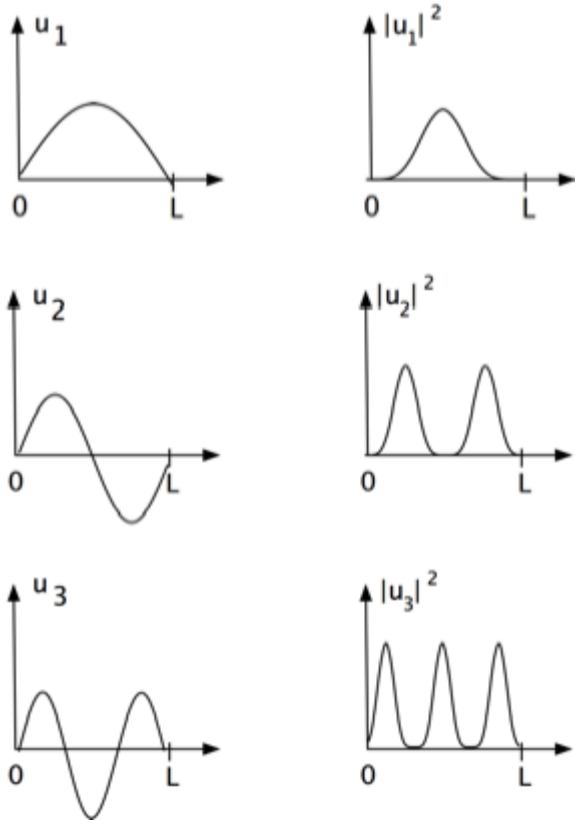


Figure 2.12: $n = 1, 2, 3$ wave functions

Since the eigenfunctions vanish for $x < 0$ and $x > L$, the probability of finding the particle (whose wave function is an energy eigenfunction) outside the region $[0, L]$ is zero. For a particle whose wave function is $u_n(x)$, the probability of finding the particle in $[x, x + dx]$ is not uniform over the region $[0, L]$ since $\wp(x, t) = |u_n(x)|^2$. This should be contrasted with the classical motion at constant speed - classically the particle spends equal amounts of time in each interval $[x, x + dx]$ throughout the region $[0, L]$.

Consider the ON set of all eigenfunctions $\{u_n\}$. Is this complete in L^2? Because all the eigenfunctions $u_n(x)$ vanish for $x < 0$ and $x > L$, a square-integrable function which is non-zero outside $[0, L]$ cannot be expanded in terms of the $u_n(x)$. However, if $\psi_0(x)$ is square-integrable and non-zero outside $[0, L]$, then

$$\langle H \rangle = \frac{\langle \psi_0 \mid H\psi_0 \rangle}{\langle \psi_0 \mid \psi_0 \rangle} = \frac{1}{\langle \psi_0 \mid \psi_0 \rangle} \int_{-\infty}^{\infty} dx \psi_0^*(x) \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi_0(x) \qquad (2.324)$$

would be infinite because $V(x) = V_0 = \infty$ outside $[0, L]$. Thus, a necessary condition for $\langle H \rangle$ to be finite is for $\psi_0(x)$ to vanish outside $[0, L]$.

It is true, however, that

$$\left\{ u_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \right\} \tag{2.325}$$

is complete for square-integrable functions which vanish outside $[0, L]$. The reasoning goes as follows. We know that

$$\left\{ e^{i \frac{2\pi n x}{2L}} \right\}_{n=0,\pm 1,\pm 2,\ldots} \tag{2.326}$$

is complete on $[-L, L]$ (just Fourier transform stuff). We have

$$e^{i \frac{\pi n x}{L}} = \cos \frac{\pi n x}{L} + i \sin \frac{\pi n x}{L} \rightarrow \left\{ \cos \frac{\pi n x}{L}, \sin \frac{\pi n x}{L} \right\} \tag{2.327}$$

for $n = 0, 1, 2, \ldots.$ is complete on $[-L, L]$.

Let $f(x)$ be an arbitrary function on $[0, L]$. Let

$$g(x) = \begin{cases} f(x) & \text{for } x \in [0, l] \\ -f(x) & \text{for } x \in [-L, 0] \end{cases} \tag{2.328}$$

$g(x)$ can be expanded in terms of

$$\left\{ \cos \frac{\pi n x}{L}, \sin \frac{\pi n x}{L} \right\} \tag{2.329}$$

that is,

$$g(x) = \sum_{n=0}^{\infty} A_n \cos \frac{\pi n x}{L} + \sum_{n=1}^{\infty} B_n \sin \frac{\pi n x}{L} \tag{2.330}$$

But,

$$A_n \propto \int_{-L}^{L} dx \cos \frac{\pi n x}{L} g(x) = 0 \tag{2.331}$$

because $g(x)$ is an odd function of x. Thus, $g(x)$ can be expanded in terms of

$$\left\{ \sin \frac{\pi n x}{L} \right\} \tag{2.332}$$

But this expansion must be valid in the subinterval $[0, L]$, where $g(x) = f(x)$. Therefore,

$$\left\{ \sin \frac{\pi n x}{L} \right\} \tag{2.333}$$

is complete on $[0, L]$.

Note: a.e. on $[0, L]$

$$f(x) = \sum_{n=1}^{\infty} B_n \sin \frac{\pi n x}{L} \tag{2.334}$$

For example, if $f(0)0$, then the endpoint $x = 0$ must be one of the points at which the expansion doesn't work (because each $\sin \pi n x/L = 0$ at $x = 0$). It is of no consequence, however, that the expansion does not hold on such a set of measure zero!

Let $\psi(x, t_0) = \psi_0(x)$ be an arbitrary wave function describing the particle constrained to move along a frictionless horizontal wire between two rigid walls. Assume that $\psi_0(x) = 0$ for $x < 0$ and $x > L$. Then we have

$$\psi_0(x) = \sum_{n=1}^{\infty} c_n u_n(x)$$

$$u_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \text{ (non - degenerate)}$$

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2} \quad , \quad \langle u_n \mid u_m \rangle = \delta_{nm}$$

which gives expansion coefficients

$$c_n = \langle u_n \mid \psi_0 \rangle = \int_0^L dx \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \psi_0(x) \tag{2.335}$$

and

$$\wp(E_n, t_0) = \frac{|c_n|^2}{\langle \psi_0 \mid \psi_0 \rangle} \tag{2.336}$$

is the probability that an energy measurement at t_0 will yield the value E_n. Only eigenvalues of H_{op} can be obtained when an energy measurement is made.

2.2.0.7. Example

Consider the wave function shown in Figure 2.13 below.

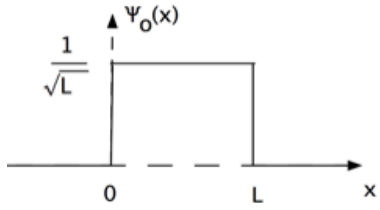


Figure 2.13: Wave Function

We have

$$\psi_0(x) = \begin{cases} 1/\sqrt{L} & \text{for } 0 \le x \le L \\ 0 & \text{otherwise} \end{cases} \tag{2.337}$$

A particle described by such a wave function can be found anywhere between 0 and L with equal probability. Note that $\psi_0(x)$ is discontinuous at $x = 0$ and $x = L$. That is fine since we only require that the energy eigenfunctions $u_n(x)$ have to be continuous!

We then have

$$\langle \psi_0 \mid \psi_0 \rangle = \int_0^L dx \frac{1}{\sqrt{L}} \frac{1}{\sqrt{L}} = 1 \tag{2.338}$$

or it is normalized. Then using

$$\psi_0(x) = \sum_{n=1}^{\infty} c_n u_n(x) \tag{2.339}$$

we have

$$\begin{aligned} c_n = \langle u_n \mid \psi_0 \rangle &= \int_0^L dx \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \psi_0(x) \\ &= \int_0^L dx \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \sqrt{\frac{1}{L}} = \frac{\sqrt{2}}{L} \frac{L}{n\pi} \left[-\cos \frac{n\pi x}{L} \right]_0^L \\ &= \frac{\sqrt{2}}{n\pi} \left[-\cos n\pi + 1 \right] = \begin{cases} 0 & \text{for } n \text{ even} \\ \frac{2\sqrt{2}}{n\pi} & \text{for } n \text{ odd} \end{cases} \end{aligned} \tag{2.340}$$

Therefore

$$\wp(E_n, t_0) = \frac{|c_n|^2}{\langle \psi_0 \mid \psi_0 \rangle} = \begin{cases} 0 & \text{for } n \text{ even} \\ \frac{8}{n^2\pi^2} & \text{for } n \text{ odd} \end{cases} \tag{2.341}$$

which is the probability of measuring the energy eigenvalue E_N when we are in the state described by $\psi_0(x)$ at t_0. Note that it is essentially the absolute square of the expansion coefficient $|c_n|^2$.

Note: Since

$$\sum_{all\ n} \wp(E_n, t_0) = 1 \tag{2.342}$$

we have

$$\sum_{n=1,3,5,\ldots} \frac{8}{n^2\pi^2} = 1 \Rightarrow \sum_{n=1,3,5,\ldots} \frac{1}{n^2} = \frac{\pi^2}{8} \tag{2.343}$$

which is a rather interesting mathematical result.

Suppose that we want to calculate $\langle H \rangle$ for the above state. We cannot use

$$\begin{aligned}\langle H \rangle &= \frac{\langle \psi_0 \mid H\psi_0 \rangle}{\langle \psi_0 \mid \psi_0 \rangle} \\ &= \frac{1}{\langle \psi_0 \mid \psi_0 \rangle} \int_{-\infty}^{\infty} dx \psi_0^*(x) \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi_0(x)\end{aligned}$$

because $\psi_0(x)$ is discontinuous at $x = 0$ and $x = L$ and therefore $d^2\psi_0(x)/dx^2$ is not defined at these points. These two isolated points cannot be omitted from the integral because $d^2\psi_0(x)/dx^2$ is infinite at these points and can give a non-zero contribution to the integral. The correct way to proceed in this case is to use the definition of the average value:

$$\langle H \rangle = \sum_{all\ n} \wp(E_n, t_0) E_n = \sum_{n=1,3,5,\ldots.} \frac{8}{n^2\pi^2} \frac{n^2\pi^2\hbar^2}{2mL^2} = \infty \tag{2.344}$$

We must now consider those physical quantities whose maximal set of ON eigenfunctions $\left\{ u_n^{(\alpha)} \right\}$ is *not* complete in L^2. An arbitrary square-integrable wave function cannot be expanded in terms of the $\left\{ u_n^{(\alpha)} \right\}$ and therefore, the results of previous discussions cannot be used to calculate the probability distribution of measurements.

Let A be the *hermitian* operator corresponding to some physical quantity. A must satisfy some additional, technical assumptions for the following discussion to be valid. We will not go into such technicalities here.

Let us generalize the *eigenvalue equation for A*:

$$A\phi(\vec{x}) = a\phi(\vec{x}) \tag{2.345}$$

where we now require

1. $\phi(\vec{x})$ is not identically zero
2. $$\langle \phi \mid \psi \rangle = \int d^3x \phi^*(\vec{x}) \psi(\vec{x})$$
   is finite for almost every square-integrable function $\psi(\vec{x})$.

Note: If $\phi(\vec{x})$ is normalizable, then $\langle \phi \mid \psi \rangle$ is finite for every square-integrable function $\psi(\vec{x})$. Thus, our generalized eigenvalue equation has all the normalizable eigenfunctions we considered before. However, there exist non-normalizable functions obeying condition (2). For example, $f(\vec{x}) = e^{i\vec{k}\cdot\vec{x}}$ has:

$$\langle f \mid f \rangle = \int d^3x \left| e^{i\vec{k}\cdot\vec{x}} \right|^2 = \infty$$

and

$$\langle f \mid \psi \rangle = \int d^3x e^{-i\vec{k}\cdot\vec{x}} \psi(\vec{x})$$

exists a.e. by the Fourier transform theorem.

We have thus enlarged the space of functions (called a rigged Hilbert space) to which an eigenfunction can belong. However, the wave function for a particle must still be normalizable.

Note: $\phi(\vec{x})$ does not obey condition (2) if $|\phi(\vec{x})| \to \infty$ as $|x| \to \infty$ or $|y| \to \infty$ or $|z| \to \infty$. For simplicity, let us demonstrate this for a function of one variable $\phi(x)$. There are square-integrable functions $\psi(x)$ which go as $1/x$ as $|x| \to \infty$ and

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

converges at the limits of integration

$$\int_{-\infty}^{\infty} dx \frac{1}{x^2} = -\frac{1}{x} \to 0$$

For such functions,

$$\langle \phi \mid \psi \rangle = \int d^3x \, \phi^*(\vec{x}) \psi(\vec{x}) \tag{2.346}$$

does not converge at the limits of integration,

$$\int_{-\infty}^{\infty} dx \frac{1}{x} \phi^* \to (\infty) \times (\ell n \infty) \to \infty \tag{2.347}$$

The spectrum of A is the set of all eigenvalues of A , where the eigenfunctions must obey conditions (1) and (2). The following results are from the spectral theory of self-adjoint operators discussed in Chapter 4 of this book). Some of the results we have already proved, others require detailed mathematical discussions because the inner product of two eigenfunctions, each obeying condition (2), may not exist, that is, $\langle \phi_1 \mid \phi_2 \rangle$ does not necessarily exist for non-normalizable ϕ_1 and ϕ_2.

2.2.0.8. Discrete Part of the Spectrum

In this case, the corresponding eigenfunctions are normalizable. Now

$$A\phi_n^{(\alpha)}(\vec{x}) = a_n \phi_n^{(\alpha)}(\vec{x}) \tag{2.348}$$

where α labels linearly independent eigenfunctions having the same eigenvalue. The eigenvalues a_n are countable ($n = 1, 2, 3, ...$), that is, the eigenvalues do not vary over a continuous range of values. This is the separability property of L^2.

1. Each a_n is real.

2. Eigenfunctions belonging to different eigenvalues are orthogonal.

3. a_n may be degenerate. g_n–fold degeneracy implies one can construct g_n orthogonal eigenfunctions belonging to a_n, $(\phi_n^{(1)}, ..., \phi_n^{(g_n)})$, such that any eigenfunction corresponding to the eigenvalue a_n can be expressed as a linear superposition of the $(\phi_n^{(1)}, ..., \phi_n^{(g_n)})$.

4. $\left\langle \phi_m^{(\alpha)} \,\middle|\, \phi_m^{(\alpha)} \right\rangle = N_m^{(\alpha)}$, which is a finite, non-zero constant (this follows from the normalizability of the $\phi_n^{(\alpha)}$. Therefore,

$$\left\langle \phi_m^{(\alpha)} \,\middle|\, \phi_n^{(\beta)} \right\rangle = N_m^{(\alpha)} \delta_{mn} \delta_{\alpha\beta} \tag{2.349}$$

Let

$$u_m^{(\alpha)} = \frac{1}{\sqrt{N_m^{(\alpha)}}} \phi_m^{(\alpha)} \tag{2.350}$$

Therefore, $\left\langle u_m^{(\alpha)} \,\middle|\, u_n^{(\beta)} \right\rangle = \delta_{mn}\delta_{\alpha\beta}$, that is, the $\left\{u_m^{(\alpha)}\right\}$ are ON eigenfunctions (normalizable) and we have

$$A u_m^{(\alpha)} = a_m u_m^{(\alpha)} \tag{2.351}$$

2.2.0.9. Continuous Part of the Spectrum

In this case, the corresponding eigenfunctions are not normalizable, but obey the conditions (1) and (2) stated earlier. Now

$$A\phi_{c\nu}^{(\alpha)}(\vec{x}) = a_{c\nu}\phi_{c\nu}^{(\alpha)}(\vec{x}) \tag{2.352}$$

where the subscript c stands for continuum. α labels linearly independent eigenfunctions having the same eigenvalue. The eigenvalues $a_{c\nu}$ vary over a continuous range of values (ν s a continuous variable).

1. Each $a_{c\nu}$ is real.

2. Eigenfunctions belonging to different eigenvalues are orthogonal.

3. $a_{c\nu}$ may be degenerate. g_ν–fold degeneracy implies one can construct g_ν orthogonal eigenfunctions belonging to $a_{c\nu}$, $(\phi_{c\nu}^{(1)}, ..., \phi_{c\nu}^{(g_\nu)})$, such that any eigenfunction corresponding to the eigenvalue $a_{c\nu}$ can be expressed as a linear superposition of the $(\phi_{c\nu}^{(1)}, ..., \phi_{c\nu}^{(g_\nu)})$.

4. $\left\langle \phi_{c\nu}^{(\alpha)} \,\middle|\, \phi_{c\nu}^{(\alpha)} \right\rangle = \infty$ because $\phi_{c\nu}^{(\alpha)}$ is not normalizable. We therefore expect $\left\langle \phi_{c\mu}^{(\alpha)} \,\middle|\, \phi_{c\nu}^{(\beta)} \right\rangle$ to be proportional to the Dirac delta function $\delta(\mu - \nu)\delta_{\alpha\beta}$.

$$\left\langle \phi_{c\mu}^{(\alpha)} \,\middle|\, \phi_{c\nu}^{(\beta)} \right\rangle = N_\mu^{(\alpha)} \delta(\mu - \nu)\delta_{\alpha\beta} = \begin{cases} 0 & \text{for } \mu \neq \nu\,,\ \alpha \neq \beta \\ \infty & \text{for } \mu = \nu\,, and \alpha = \beta \end{cases} \tag{2.353}$$

Let

$$u_{c\mu}^{(\alpha)} = \frac{1}{\sqrt{N_\mu^{(\alpha)}}} \phi_{c\mu}^{(\alpha)} \tag{2.354}$$

Therefore, $\left\langle u_{c\mu}^{(\alpha)} \,\middle|\, u_{c\nu}^{(\beta)} \right\rangle = \delta(\mu-\nu)\delta_{\alpha\beta}$ where $A u_{c\mu}^{(\alpha)} = a_{c\mu} u_{c\mu}^{(\alpha)}$.

5. Continuum eigenfunctions are orthogonal to discrete eigenfunctions

$$\left\langle u_n^{(\alpha)} \,\middle|\, u_{c\nu}^{(\beta)} \right\rangle = 0 \tag{2.355}$$

2.2.0.10. Theorem(proof omitted)

Let $\left\{u_n^{(\alpha)}, u_{c\nu}^{(\beta)}\right\}$ be a maximal ON set of discrete and continuum eigenfunctions of the hermitian operator A. Here, maximal means that the set contains eigenfunctions for all eigenvalues with α and β going through their full set of values for each eigenvalue ($\alpha = 1, .., g_n$ for a_n and $\beta = 1, ..., g_\nu$ for $a_{c\nu}$). Then $\left\{u_n^{(\alpha)}, u_{c\nu}^{(\beta)}\right\}$ is complete in L^2, that is, any square-integrable $\psi(\vec{x})$ can be written:

$$\psi(\vec{x}) = \sum_n \sum_{\alpha=1}^{g_n} c_n^{(\alpha)} u_n^{(\alpha)}(\vec{x}) + \int\limits_{\substack{entire \\ continuum}} d\nu \sum_{\beta=1}^{g_\nu} d_\nu^{(\beta)} u_{c\nu}^{(\beta)}(\vec{x}) \tag{2.356}$$

Note: The continuum eigenvalues may require labeling by more than one continuous index $\nu = (\nu_1, \nu_2, ...)$. In such a case, $d\nu = d\nu_1\, d\nu_2 .....$ and

$$\delta(\nu-\mu) = \delta(\nu_1-\mu_1)\delta(\nu_2-\mu_2).....\tag{2.357}$$

One can easily solve for the coefficients in the expansion.

$$\begin{aligned}\left\langle u_m^{(\gamma)} \,\middle|\, \psi \right\rangle &= \sum_n \sum_{\alpha=1}^{g_n} c_n^{(\alpha)} \left\langle u_m^{(\gamma)} \,\middle|\, u_n^{(\alpha)} \right\rangle + \int\limits_{\substack{entire \\ continuum}} d\nu \sum_{\beta=1}^{g_\nu} d_\nu^{(\beta)} \left\langle u_m^{(\gamma)} \,\middle|\, u_{c\nu}^{(\beta)} \right\rangle \\ &= \sum_n \sum_{\alpha=1}^{g_n} c_n^{(\alpha)} \delta_{mn}\delta_{\gamma\alpha} + \int\limits_{\substack{entire \\ continuum}} d\nu \sum_{\beta=1}^{g_\nu} d_\nu^{(\beta)}(0) = c_m^{(\gamma)}\end{aligned} \tag{2.358}$$

which is finite by earlier condition (2) and

$$\begin{aligned}\left\langle u_{c\mu}^{(\gamma)} \,\middle|\, \psi \right\rangle &= \sum_n \sum_{\alpha=1}^{g_n} c_n^{(\alpha)} \left\langle u_{c\mu}^{(\gamma)} \,\middle|\, u_n^{(\alpha)} \right\rangle + \int\limits_{\substack{entire \\ continuum}} d\nu \sum_{\beta=1}^{g_\nu} d_\nu^{(\beta)} \left\langle u_{c\mu}^{(\gamma)} \,\middle|\, u_{c\nu}^{(\beta)} \right\rangle \\ &= \sum_n \sum_{\alpha=1}^{g_n} c_n^{(\alpha)}(0) + \int\limits_{\substack{entire \\ continuum}} d\nu \sum_{\beta=1}^{g_\nu} d_\nu^{(\beta)} \delta(\mu-\nu)\delta_{\gamma\beta} = d_\mu^{(\gamma)}\end{aligned} \tag{2.359}$$

which is finite by earlier condition (2).

Note: The wave function for a particle must be normalizable (so that a probability interpretation is possible). However, the CON set $\left\{u_n^{(\alpha)}, u_{c\nu}^{(\beta)}\right\}$, in terms of which the wave function can be expanded, may contain non-normalizable eigenfunctions. Let $\psi(\vec{x}, t_0)$ be the wave function for the particle at t_0.

$$\psi(\vec{x}, t_0) = u_n^{(\alpha)}(\vec{x}) \text{ is possible } (u_n^{(\alpha)} \text{ normalizable})$$
$$\psi(\vec{x}, t_0) = u_{c\nu}^{(\alpha)}(\vec{x}) \text{ is } \textit{not} \text{ allowed } (u_{c\nu}^{(\alpha)} \text{ not normalizable})$$

However,

$$\psi(\vec{x}, t_0) = \left(\frac{1}{\Delta\nu}\right)^{1/2} \int\limits_{\substack{\Delta\nu \\ region}} d\nu \, u_{c\nu}^{(\alpha)}(\vec{x}) \tag{2.360}$$

with α fixed and $\Delta\nu$ some region in the continuum, is a normalizable wave function for any $\Delta\nu \neq 0$ (no matter how small but non-zero). Then

$$\begin{aligned}\langle\psi \mid \psi\rangle &= \left(\frac{1}{\Delta\nu}\right) \int\limits_{\Delta\nu} d\nu \int\limits_{\Delta\nu} d\nu' \left\langle u_{c\nu}^{(\alpha)} \,\middle|\, u_{c\nu'}^{(\alpha)} \right\rangle \\ &= \left(\frac{1}{\Delta\nu}\right) \int\limits_{\Delta\nu} d\nu \int\limits_{\Delta\nu} d\nu' \delta(\nu - \nu') \\ &= \left(\frac{1}{\Delta\nu}\right) \int\limits_{\Delta\nu} d\nu = 1\end{aligned}$$

which is thus normalizable. The spread of values produces a normalizable wave function.

2.2.0.11. Basic Problem

Suppose we are given a physical quantity A (hermitian). We then solve the eigenvalue equation as described earlier and form the CON set of eigenfunctions $\left\{u_n^{(\alpha)}, u_{c\nu}^{(\beta)}\right\}$. Let $\psi(\vec{x}, t_0) = \psi_0(\vec{x})$ be the wave function for the particle at time t_0. A measurement of A is made at time t_0.

What values can be obtained from the measurement and with what probability?

We have

$$\psi_0(\vec{x}) = \sum_{n,\alpha} c_n^{(\alpha)} u_n^{(\alpha)}(\vec{x}) + \int d\nu \sum_{\beta} d_\nu^{(\beta)} u_{c\nu}^{(\beta)}(\vec{x}) \tag{2.361}$$

so that

$$\left\langle \psi_0 \mid A^N \psi_0 \right\rangle = \left\langle \begin{array}{l} \sum\limits_{n,\alpha} c_n^{(\alpha)} u_n^{(\alpha)}(\vec{x}) \\ + \int d\nu \sum\limits_{\beta} d_\nu^{(\beta)} u_{c\nu}^{(\beta)}(\vec{x}) \end{array} \middle| A^N \left(\begin{array}{l} \sum\limits_{n,\alpha} c_n^{(\alpha)} u_n^{(\alpha)}(\vec{x}) \\ + \int d\nu \sum\limits_{\beta} d_\nu^{(\beta)} u_{c\nu}^{(\beta)}(\vec{x}) \end{array} \right) \right\rangle$$

$$= \left\langle \begin{array}{l} \sum\limits_{n,\alpha} c_n^{(\alpha)} u_n^{(\alpha)}(\vec{x}) \\ + \int d\nu \sum\limits_{\beta} d_\nu^{(\beta)} u_{c\nu}^{(\beta)}(\vec{x}) \end{array} \middle| \begin{array}{l} \sum\limits_{n,\alpha} c_n^{(\alpha)} a_n^N u_n^{(\alpha)}(\vec{x}) \\ + \int d\nu \sum\limits_{\beta} d_\nu^{(\beta)} a_{c\nu}^N u_{c\nu}^{(\beta)}(\vec{x}) \end{array} \right\rangle$$

$$= \sum_{n,\alpha} a_n^N \left| c_n^{(\alpha)} \right|^2 + \int d\nu \sum_{\beta} a_{c\nu}^N \left| d_\nu^{(\beta)} \right|^2 \tag{2.362}$$

where we have used orthonormality. Therefore, the N^{th} moment of the probability distribution of measurements of A is:

$$\left\langle A^N \right\rangle = \frac{\left\langle \psi_0 \mid A^N \psi_0 \right\rangle}{\langle \psi_0 \mid \psi_0 \rangle}$$

$$= \sum_n a_n^N \left\{ \frac{\sum\limits_{\alpha} \left| c_n^{(\alpha)} \right|^2}{\langle \psi_0 \mid \psi_0 \rangle} \right\} + \int d\nu a_{c\nu}^N \left\{ \frac{\sum\limits_{\beta} \left| d_\nu^{(\beta)} \right|^2}{\langle \psi_0 \mid \psi_0 \rangle} \right\} \tag{2.363}$$

The moments $\left\langle A^N \right\rangle$ for $N = 0, 1, 2, ...$ *uniquely* determine the probability distribution of measurements of A. Therefore, we need only construct a probability distribution which gives the above moments.

1. Let $\wp(a_n, t_0)$ be the probability that a measurement of A at t_0 will yield the *discrete* eigenvalue a_n.

$$\wp(a_n, t_0) = \frac{1}{\langle \psi_0 \mid \psi_0 \rangle} \sum_{\alpha} \left| c_n^{(\alpha)} \right|^2 \tag{2.364}$$

2. Let $\tilde{\wp}(a_{c\nu}, t_0)$ be the probability that a measurement of A at t_0 will yield a value in the *continuum* between $a_{c\nu}$ and $a_{c\nu+d\nu}$. ($\tilde{\wp}(a_{c\nu}, t_0)$ is actually the probability density).

$$\tilde{\wp}(a_{c\nu}, t_0) = \frac{1}{\langle \psi_0 \mid \psi_0 \rangle} \sum_{\beta} \left| d_\nu^{(\beta)} \right|^2 \tag{2.365}$$

3. The probability a measurement of A at t_0 will yield a value not in the spectrum of A is zero.

For non-degenerate eigenvalues, the sums over α and β do not appear.

Example: Consider one-dimensional motion ($x-$axis). Let

$$A = p_{xop} = \frac{\hbar}{i} \frac{d}{dx} \tag{2.366}$$

Then

$$A\phi_p = p_{xop}\phi_p = \frac{\hbar}{i}\frac{d\phi_p}{dx} = p\phi_p \tag{2.367}$$

where p = constant eigenvalue. Therefore,

$$\frac{d\phi_p}{dx} = \frac{ip}{\hbar}\phi_p \Rightarrow \phi_p(x) = N_p e^{i\frac{px}{\hbar}} \tag{2.368}$$

First we show that p must be real. Let $p = \alpha + i\beta$. Then

$$\phi_p(x) = N_p e^{i\frac{\alpha x}{\hbar}} e^{-\frac{\beta x}{\hbar}} \tag{2.369}$$

The term $e^{-\beta x/\hbar}$ goes to ∞ for $x \to +\infty$ when $\beta < 0$ and goes to ∞ for $x \to -\infty$ when $\beta > 0$. Therefore, we must have $\beta = 0$ for condition (2) to be satisfied. Thus,

$$\phi_p(x) = N_p e^{i\frac{px}{\hbar}} \tag{2.370}$$

with p any real number in the interval $[-\infty, +\infty]$, which is therefore the *spectrum of p*. Note that the spectrum of p is entirely a *continuum*. Contrast this with the spectrum of L_{zop}, which is entirely discrete.
12pt] Now,

$$\begin{aligned}\langle \phi_{p'} \mid \phi_p \rangle &= N^*_{p'} N_p \int_{-\infty}^{\infty} dx e^{-i\frac{p'x}{\hbar}} e^{i\frac{px}{\hbar}} = N^*_{p'} N_p \hbar \int_{-\infty}^{\infty} dy e^{iy(p-p')} \\ &= N^*_{p'} N_p \hbar (2\pi)\delta(p-p') = (2\pi\hbar)\left|N_p\right|^2 \delta(p-p')\end{aligned} \tag{2.371}$$

since the expression vanishes for $p \neq p'$. Letting $N_p = 1/\sqrt{2\pi\hbar}$, we obtain ON eigenfunctions

$$u_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{px}{\hbar}} \text{ with } \langle u_{p'} \mid u_p \rangle = \delta(p-p') \tag{2.372}$$

Notice that we are using p for the eigenvalue $a_{c\nu}$ as well as for the continuous index ν.

Now let $\psi(\vec{x}, t_0)$ be a square-integrable wave function. The completeness of $\{u_p(x)\}$ implies that

$$\psi(x, t_0) = \int_{-\infty}^{\infty} dp\, \tilde{\psi}(p, t_0) u_p(x) \tag{2.373}$$

so that

$$\psi(x, t_0) = \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi\hbar}} e^{i\frac{px}{\hbar}} \tilde{\psi}(p, t_0) \tag{2.374}$$

ON implies that the expansion coefficient is

$$\tilde{\psi}(p, t_0) = \langle u_p \mid \psi \rangle = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\hbar}} e^{-i\frac{px}{\hbar}} \psi(x, t_0) \tag{2.375}$$

which agrees with the Fourier transform theorem. Furthermore,

$$\tilde{\wp}(p,t_0) = \frac{1}{\langle\psi_0 \mid \psi_0\rangle}\left|\tilde{\psi}(p,t_0)\right|^2 \tag{2.376}$$

using the recipe we developed earlier for $\tilde{\wp}(p,t_0)$. This result agrees with Postulate 2 with $\tilde{\wp}(p,t_0)$ a new notation for the momentum probability distribution.

2.2.0.12. Notes

1. Let me stress that the above derivations of $\wp(a_n,t_0)$ and $\tilde{\wp}(a_{c\nu},t_0)$ are valid only if the eigenfunctions $\left\{u_n^{(\alpha)}, u_{c\nu}^{(\beta)}\right\}$ are *orthonormal*:

   $$\left\langle u_{n'}^{(\alpha')} \,\middle|\, u_n^{(\alpha)}\right\rangle = \delta_{n'n}\delta_{\alpha'\alpha}\ ,\ \left\langle u_{c\nu'}^{(\beta')} \,\middle|\, u_{c\nu}^{(\beta)}\right\rangle = \delta(\nu'-\nu)\delta_{\beta'\beta}\ ,\ \left\langle u_n^{(\alpha)} \,\middle|\, u_{c\nu}^{(\beta)}\right\rangle = 0$$

   Although the eigenfunctions $\left\{u_n^{(\alpha)}, u_{c\nu}^{(\beta)}\right\}$ must be *normalized* (the continuum eigenfunctions are *normalized* to a Dirac delta function), $\psi(\vec{x},t_0) = \psi_0(\vec{x})$ need not be normalized ($\langle\psi_0\,|\,\psi_0\rangle$ is only required to be finite and non-zero).

2. Consider the 2 wave functions $\psi_0(\vec{x})$ and $\hat{\psi}_0(\vec{x}) = Z\psi_0(\vec{x})$, where Z is some complex constant. $\psi_0(\vec{x})$ and $\hat{\psi}_0(\vec{x})$ determine the same probability distributions $\wp(a_n,t_0)$ and $\tilde{\wp}(a_{c\nu},t_0)$.

   #### 2.2.0.13. Proof

   $$\begin{aligned}\left\langle\hat{\psi}_0 \,\middle|\, \hat{\psi}_0\right\rangle &= |Z|^2\langle\psi_0 \mid \psi_0\rangle\\ \hat{c}_n^{(\alpha)} &= \left\langle u_n^{(\alpha)} \,\middle|\, \hat{\psi}_0\right\rangle = Z\left\langle u_n^{(\alpha)} \,\middle|\, \psi_0\right\rangle = Zc_n^{(\alpha)}\end{aligned}$$

   Similarly,

   $$\hat{d}_\nu^{(\beta)} = Zd_\nu^{(\beta)} \tag{2.377}$$

   Therefore,

   $$\hat{\wp}(a_n,t_0) = \frac{1}{\left\langle\hat{\psi}_0 \,\middle|\, \hat{\psi}_0\right\rangle}\left|\hat{c}_n^{(\alpha)}\right|^2 = \frac{1}{\langle\psi_0 \mid \psi_0\rangle}\left|c_n^{(\alpha)}\right|^2 = \wp(a_n,t_0) \tag{2.378}$$

   If the wave function at t_0 is known, then the probability distribution of measurements of any physical quantity at time t_0 can be determined.

2.3. Collapse

2.3.0.1. A Question

A natural question now arises: *How can one prepare a particle so that its wave function at t_0 is completely determined* (up to an arbitrary multiplicative constant, which has no physical significance according to note (2) above)?

Experimental Result: If a measurement of A at time t yields the value a_n (or a continuum value in the range $a_{c\nu}$ to $a_{c\nu+d\nu}$), then a subsequent measurement of A performed *immediately* after the first measurement will yield the value a_n (or a continuum value in the same range as before) with *certainty*. The second measurement must be made immediately after the first so that the forces acting on the particle do not have time enough to alter the state of the particle. Thus, a measurement tells us something about a particle right after the measurement - an immediate repetition of the measurement will yield the same result as did the first measurement. We note here that this assumption of *repeatable* measurements is an assumption which is it is not always possible to accomplish in the laboratory.

This experimental result motivates the following postulate.

2.3.1. Postulate 4: Collapse of the Wave Function

Let $\left\{u_n^{(\alpha)}, u_{c\nu}^{(\beta)}\right\}$ be a CON set of eigenfunctions of the physical quantity A. Let $\psi(\vec{x}, t_0) = \psi_0(\vec{x})$ so that

$$\psi_0(\vec{x}) = \sum_{n,\alpha} c_n^{(\alpha)} u_n^{(\alpha)}(\vec{x}) + \int d\nu \sum_{\beta} d_\nu^{(\beta)} u_{c\nu}^{(\beta)}(\vec{x}) \tag{2.379}$$

1. If a measurement of A at t_0 yields the value a_n (we are assuming that this measurement is made with sufficient accuracy so that no other discrete eigenvalue lies within the experimental uncertainty), then the particle's wave function right after this measurement is

$$\psi_0'(\vec{x}) = \sum_{\alpha} c_n^{(\alpha)} u_n^{(\alpha)}(\vec{x}) \tag{2.380}$$

that is, the wave function *collapses* to that part of $\psi_0(\vec{x})$ which is an eigenfunction of A with eigenvalue a_n (linear superposition of degenerate states or a single state if eigenvalue is non-degenerate). A measurement of A for the state $\psi_0'(\vec{x})$ will yield the result a_n with certainty. Note that $\psi_0'(\vec{x})$ cannot be identically zero because a_n can be obtained from the measurement only if

$$\wp(a_n, t_0) = \frac{1}{\langle \psi_0 \mid \psi_0 \rangle} \sum_{\alpha} \left| c_n^{(\alpha)} \right|^2 \neq 0 \tag{2.381}$$

2. If a measurement of A at t_0 yields a continuum value measured to an accuracy such that this value lies in the range $a_{c\nu}$ to $a_{c\nu+d\nu}$, then the particle's wave function right after this measurement is

$$\psi_0'(\vec{x}) = \int_{\nu}^{\nu+d\nu} d\nu \sum_{\beta} d_\nu^{(\beta)} u_{c\nu}^{(\beta)}(\vec{x}) \tag{2.382}$$

that is, the wave function *collapses* to that part of $\psi_0(\vec{x})$ which is an eigenfunction of A with eigenvalues in the range $a_{c\nu}$ to $a_{c\nu+d\nu}$ (with certainty). Note that $\psi_0'(\vec{x})$ cannot be identically zero because a measurement will yield a value in the range $a_{c\nu}$ to $a_{c\nu+d\nu}$ only if

$$\int_{\nu}^{\nu+d\nu} d\nu \tilde{\wp}(a_{c\nu}, t_0) = \frac{1}{\langle \psi_0 \mid \psi_0 \rangle} \int_{\nu}^{\nu+d\nu} d\nu \sum_{\beta} \left| d_{\nu}^{(\beta)} \right|^2 \neq 0 \tag{2.383}$$

The collapse of the wave function has a simple geometric interpretation when the spectrum of A is entirely discrete, that is

$$\psi_0(\vec{x}) = \sum_{n,\alpha} c_n^{(\alpha)} u_n^{(\alpha)}(\vec{x}) \tag{2.384}$$

with no continuum eigenfunctions present. ψ_0 belongs to the vector space of square-integrable functions and $\left\{u_n^{(\alpha)}\right\}$ is a CON set of basis vectors in this infinite-dimensional vector space. I will draw only three of the orthogonal basis vectors - the other basis vectors are in orthogonal directions. In general, the coefficients $c_n^{(\alpha)}$ are complex; however, my diagrams below are necessarily of a real vector space, $c_n^{(\alpha)}$ real. The superscript α is not needed for eigenfunctions corresponding to non-degenerate eigenvalues.

Case #1: All non-degenerate eigenvalues. Eigenfunctions and corresponding eigenvalues are:

$$u_1 \leftrightarrow a_1 \quad , \quad u_2 \leftrightarrow a_2 \quad , \quad u_3 \leftrightarrow a_3 \tag{2.385}$$

as shown in Figure 2.14 below.

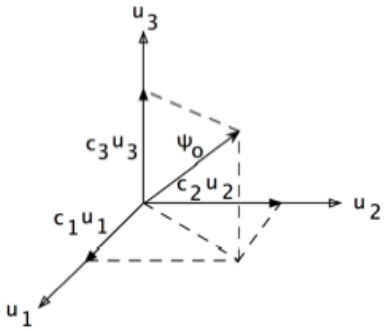


Figure 2.14: Vectors in Hilbert Space

Let $\langle \psi_0 \mid \psi_0 \rangle = 1$ and $\psi_0 = c_1 u_1 + c_2 u_2 + c_3 u_3 + \ldots\ldots$ as shown above. We then have $\wp(a_1, t_0) = |c_1|^2$. If a measurement of A yields a_1, the wave function collapses to the vector $c_1 u_1$, which is physically equivalent to u_1 and similarly for a_2

and a_3. **Case #2**: 2-fold degenerate eigenvalue and non-degenerate eigenvalue. Eigenfunctions and corresponding eigenvalues are:

$$u_1^{(1)} \leftrightarrow a_1 \quad , \quad u_1^{(2)} \leftrightarrow a_1 \quad , \quad u_2 \leftrightarrow a_2 \tag{2.386}$$

as shown in Figure 2.15 below:

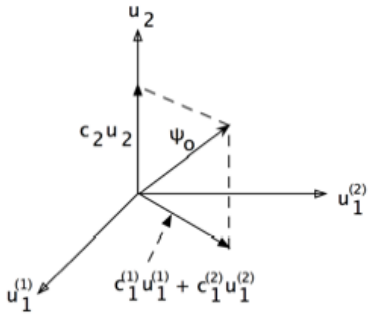


Figure 2.15: Vectors in Hilbert Space

Let $\langle \psi_0 \mid \psi_0 \rangle = 1$ and $\psi_0 = c_1^{(1)} u_1^{(1)} + c_1^{(2)} u_1^{(2)} + c_2 u_2 + ...$ as shown above. We then have $\wp(a_1, t_0) = \left| c_1^{(1)} \right|^2 + \left| c_1^{(2)} \right|^2$. If a measurement of A yields a_1, the wave function collapses to the vector $c_1^{(1)} u_1^{(1)} + c_1^{(2)} u_1^{(2)}$. We also have $\wp(a_2, t_0) = |c_2|^2$. If a measurement of A yields a_2, the wave function collapses to the vector $c_2 u_2$, which is physically equivalent to u_2.

This simple geometrical picture does not hold when the spectrum of A has a continuum part because the continuum eigenfunctions are not square-integrable and therefore do not belong to L^2, the space in which ψ_0 lies. The collapse of the wave function onto continuum eigenfunctions cannot be pictured as a simple *projection* onto basis vectors in L^2.

For the following discussion, I will assume that the spectrum of A is entirely discrete so that $\left\{ u_n^{(\alpha)} \right\}$ is a CON set of eigenfunctions. This is done only for simplicity of notation; all of the following results generalize in an obvious manner when A has both discrete and continuum parts to its spectrum.

I would like to make a set of measurements on a particle so that, from the results of these measurements, I will know what the particle's wave function is (up to an unimportant multiplicative constant) immediately after the measurements, that is, I would like to prepare the particle (by making certain measurements) so that its wave function is known at a specified time.

Suppose we write

$$\psi(\vec{x}, t_0) = \psi_0(\vec{x}) = \sum_{n,\alpha} c_n^{(\alpha)} u_n^{(\alpha)}(\vec{x}) \tag{2.387}$$

In this situation, the eigenfunctions $\left\{u_n^{(\alpha)}\right\}$ are *known* from solving the eigenvalue equation for A. However, $\psi_0(\vec{x})$ and the $c_n^{(\alpha)}$ have not yet been determined.

A measurement of A at t_0 yields the value a_N. If a_N is non-degenerate (eigenfunction $u_N^{(1)}$), the wave function collapses to $\psi_0'(\vec{x}) = c_N^{(1)} u_N^{(1)}$ and the wave function right after the measurement is known up to the multiplicative constant $c_N^{(1)}$. If a_N is degenerate (eigenfunctions $u_N^{(1)}, u_N^{(2)}, ..., u_N^{(g)}$), the wave function collapses to

$$\psi_0'(\vec{x}) = \sum_{\alpha=1}^{g} c_N^{(\alpha)} u_N^{(\alpha)}(\vec{x}) \tag{2.388}$$

and the wave function right after the measurement is not known up to a multiplicative constant because just knowing the eigenvalue a_N does not tell us the particular linear superposition of $u_N^{(1)}, u_N^{(2)}, ..., u_N^{(g)}$ that results, that is, the coefficients $c_N^{(1)}, c_N^{(2)}, ..., c_N^{(g)}$ have not yet been determined. More measurements must be performed on the particle in order to collapse the wave function further.

However, one must be careful in choosing which subsequent measurements to make. A measurement of another physical quantity B will usually *disturb* the wave function $\psi_0'(\vec{x})$, that is, collapse $\psi_0'(\vec{x})$ to $\psi_0''(\vec{x})$, an eigenfunction of B such that the wave function $\psi_0''(\vec{x})$ after this second measurement is no longer an eigenfunction of A with eigenvalue a_N. That means that the subsequent measurement of B will usually disturb the particle so that we destroy any preparation of the particle accomplished by the first measurement (of A).

An outline of this argument is as follows:

$\psi(\vec{x}, t_0) = \psi_0(\vec{x})$
Measurement of A yields a_N
Wave function collapses to $\psi_0'(\vec{x})$ where $A\psi_0'(\vec{x}) = a_N \psi_0'(\vec{x})$
Subsequent measurement of B yields b_M
Wave function collapses to $\psi_0''(\vec{x})$ where $B\psi_0''(\vec{x}) = b_M \psi_0''(\vec{x})$
Is $\psi_0''(\vec{x})$ still an eigenfunction of A with eigenvalue a_N?

Assume that it is. Then we have

$A\psi_0''(\vec{x}) = a_N \psi_0''(\vec{x})$
$BA\psi_0''(\vec{x}) = Ba_N \psi_0''(\vec{x}) = a_N B\psi_0''(\vec{x}) = a_N b_M \psi_0''(\vec{x})$
$AB\psi_0''(\vec{x}) = Ab_M \psi_0''(\vec{x}) = b_M A\psi_0''(\vec{x}) = b_M a_N \psi_0''(\vec{x})$
$[A, B]\,\psi_0''(\vec{x}) = 0$

Therefore, for $\psi_0''(\vec{x})$ to be an eigenfunction of both A and B, we must have $[A, B]\,\psi_0''(\vec{x}) = 0$ or $[A, B] = 0$. For arbitrary observable quantities A and B,

this is usually not true, because $[A, B]$ is not necessarily zero. Thus, $\psi_0''(\vec{x})$ will usually not remain an eigenfunction of A.

Definition: Let A and B be the hermitian operators corresponding to two physical quantities. A and B are said to be *compatible* if one can find a CON set of functions which are simultaneously eigenfunctions of A and B. We say there exists a *CON set of simultaneous eigenfunctions of A and B if A and B are compatible.*

Note that 2 operators need not be compatible for them to possess some simultaneous eigenfunctions. Compatibility requires that the 2 operators possess a *complete* set of simultaneous eigenfunctions.

Therefore, if $\left\{v_{m,n}^{(\alpha)}(\vec{x})\right\}$ = CON set of simultaneous eigenfunction of A and B, then

$$Av_{m,n}^{(\alpha)}(\vec{x}) = a_m v_{m,n}^{(\alpha)}(\vec{x}) \quad , \quad Bv_{m,n}^{(\alpha)}(\vec{x}) = b_n v_{m,n}^{(\alpha)}(\vec{x}) \tag{2.389}$$

where α labels the linearly independent eigenfunctions having the same a_N and b_M.

2.3.1.1. Comments

1. $\left\{v_{m,n}^{(\alpha)}(\vec{x})\right\}$ is a CON set of wave functions for which both A and B have precise values, that is, $\Delta A = 0 = \Delta B$ for each wave function $v_{m,n}^{(\alpha)}(\vec{x})$.

2. Let
$$\psi(\vec{x}, t_0) = \psi_0(\vec{x}) = \sum_{m,n,\alpha} c_{m,n}^{(\alpha)} v_{m,n}^{(\alpha)}(\vec{x}) \tag{2.390}$$
Note that the eigenfunctions $\left\{v_{m,n}^{(\alpha)}(\vec{x})\right\}$ are known from solving the eigenvalue equations for A and B. However, $\psi_0(\vec{x})$ and $c_{m,n}^{(\alpha)}$ have not yet been determined.

   Suppose that we measure A and obtain the value a_M. The wave function collapses to
$$\psi_0'(\vec{x}) = \sum_{n,\alpha} c_{M,n}^{(\alpha)} v_{M,n}^{(\alpha)}(\vec{x}) \tag{2.391}$$
   Suppose that we measure B and obtain the value b_N. The wave function collapses to
$$\psi_0''(\vec{x}) = \sum_{\alpha} c_{M,N}^{(\alpha)} v_{M,N}^{(\alpha)}(\vec{x}) \tag{2.392}$$
   Notice that $\psi_0''(\vec{x})$ is still an eigenfunction of A with eigenvalue a_M. The measurement of B has not disturbed the value of A (when A and B are compatible). In this sense A and B are truly compatible.

3. Let A and B be compatible. Let $\left\{u_m^{(\beta)}(\vec{x})\right\}$ be any CON set of eigenfunctions of A. This is not the only CON set of eigenfunctions of A if some of the eigenvalues are degenerate - there are different possible choices for the linearly independent eigenfunctions belonging to a degenerate eigenvalue. The given eigenfunctions $\left\{u_m^{(\beta)}(\vec{x})\right\}$ need not be simultaneous eigenfunctions of B. The compatibility of A and B implies only that *there exists some* CON set of eigenfunctions of both A and B simultaneously.

Suppose A and B are compatible. Suppose we measure A (obtaining the value a_M) and then B (obtaining the value b_N). As in comment (2) above, the wave function right after these compatible measurements is

$$\psi_0''(\vec{x}) = \sum_\alpha c_{M,N}^{(\alpha)} v_{M,N}^{(\alpha)}(\vec{x}) \tag{2.393}$$

If there are two or more ON eigenfunctions corresponding to a_M and b_N, $\psi_0''(\vec{x})$ is still not completely known (up to a multiplicative constant) because we do not yet know the individual coefficients $c_{M,N}^{(1)}, c_{M,N}^{(2)}, ...$ For such a case, other compatible measurements must be made on the particle until the wave function has collapsed to a function that is completely known (up to a multiplicative constant).

Definition: Let A, B, C, ..., Q be the hermitian operators corresponding to some physical quantities. A, B, C, ..., Q are said to from a complete set of compatible observables if there exists one, and only one, CON set of simultaneous eigenfunctions of A, B, C, ..., Q. (2 CON sets are not considered different if the functions of one set differ from the functions of the other set by multiplicative constants of modulus unity). One can prove the existence of complete sets of compatible observables, but we will not do that here.

Therefore, if $\{v_{\ell mn....}(\vec{x})\}$ = CON set of simultaneous eigenfunction of A, B, C, ..., Q, then

$$\begin{aligned}
&Av_{\ell mn....}(\vec{x}) = a_\ell v_{\ell mn....}(\vec{x}) \\
&Bv_{\ell mn....}(\vec{x}) = b_m v_{\ell mn....}(\vec{x}) \\
&Cv_{\ell mn....}(\vec{x}) = c_n v_{\ell mn....}(\vec{x}) \\
&..... \\
&.....
\end{aligned}$$

Note that we have used the fact that if A, B, C, ..., Q form a complete set of compatible observables, then that implies that there is only one eigenfunction (determined up to an arbitrary multiplicative constant) corresponding to given eigenvalues $a_\ell, b_m, c_n, ...$

1. It is possible for a single operator A by itself to form a *complete set of compatible observables*. The operator A need only have eigenvalues which

are all non-degenerate: if the eigenvalues of A are all non-degenerate, then a given eigenvalue has only one linearly independent corresponding eigenfunction and there exists only one CON set of eigenfunctions of A.

Two different complete sets of compatible observables A, B, C, ... and A', B', C', ... need not have the same number of operators.

2. For
$$\psi(\vec{x}, t_0) = \psi_0(\vec{x}) = \sum_{\ell,m,n,....} K_{\ell mn...} v_{\ell mn...}(\vec{x}) \tag{2.394}$$

Note that the eigenfunctions $\{v_{\ell mn...}(\vec{x})\}$ are known from solving the eigenvalue equations for A, B, C, ... However, $\psi_0(\vec{x})$ and the expansion coefficients $K_{\ell mn...}$ have not yet been determined.

Suppose we measure A and obtain a_L. The wave function then collapses to
$$\psi_0'(\vec{x}) = \sum_{m,n,....} K_{Lmn...} v_{Lmn...}(\vec{x}) \tag{2.395}$$

Suppose we measure B and obtain b_M. The wave function then collapses to
$$\psi_0''(\vec{x}) = \sum_{n,....} K_{LMn...} v_{LMn...}(\vec{x}) \tag{2.396}$$

Suppose we measure all the remaining quantities C,.... in the complete set of compatible observables A, B, C, ... and obtain the values $c_N, ...$ The wave function will finally collapse to
$$\psi_0'''^{....}(\vec{x}) = K_{LMN...} v_{LMN...}(\vec{x}) \tag{2.397}$$

where no sum is present now.

Notice that $\psi_0'''^{....}(\vec{x})$ *is now completely known* (up to a multiplicative constant $K_{LMN.....}$). Thus, *measurements made of a complete set of compatible observables collapse the wave function to a simultaneous eigenfunction of all these observables - the experimental results* $a_L, b_M, c_N, ...$ *completely determine this simultaneous eigenfunction* $v_{LMN...}(\vec{x})$. Thus, the wave function of the particle immediately after the measurements has been experimentally determined (up to a multiplicative constant), that is, the measurements have prepared the particle so that its wave function is known at a specified time.

Chapter 3

Formulation of Wave Mechanics - Part 2

3.1. Complete Orthonormal Sets

Our earlier discussions give a simple criterion for observables to be compatible. In particular, we showed that

A and B are compatible implies that $[A, B] = 0$

In addition we have the following theorem:

$[A, B] = 0$ implies that A and B are compatible

The proof of this theorem provides a practical way to construct a CON set of simultaneous eigenfunctions of two compatible observables.

Proof: Let $\left\{u_n^{(\beta)}(\vec{x})\right\}$ be any CON set of eigenfunctions of A.

$$Au_n^{(\beta)}(\vec{x}) = a_n u_n^{(\beta)}(\vec{x}) \tag{3.1}$$

and assume that $[A, B] = 0$. The above eigenfunctions of A need not be eigenfunctions of B. We will now show how to construct from the $\left\{u_n^{(\beta)}(\vec{x})\right\}$ a CON set of simultaneous eigenfunctions of A and B - this will prove that A and B are compatible.

(a) Consider a particular eigenvalue a_n. If it is *non-degenerate*, then the following is valid:

$u_n^{(1)}$ is the only linearly independent
eigenfunction corresponding to a_n

Claim: $u_n^{(1)}$ is necessarily an eigenfunction of B also.

Proof: We have

$$ABu_n^{(1)} = BAu_n^{(1)} = Ba_n u_n^{(1)} = a_n Bu_n^{(1)} \tag{3.2}$$

Therefore, $Bu_n^{(1)}$ is an eigenfunction of A with eigenvalue a_n and since a_n is non-degenerate, we must have $Bu_n^{(1)} = (constant)u_n^{(1)}$. But this says that $u_n^{(1)}$ is an eigenfunction of B.

Therefore, *eigenfunctions of A corresponding to non-degenerate eigenvalues are necessarily eigenfunctions of B also.*

(b) Consider a particular eigenvalue a_n. If it is *degenerate*, then the following is valid:

> g-fold degeneracy implies that $u_n^{(1)}, u_n^{(2)}, ..., u_n^{(g)}$
> are ON eigenfunctions of A with eigenvalue a_n
> and any eigenfunction of A with eigenvalue a_n
> can be expressed as a linear superposition of
> these g eigenfucntions.

Now, consider the case where $u_n^{(\beta)}$ is not necessarily an eigenfunction of B. We have

$$ABu_n^{(\beta)} = BAu_n^{(\beta)} = Ba_n u_n^{(\beta)} = a_n Bu_n^{(\beta)} \tag{3.3}$$

so that $Bu_n^{(\beta)}$ is an eigenfunction of A with eigenvalue a_n and can be expressed as a linear superposition of $u_n^{(1)}, u_n^{(2)}, ..., u_n^{(g)}$:

$$Bu_n^{(\beta)}(\vec{x}) = \sum_{\alpha=1}^{g} b_{\alpha\beta}^{(n)} u_n^{(\alpha)}(\vec{x}) \text{for} \beta = 1, 2, ..., g \tag{3.4}$$

Relabeling indices: $b_{\alpha\beta}^{(n)} = \left\langle u_n^{(\alpha)} \,\middle|\, Bu_n^{(\beta)} \right\rangle$. Note that α is the first index and β is the second index on both sides of this equation.

$b^{(n)}$ is a $g \times g$ matrix where the matrix elements of $b^{(n)}$ are computed from the given ON eigenfunctions of A corresponding to the eigenvalue a_n.

$$b^{(n)} = \begin{pmatrix} b_{11}^{(n)} & b_{12}^{(n)} & . & . \\ b_{21}^{(n)} & b_{22}^{(n)} & . & . \\ . & . & . & . \\ . & . & . & . \end{pmatrix} \tag{3.5}$$

The matrix $b^{(n)}$ is hermitian, that is, the matrix is equal to the complex conjugate of its transposed matrix:

$$b_{\alpha\beta}^{(n)} = \left\langle u_n^{(\alpha)} \,\middle|\, Bu_n^{(\beta)} \right\rangle = \left\langle Bu_n^{(\alpha)} \,\middle|\, u_n^{(\beta)} \right\rangle = \left\langle u_n^{(\beta)} \,\middle|\, Bu_n^{(\alpha)} \right\rangle^* = b_{\beta\alpha}^{(n)*} \tag{3.6}$$

Claim: We can find g linearly independent functions, each of the form

$$\sum_{\alpha=1}^{g} c_\alpha u_n^{(\alpha)} \tag{3.7}$$

which are eigenfunctions of B (they are obviously eigenfunctions of A corresponding to eigenvalue a_n).

Proof: Let us show how to find the c_α such that

$$\sum_{\alpha=1}^{g} c_\alpha u_n^{(\alpha)}$$

is an eigenfunction of B. We have

$$B\sum_{\alpha=1}^{g} c_\alpha u_n^{(\alpha)} = b\sum_{\alpha=1}^{g} c_\alpha u_n^{(\alpha)} \text{ where b = yet to be determined eigenvalue}$$

$$B\sum_{\alpha=1}^{g} c_\alpha u_n^{(\alpha)} = \sum_{\alpha=1}^{g} c_\alpha B u_n^{(\alpha)} = \sum_{\alpha=1}^{g} c_\alpha \sum_{\beta=1}^{g} b_{\beta\alpha}^{(n)} u_n^{(\beta)} = b\sum_{\alpha=1}^{g} c_\alpha u_n^{(\alpha)} = b\sum_{\beta=1}^{g} c_\beta u_n^{(\beta)}$$

$$\sum_{\alpha=1}^{g}\sum_{\beta=1}^{g} c_\alpha b_{\beta\alpha}^{(n)} u_n^{(\beta)} = b\sum_{\beta=1}^{g} c_\beta u_n^{(\beta)}$$

$$\sum_{\beta=1}^{g} u_n^{(\beta)}\left(\sum_{\alpha=1}^{g} b_{\beta\alpha}^{(n)} c_\alpha - b c_\beta\right) = 0 \Rightarrow \left(\sum_{\alpha=1}^{g} b_{\beta\alpha}^{(n)} c_\alpha\right) - b c_\beta = 0$$

for $\beta = 1, 2, ..., g$. This result is true because the $u_n^{(1)}, u_n^{(2)}, ..., u_n^{(g)}$ are linearly independent.

Using the notation

$$\vec{c} = \begin{pmatrix} c_1 \\ c_2 \\ . \\ c_g \end{pmatrix} = \text{ column vector} \tag{3.8}$$

this equation becomes

$$b^{(n)}\vec{c} = b\vec{c} \tag{3.9}$$

which is an eigenvalue equation for the $g \times g$ hermitian matrix $b^{(n)}$. Now $(b^{(n)} - b)\vec{c} = 0$ has a non-trivial solution for $\vec{c}$ provided that $(b^{(n)} - b)$ is not invertible, that is,

$$\det(b^{(n)} - b) = 0 \tag{3.10}$$

or

$$\det\begin{pmatrix} b_{11}^{(n)} - b & b_{12}^{(n)} & . & . \\ b_{21}^{(n)} & b_{22}^{(n)} - b & . & . \\ . & . & . & . \\ . & . & . & . \end{pmatrix} = 0 \tag{3.11}$$

The various possible eigenvalues b can be found by solving this algebraic equation for b. For each b found, we can then find at least one non-trivial $\vec{c}$ satisfying $b^{(n)}\vec{c} = b\vec{c}$ (just solve this equation for $\vec{c}$ with b given). It is a basic result of linear algebra that the eigenfunctions of a hermitian matrix are complete (the spectral theorem we stated in Chapter 2 is a generalization of this theorem to hermitian operators on the infinite-dimensional space L^2). This means that, for the $g \times g$ hermitian matrix $b^{(n)}$, one can find g linearly independent column vectors $\vec{c}$,

$$\vec{c}^{(1)} = \begin{pmatrix} c_1^{(1)} \\ c_2^{(1)} \\ . \\ c_g^{(1)} \end{pmatrix}, \vec{c}^{(2)} = \begin{pmatrix} c_1^{(2)} \\ c_2^{(2)} \\ . \\ c_g^{(2)} \end{pmatrix}, ..., \vec{c}^{(g)} = \begin{pmatrix} c_1^{(g)} \\ c_2^{(g)} \\ . \\ c_g^{(g)} \end{pmatrix}$$

Several of these column vectors may correspond to the same eigenvalue b, while others correspond to different eigenvalues. We have thus shown how to find g linearly independent functions, each of the form

$$\sum_{\alpha=1}^{g} c_\alpha u_n^{(\alpha)} \tag{3.12}$$

which are eigenfunctions of B (the eigenvalue is the value of b which determined this $\vec{c}$) and of A (the eigenvalue is a_n).

Let me summarize the results (a) and (b) obtained so far in the proof of the theorem.

$[A, B] = 0$ and $\left\{u_n^{(\beta)}(\vec{x})\right\}$ is any CON set of eigenfunctions of A

(a) If a_n is *non-degenerate*, then the only eigenfunction corresponding to a_n is $u_n^{(1)}$ and $u_n^{(1)}$ is automatically a simultaneous eigenfunction of B.

(b) If a_n is *degenerate*(g-fold degeneracy), then $u_n^{(1)}, u_n^{(2)}, ..., u_n^{(g)}$ are the corresponding ON eigenfunctions and $u_n^{(\beta)}$ is not necessarily an eigenfunction of B. Now form the $g \times g$ hermitian matrix $b^{(n)}$, whose matrix elements are $b_{\alpha\beta}^{(n)} = \left\langle u_n^{(\alpha)} \,\middle|\, Bu_n^{(\beta)} \right\rangle$, $\alpha, \beta = 1, 2, ..., g$. Solve the equation $b^{(n)}\vec{c} = b\vec{c}$. The eigenvalues b are obtained by solving $\det(b^{(n)} - b) = 0$. Knowing the eigenvalues b, we can then find g linearly independent column vectors $\vec{c}^{(1)}, \vec{c}^{(2)}, ..., \vec{c}^{(g)}$ which solve the eigenvalue equation. The g linearly independent functions

$$\phi_n^{(\beta)}(\vec{x}) = \sum_{\alpha=1}^{g} c_\alpha^{(\beta)} u_n^{(\alpha)}(\vec{x}) \quad , \quad \beta = 1, 2, ..., g \tag{3.13}$$

are eigenfunctions of B (the eigenvalue is the value of b which determined

this

$$\vec{c}^{(\beta)} = \begin{pmatrix} c_1^{(\beta)} \\ c_2^{(\beta)} \\ . \\ c_g^{(\beta)} \end{pmatrix} \tag{3.14}$$

and of A (the eigenvalue is a_n). The $\phi_n^{(\beta)}$'s which correspond to different eigenvalues b are necessarily orthogonal; the $\phi_n^{(\beta)}$'s which belong to the same eigenvalue b can be constructed to be orthogonal by the *Gram-Schmidt process*. All the $\phi_n^{(\beta)}$'s can be normalized. Thus, one can always find $\phi_n^{(\beta)}$'s satisfying $\left\langle \phi_n^{(\alpha)} \,\middle|\, \phi_n^{(\beta)} \right\rangle = \delta_{\alpha\beta}$.

We now have a method for constructing a CON set of simultaneous eigenfunctions of A and B. For each eigenvalue of A, we can find g CON simultaneous eigenfunctions of A and B when the eigenvalue is g-fold degenerate ($g = 1$ means a non-degenerate eigenvalue). Doing this for all the eigenvalues of A yields a CON set of simultaneous eigenfunctions of A and B. The existence of a CON set of simultaneous eigenfunctions implies that A and B are compatible.

Example: Construction of a CON set of simultaneous eigenfunctions of two commuting hermitian operators.

Let the functions $u_1^{(1)}(\vec{x}), u_1^{(2)}(\vec{x}), u_2(\vec{x}), u_3(\vec{x}), u_4(\vec{x}), ...$ be a CON set in L^2. Define the linear operators A and B by their action on this CON set:

A	B
$Au_1^{(1)} = u_1^{(1)}$	$Bu_1^{(1)} = u_1^{(2)}$
$Au_1^{(2)} = u_1^{(2)}$	$Bu_1^{(2)} = u_1^{(1)}$
$Au_2 = 2u_2$	$Bu_2 = 2u_2$
$Au_3 = 3u_3$	$Bu_3 = 3u_3$
.....	.....
$Au_n = nu_n$	$Bu_n = nu_n$
.....	.....

Table 3.1: Definition of A and B

Note that $u_2(\vec{x}), u_3(\vec{x}), u_4(\vec{x}), ...$ are simultaneous eigenfunctions of A and B, while $u_1^{(1)}(\vec{x}), u_1^{(2)}(\vec{x})$ are degenerate eigenfunctions of A (eigenvalue = +1), but are not eigenfunctions of B.

Notes:

1. A linear operator A is completely defined by specifying its action on some CON set $\left\{v_n^{(\alpha)}(\vec{x})\right\}$: $Av_n^{(\alpha)}(\vec{x})$ given for all n, α. This is true because an

arbitrary $\phi(\vec{x})$ can be written as

$$\phi(\vec{x}) = \sum_{n,\alpha} c_n^{(\alpha)} v_n^{(\alpha)}(\vec{x}) \tag{3.15}$$

Therefore,

$$A\phi(\vec{x}) = \sum_{n,\alpha} c_n^{(\alpha)} \underbrace{A v_n^{(\alpha)}(\vec{x})}_{given} \tag{3.16}$$

and thus, the action of A on any $\phi(\vec{x})$ is determined. For example,

$$[A,B] = 0 \text{ if } [A,B]\, v_n^{(\alpha)}(\vec{x}) = 0 \text{ for all } n, \alpha$$

2. A linear operator A is hermitian if $\langle \phi \mid A\phi \rangle = \langle A\phi \mid \phi \rangle$ for all $\phi(\vec{x})$. But an arbitrary $\phi(\vec{x})$ can be written

$$\phi(\vec{x}) = \sum_{n,\alpha} c_n^{(\alpha)} v_n^{(\alpha)}(\vec{x}) \tag{3.17}$$

when $\left\{ v_n^{(\alpha)}(\vec{x}) \right\}$ is some CON set. Therefore, A is hermitian if

$$\left\langle \sum_{n,\alpha} c_n^{(\alpha)} v_n^{(\alpha)}(\vec{x}) \,\middle|\, A \sum_{m,\beta} c_m^{(\beta)} v_m^{(\beta)}(\vec{x}) \right\rangle = \left\langle A \sum_{n,\alpha} c_n^{(\alpha)} v_n^{(\alpha)}(\vec{x}) \,\middle|\, \sum_{m,\beta} c_m^{(\beta)} v_m^{(\beta)}(\vec{x}) \right\rangle$$

$$\sum_{n,\alpha} c_n^{(\alpha)*} \sum_{m,\beta} c_m^{(\beta)} \left\langle v_n^{(\alpha)}(\vec{x}) \,\middle|\, A v_m^{(\beta)}(\vec{x}) \right\rangle = \sum_{n,\alpha} c_n^{(\alpha)*} \sum_{m,\beta} c_m^{(\beta)} \left\langle A v_n^{(\alpha)}(\vec{x}) \,\middle|\, v_m^{(\beta)}(\vec{x}) \right\rangle$$

Because this must hold for arbitrary coefficients $c_n^{(\alpha)}$, we conclude that A is hermitian if $\left\langle v_n^{(\alpha)}(\vec{x}) \,\middle|\, A v_m^{(\beta)}(\vec{x}) \right\rangle = \left\langle A v_n^{(\alpha)}(\vec{x}) \,\middle|\, v_m^{(\beta)}(\vec{x}) \right\rangle$ for all $n, m.\alpha, \beta$. This is a simple test for hermiticity when the action of A on a CON set is known.

Because A and B commute, we can find a CON set of simultaneous eigenfunctions.

A's eigenvalues $2, 3, 4, \ldots.$ are non-degenerate and therefore the corresponding eigenfunctions $u_2(\vec{x}), u_3(\vec{x}), u_4(\vec{x}), \ldots\ldots$ are necessarily eigenfunctions of B also.

A's eigenvalue 1 is 2–fold degenerate. $u_1^{(1)}(\vec{x}), u_1^{(2)}(\vec{x})$ are not eigenfunctions of B. We form the 2×2 matrix $b^{(n=1)}$ where

$$b_{\alpha\beta}^{(1)} = \left\langle u_1^{(\alpha)} \,\middle|\, B u_1^{(\beta)} \right\rangle \tag{3.18}$$

so that

$$b_{11}^{(1)} = \left\langle u_1^{(1)} \,\middle|\, B u_1^{(1)} \right\rangle = \left\langle u_1^{(1)} \,\middle|\, u_1^{(2)} \right\rangle = 0$$

$$b_{22}^{(1)} = \left\langle u_1^{(2)} \,\middle|\, B u_1^{(2)} \right\rangle = \left\langle u_1^{(2)} \,\middle|\, u_1^{(1)} \right\rangle = 0$$

$$b_{12}^{(1)} = \left\langle u_1^{(1)} \,\middle|\, B u_1^{(2)} \right\rangle = \left\langle u_1^{(1)} \,\middle|\, u_1^{(1)} \right\rangle = 1$$

$$b_{21}^{(1)} = \left\langle u_1^{(2)} \,\middle|\, B u_1^{(1)} \right\rangle = \left\langle u_1^{(2)} \,\middle|\, u_1^{(2)} \right\rangle = 1$$

Therefore

$$b^{(n=1)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{3.19}$$

and we have

$$\det(b^{(1)} - b) = 0 \Rightarrow \det\begin{pmatrix} -b & 1 \\ 1 & -b \end{pmatrix} = 0 = b^2 - 1 \Rightarrow b = \pm 1 \tag{3.20}$$

Case #1: $b = +1$

$$b^{(1)}\vec{c}^{\,+} = \vec{c}^{\,+} \Rightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} c_1^+ \\ c_2^+ \end{pmatrix} = \begin{pmatrix} c_1^+ \\ c_2^+ \end{pmatrix} \Rightarrow c_2^+ = c_1^+ \tag{3.21}$$

Case #2: $b = -1$

$$b^{(1)}\vec{c}^{\,-} = \vec{c}^{\,-} \Rightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} c_1^- \\ c_2^- \end{pmatrix} = -\begin{pmatrix} c_1^- \\ c_2^- \end{pmatrix} \Rightarrow c_2^- = -c_1^- \tag{3.22}$$

Therefore, $c_1^+ u_1^{(1)} + c_2^+ u_1^{(2)} = c_1^+(u_1^{(1)} + u_1^{(2)})$ is a simultaneous eigenfunction of A (eigenvalue = +1) and of B (eigenvalue = +1) and $c_1^- u_1^{(1)} + c_2^- u_1^{(2)} = c_1^-(u_1^{(1)} - u_1^{(2)})$ is a simultaneous eigenfunction of A (eigenvalue = +1) and of B (eigenvalue = −1).

To normalize these functions we note that

$$\left\langle u_1^{(1)} \pm u_1^{(2)} \,\middle|\, u_1^{(1)} \pm u_1^{(2)} \right\rangle = 2 \Rightarrow c_1^{\pm} = \frac{1}{\sqrt{2}} \tag{3.23}$$

Thus,

$$\frac{1}{\sqrt{2}}(u_1^{(1)} + u_1^{(2)}), \frac{1}{\sqrt{2}}(u_1^{(1)} - u_1^{(2)}), u_2, u_3, u_4, ... \tag{3.24}$$

with eigenvalues

$$+1(A), +1(B) \quad +1(A), -1(B) \quad 2(A,B) \quad 3(A,B) \quad 4(A,B) \quad ..... \tag{3.25}$$

form a CON set of simultaneous eigenfunctions of A and B.

Summarizing our results: Two hermitian operators are compatible if, and only if, they commute: *compatibility is equivalent to commutativity.* Compatible physical quantities are important when one wants to prepare a particle so that its wave function is known (up to a multiplicative constant) at a specified time: measurements made of a complete set of compatible observables collapse the wave function to a simultaneous eigenfunction of all these observables and the experimental results from these measurements uniquely determine the simultaneous eigenfunction to which the wave function collapsed.

There is another important use of commuting observables. Suppose we want

to find the eigenfunctions and eigenvalues of some physical quantity A. If we already know the eigenfunctions of a physical quantity B *which commutes with* A, then our task is greatly simplified because there must exist a CON set of eigenfunctions of B which are simultaneous eigenfunctions of A.

Example: Free Particle in Three Dimensions(no forces present): We have

$$H_{op} = \frac{p_{xop}^2 + p_{yop}^2 + p_{zop}^2}{2m} \tag{3.26}$$

Let us find the eigenfunctions and eigenvalues of H_{op} (discrete and continuum parts) using the eigenvalue equation

$$H_{op}\phi(\vec{x}) = E\phi(\vec{x}) \tag{3.27}$$

Method #1: $p_{xop}, p_{yop}, p_{zop}, H_{op}$ are obviously mutually commuting operators, that is, any pair of these operators commute. Therefore, we can find a CON set of simultaneous eigenfunctions of these 4 operators. Now, the eigenfunctions of $p_{xop}, p_{yop}, p_{zop}$ have already been derived.

$$\text{eigenfunctions of } p_{xop} \to N_x(y,z)e^{\frac{ip_x x}{\hbar}} \text{ with eigenvalues } p_x \in (-\infty, +\infty)$$

$$\text{eigenfunctions of } p_{yop} \to N_y(x,z)e^{\frac{ip_y y}{\hbar}} \text{ with eigenvalues } p_y \in (-\infty, +\infty)$$

$$\text{eigenfunctions of } p_{zop} \to N_z(x,y)e^{\frac{ip_z z}{\hbar}} \text{ with eigenvalues } p_z \in (-\infty, +\infty)$$

Clearly, the simultaneous eigenfunctions of $p_{xop}, p_{yop}, p_{zop}$ are

$$u_{p_x p_y p_z}(\vec{x}) = Ne^{\frac{ip_x x}{\hbar}} e^{\frac{ip_y y}{\hbar}} e^{\frac{ip_z z}{\hbar}} = Ne^{\frac{i}{\hbar}(p_x x + p_y y + p_z z)} \tag{3.28}$$

where N is independent of x, y, z, form a complete set. Given p_x, p_y, p_z, there exists (no degeneracy remains after p_x, p_y, p_z given) *only one linearly independent* eigenfunction. Therefore, the functions $u_{p_x p_y p_z}(\vec{x})$ are also eigenfunctions of H_{op}. Finding the eigenvalues of H_{op} is simple:

$$\begin{aligned} H_{op}u_{p_x p_y p_z} &= \left(\frac{p_{xop}^2 + p_{yop}^2 + p_{zop}^2}{2m}\right) u_{p_x p_y p_z} \\ &= \left(\frac{p_x^2 + p_y^2 + p_z^2}{2m}\right) u_{p_x p_y p_z} = E u_{p_x p_y p_z} \end{aligned} \tag{3.29}$$

so that

$$E = \left(\frac{p_x^2 + p_y^2 + p_z^2}{2m}\right) \quad , \quad p_x, p_y, p_z \in (-\infty, +\infty) \tag{3.30}$$

Thus, the spectrum of H_{op} has only a continuum part, with the eigenvalue E anywhere in $[0, +\infty]$.

Method #2: Separation of variables(SOV): This is the method used to solve certain partial differential equations. We have

$$H_{op}\phi(\vec{x}) = E\phi(\vec{x}) \tag{3.31}$$

We look for eigenfunctions satisfying earlier conditions (a) and (b) so that the eigenfunctions must not become infinite as $|\vec{x}| \to \infty$.

Now, inserting differential operators, the eigenvalue equation becomes

$$\begin{aligned} H_{op}\phi(\vec{x}) &= \left(\frac{p_{xop}^2 + p_{yop}^2 + p_{zop}^2}{2m} \right) \phi(\vec{x}) \\ &= -\frac{\hbar^2}{2m} \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial x^2} \right) = E\phi \end{aligned} \tag{3.32}$$

for fixed E. The allowed values of E are then determined by requiring that $\phi(\vec{x})$ does not become infinite as $|\vec{x}| \to \infty$. This is called a *boundary condition*.

In this SOV method, we look for solutions of the form $\phi(\vec{x}) = X(x)Y(y)Z(z)$, i.e., separated variables. Substituting into the partial differential equation we have

$$-\frac{\hbar^2}{2m} \left(YZ\frac{\partial^2 X}{\partial x^2} + XZ\frac{\partial^2 Y}{\partial y^2} + XY\frac{\partial^2 Z}{\partial x^2} \right) = E(XYZ) \tag{3.33}$$

Dividing by XYZ (recall that $\phi(\vec{x})$ is not identically zero) we get

$$\underbrace{\left(-\frac{\hbar^2}{2m}\frac{1}{X}\frac{\partial^2 X}{\partial x^2} \right)}_{\substack{function\ of\ x\ only \\ =F_1(x)}} + \underbrace{\left(-\frac{\hbar^2}{2m}\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} \right)}_{\substack{function\ of\ y\ only \\ =F_2(y)}} + \underbrace{\left(-\frac{\hbar^2}{2m}\frac{1}{Z}\frac{\partial^2 Z}{\partial x^2} \right)}_{\substack{function\ of\ z\ only \\ =F_3(z)}} = E = \text{constant} \tag{3.34}$$

This equation must be true for all x, y, z where x, y, z are independent variables. In particular, the equation must be valid as x varies while y and z are kept fixed. Thus, $F_1(x)$ must be independent of x. In a similar manner, we arrive at the conclusion that $F_2(y)$ must be independent of y and $F_3(z)$ must be independent of z. Therefore,

$$F_1(x) = constant \quad , \quad F_2(y) = constant \quad , \quad F_3(z) = constant \tag{3.35}$$

We let

$$F_1(x) = \frac{\hbar^2 k_1^2}{2m} \quad , \quad F_2(y) = \frac{\hbar^2 k_2^2}{2m} \quad , \quad F_3(z) = \frac{\hbar^2 k_3^2}{2m} \tag{3.36}$$

where k_1, k_2, k_3 are constants (in principle, complex constants). The quantities

$$\frac{\hbar^2 k_1^2}{2m} \, , \, \frac{\hbar^2 k_2^2}{2m} \, , \, \frac{\hbar^2 k_3^2}{2m} \tag{3.37}$$

are called *separation constants*. We then obtain the eigenvalues in terms of these three unknown constants as

$$E = \frac{\hbar^2 k_1^2}{2m} + \frac{\hbar^2 k_2^2}{2m} + \frac{\hbar^2 k_3^2}{2m} \tag{3.38}$$

and the three equations

$$\frac{\partial^2 X}{\partial x^2} = -k_1^2 X \rightarrow X = e^{\pm ik_1 x} \tag{3.39}$$

$$\frac{\partial^2 Y}{\partial x^2} = -k_2^2 Y \rightarrow Y = e^{\pm ik_2 y} \tag{3.40}$$

$$\frac{\partial^2 Z}{\partial x^2} = -k_3^2 Z \rightarrow Z = e^{\pm ik_3 z} \tag{3.41}$$

Since X, Y, Z must not become infinite as $|x| \rightarrow \infty, |y| \rightarrow \infty, |z| \rightarrow \infty$, the constants k_1, k_2, k_3 must be *pure real* (positive or negative).

It is sufficient to write

$$X = e^{+ik_1 x} \quad , \quad Y = e^{+ik_2 y} \quad , \quad Z = e^{+ik_3 z} \tag{3.42}$$

because k_1, k_2, k_3 may be positive or negative.

Therefore,

$$\phi(\vec{x}) = Ne^{+i(k_1 x + k_2 y + k_3 z)}$$

$$E = \frac{\hbar^2}{2m}\left(k_1^2 + k_2^2 + k_3^2\right) \in [0, +\infty]$$

k_1, k_2, k_3 pure real

With $k_i = p_i/\hbar$ these results agree with those from Method #1. One might ask how we know that the eigenfunctions of the form $\phi(\vec{x}) = X(x)Y(y)Z(z)$ give a *complete* set of eigenfunctions. Method #2 does not tell us. Only Method #1 really shows that the eigenfunctions we have obtained are complete.

3.2. Time Development

We have discussed in detail how a measurement collapses the wave function in Chapter 2. By measuring a complete set of compatible observables, one prepares a particle so that its wave function immediately after the measurements (at time t_0) is known (up to a multiplicative constant). $\psi(\vec{x}, t_0)$ is therefore known (up to a normalization factor). Suppose another measurement is made at some later time t_1 ($t_1 > t_0$). The probability distribution of results of such a measurement can be determined if one knows the wave function $\psi(\vec{x}, t_1)$ right before this measurement is made. We must therefore specify the *time-development of the wave function between measurements*, that is, between t_0 and t_1, so that $\psi(\vec{x}, t_1)$ can be calculated in terms of $\psi(\vec{x}, t_0)$. Naturally, the time-development depends on the forces acting on the particle.

3.2.1. Mathematical Preliminaries

1. Let A and B be linear operators. If $\langle \phi_1 \mid A\phi_2 \rangle = \langle \phi_1 \mid B\phi_2 \rangle$ for all ϕ_1, ϕ_2, then $A = B$.

Proof: We have $0 = \langle\phi_1 \mid A\phi_2\rangle - \langle\phi_1 \mid B\phi_2\rangle = \langle\phi_1 \mid (A-B)\phi_2\rangle$. Now choose $\phi_1 = (A-B)\phi_2$. Then $0 = \langle(A-B)\phi_2 \mid (A-B)\phi_2\rangle \Rightarrow (A-B)\phi_2$ for all ϕ_2 or $A - B = 0$.

2. Let A and B be linear operators. If $\langle\phi \mid A\phi\rangle = \langle\phi \mid B\phi\rangle$ for all ϕ, that is, if $\langle A\rangle = \langle B\rangle$ for all states, then $A = B$.

   Proof: Let $\phi = \phi_1 + \lambda\phi_2$, where λ is an arbitrary complex constant. Therefore,

$$\begin{aligned}
\langle\phi \mid A\phi\rangle &= \langle\phi_1 + \lambda\phi_2 \mid A(\phi_1 + \lambda\phi_2)\rangle \\
&= \langle\phi_1 \mid A\phi_1\rangle + |\lambda|^2 \langle\phi_2 \mid A\phi_2\rangle + \lambda\langle\phi_1 \mid A\phi_2\rangle + \lambda^* \langle\phi_2 \mid A\phi_1\rangle \\
\langle\phi \mid B\phi\rangle &= \langle\phi_1 + \lambda\phi_2 \mid B(\phi_1 + \lambda\phi_2)\rangle \\
&= \langle\phi_1 \mid B\phi_1\rangle + |\lambda|^2 \langle\phi_2 \mid B\phi_2\rangle + \lambda\langle\phi_1 \mid B\phi_2\rangle + \lambda^* \langle\phi_2 \mid B\phi_1\rangle
\end{aligned}$$

   But $\langle\phi_1 \mid A\phi_1\rangle = \langle\phi_1 \mid B\phi_1\rangle$ and $\langle\phi_2 \mid A\phi_2\rangle = \langle\phi_2 \mid B\phi_2\rangle$. Therefore,

$$\lambda\langle\phi_1 \mid A\phi_2\rangle + \lambda^* \langle\phi_2 \mid A\phi_1\rangle = \lambda\langle\phi_1 \mid B\phi_2\rangle + \lambda^* \langle\phi_2 \mid B\phi_1\rangle \text{ for all } \lambda \quad (3.43)$$

   and

$$\lambda = 1 \rightarrow \langle\phi_1 \mid A\phi_2\rangle + \langle\phi_2 \mid A\phi_1\rangle = \langle\phi_1 \mid B\phi_2\rangle + \langle\phi_2 \mid B\phi_1\rangle \quad (3.44)$$

$$\lambda = i \rightarrow \langle\phi_1 \mid A\phi_2\rangle - \langle\phi_2 \mid A\phi_1\rangle = \langle\phi_1 \mid B\phi_2\rangle - \langle\phi_2 \mid B\phi_1\rangle \quad (3.45)$$

   Therefore, $\langle\phi_1 \mid A\phi_2\rangle = \langle\phi_1 \mid B\phi_2\rangle$ for all ϕ_1, ϕ_2 so that $A = B$.

3. We have

$$[x_i, p_j] = i\hbar\delta_{ij} \quad , \quad [x_i, x_j] = 0 \quad , \quad [p_i, p_j] = 0 \quad (3.46)$$

   We can cleverly rewrite these equations by letting A be one of the operators x, y, z, p_x, p_y or p_z:

$$[x_i, A] = i\hbar\frac{\partial A}{\partial p_i} \quad , \quad [A, p_j] = i\hbar\frac{\partial A}{\partial x_j} \quad (3.47)$$

   where

$$\frac{\partial x_i}{\partial p_j} = 0 \quad , \quad \frac{\partial p_j}{\partial p_i} = \delta_{ij} \quad , \quad \frac{\partial p_i}{\partial x_j} = 0 \quad , \quad \frac{\partial p_i}{\partial x_j} = 0 \quad (3.48)$$

   Let $f = f(\vec{x}, \vec{p}) = \sum(ABCD...)$ = sum of terms of the form $(ABCD...)$, where each operator $A, B, C.D, ...$ is one of the operators x, y, z, p_x, p_y or p_z. For example,

$$f(\vec{x}, \vec{p}) = xp_xxz + p_y^2x \quad (3.49)$$

Now,

$$\begin{aligned}[x_i, f(\vec{x},\vec{p})] &= \left[x_i, \sum (ABCD...)\right] = \sum [x_i, ABCD...] \\ &= \sum \left([x_i, A]\, BCD... + A\,[x_i, B]\, CD... + AB\,[x_i, C]\, D...+\right) \\ &= \sum \left(i\hbar \frac{\partial A}{\partial p_i} BCD... + Ai\hbar \frac{\partial B}{\partial p_i} CD... + ABi\hbar \frac{\partial C}{\partial p_i} D...+\right) \\ &= i\hbar \sum \left(\frac{\partial A}{\partial p_i} BCD... + A\frac{\partial B}{\partial p_i} CD... + AB\frac{\partial C}{\partial p_i} D...+\right) \\ &= i\hbar \frac{\partial}{\partial p_i} \sum (ABCD...) = i\hbar \frac{\partial f(\vec{x},\vec{p})}{\partial p_i} \end{aligned} \tag{3.50}$$

and in a similar manner we have

$$[f(\vec{x},\vec{p}), p_j] = i\hbar \frac{\partial f(\vec{x},\vec{p})}{\partial x_j} \tag{3.51}$$

Note: When differentiating an operator of the form $ABCD....$, one must maintain the order of the operators $A, B, C, D, ...$ because the operators do not necessarily commute.

Example: Let

$$f(\vec{x},\vec{p}) = xp_x xz + p_y^2 x \tag{3.52}$$

Then

$$[x, f(\vec{x},\vec{p})] = i\hbar \frac{\partial f}{\partial p_x} = i\hbar\,(x(1)xz + 0) = i\hbar x^2 z \tag{3.53}$$

We now proceed to consider the *time-development of the wave function between measurements*. This time-development will be our final postulate. We will motivate this postulate by *deriving* it from several rather *reasonable* assumptions.

Consider a particle under the influence of a conservative force:

$$H = \frac{\vec{p}\cdot\vec{p}}{2m} + V(\vec{x}) \tag{3.54}$$

Let us try to obtain a differential equation which will determine the behavior of $\psi(\vec{x}, t)$ with time.

Assumption (a) $\psi(\vec{x}, t)$ is completely determined by knowing the wave function at some initial time t_0, that is, $\psi(\vec{x}, t_0)$ at all $\vec{x}$ determines $\psi(\vec{x}, t)$ for all time t. In particular, we are assuming that $\partial\psi(\vec{x}, t_0)/\partial t$ need not be given as an initial condition. Thus, the differential equation obeyed by $\psi(\vec{x}, t)$ must be *first order in time*:

$$\frac{\partial\psi}{\partial t} = \frac{1}{i\hbar}\left[\theta(\vec{x},\vec{p},t)\right]\psi \quad , \quad \vec{p} = \frac{\hbar}{i}\nabla \tag{3.55}$$

where $\theta(\vec{x},\vec{p},t)$ is some complicated operator which, in principle, might be non-linear. The factor $1/i\hbar$ has been separated out for later convenience.

Assumption (b) If $\psi_1(\vec{x},t)$ and $\psi_2(\vec{x},t)$ are solutions of (3.55), then any linear superposition $\lambda_1\psi_1(\vec{x},t)+\lambda_2\psi_2(\vec{x},t)$ is also a solution. This is essentially Postulate (1b) from earlier (*linear superposition*). Therefore, if we have

$$\frac{\partial\psi_1}{\partial t}=\frac{1}{i\hbar}\theta\psi_1 \text{ and } \frac{\partial\psi_2}{\partial t}=\frac{1}{i\hbar}\theta\psi_2 \tag{3.56}$$

then this implies that

$$\frac{\partial}{\partial t}(\lambda_1\psi_1+\lambda_2\psi_2)=\frac{1}{i\hbar}\theta(\lambda_1\psi_1+\lambda_2\psi_2) \tag{3.57}$$

for all constants λ_1,λ_2. Therefore,

$$\begin{aligned}\frac{1}{i\hbar}\theta(\lambda_1\psi_1+\lambda_2\psi_2)&=\frac{\partial}{\partial t}(\lambda_1\psi_1+\lambda_2\psi_2)\\&=\lambda_1\frac{\partial\psi_1}{\partial t}+\lambda_2\frac{\partial\psi_2}{\partial t}=\frac{1}{i\hbar}\lambda_1\theta\psi_1+\frac{1}{i\hbar}\lambda_2\theta\psi_2\end{aligned}$$

or

$$\theta(\lambda_1\psi_1+\lambda_2\psi_2)=\lambda_1\theta\psi_1+\lambda_2\theta\psi_2 \tag{3.58}$$

which says that $\theta=\theta(\vec{x},\vec{p},t)$ must be *linear*.

Assumption (c) $\psi(\vec{x},t)$ must be normalizable for all t in order to be a physical wave function (Postulate (1a) from earlier). The simplest way to guarantee this is to require

$$\int d^3x\psi^*(\vec{x},t)\psi(\vec{x},t)=\int d^3x\psi^*(\vec{x},t_0)\psi(\vec{x},t_0) \tag{3.59}$$

where the initial wave function $\psi(\vec{x},t_0)$ is assumed to be normalizable. This should be regarded as a *convenient choice* for preserving normalization. We note that this property fails if we were considering relativistic quantum mechanics!

Notation: We have

$$\langle\psi_1(t)\mid\psi_2(t)\rangle=\int d^3x\psi^*(\vec{x},t)\psi(\vec{x},t) \tag{3.60}$$

where the variable $\vec{x}$ has been omitted on the left hand side because it is integrated over so that the resulting inner product depends only on t.

Therefore, assumption (c) can be written

$$\langle\psi(t)\mid\psi(t)\rangle=\langle\psi(t_0)\mid\psi(t_0)\rangle \tag{3.61}$$

or

$$\frac{d}{dt}\langle\psi(t)\mid\psi(t)\rangle=0 \tag{3.62}$$

which gives

$$\begin{aligned} 0 &= \frac{d}{dt}\int d^3x\psi^*(\vec{x},t)\psi(\vec{x},t) \\ &= \int d^3x\left[\frac{\partial\psi^*(\vec{x},t)}{\partial t}\psi(\vec{x},t)+\psi^*(\vec{x},t)\frac{\partial\psi(\vec{x},t)}{\partial t}\right] \\ &= \left\langle\frac{\partial\psi(t)}{\partial t}\,\middle|\,\psi(t)\right\rangle+\left\langle\psi(t)\,\middle|\,\frac{\partial\psi(t)}{\partial t}\right\rangle \\ &= -\frac{1}{i\hbar}\langle\theta\psi(t)\mid\psi(t)\rangle+\frac{1}{i\hbar}\langle\psi(t)\mid\theta\psi(t)\rangle \end{aligned} \tag{3.63}$$

or

$$\langle\theta\psi(t)\mid\psi(t)\rangle=\langle\psi(t)\mid\theta\psi(t)\rangle \text{ for arbitrary } \psi(\vec{x},t) \tag{3.64}$$

Note that $\psi(\vec{x},t)$ can be practically any square-integrable function because $\psi(\vec{x},t_0)$ may be chosen arbitrarily.

This result says that $\theta=\theta(\vec{x},\vec{p},t)$ must be *hermitian*.

Assumption (d) This is the important assumption. We must construct a quantum theory which, for macroscopic phenomena, reduces to the equations of classical physics (Newton's laws of motion). This constraint on the quantum theory is called the *correspondence principle*, and we will impose it on our theory by assuming the following, which is experimentally verified for microscopic and macroscopic phenomena:

> Even though the results if *individual* measurements do not obey the equations of classical physics in detail, the *average values* of measurements obey the classical equations of motion

Basic Assumption (will determine $\theta=\theta(\vec{x},\vec{p},t)$):

$$\frac{d}{dt}\langle p_i\rangle=+\langle F_i\rangle=\left\langle-\frac{\partial V(\vec{x})}{\partial x_i}\right\rangle \text{ where } \frac{d}{dt}\langle x_i\rangle=\left\langle\frac{p_i}{m}\right\rangle \tag{3.65}$$

These equations correspond (are the quantum analogues) to the classical equations of motion:

$$\frac{dp_i}{dt}=F_i=-\frac{\partial V(\vec{x})}{\partial x_i} \text{ and } \frac{dx_i}{dt}=\frac{p_i}{m} \tag{3.66}$$

The average values

$$\langle p_i\rangle=\frac{\langle\psi(t)\mid p_i\psi(t)\rangle}{\langle\psi(t)\mid\psi(t)\rangle} \text{ and } \langle x_i\rangle=\frac{\langle\psi(t)\mid x_i\psi(t)\rangle}{\langle\psi(t)\mid\psi(t)\rangle} \tag{3.67}$$

depend on time because $\psi(\vec{x},t)$ depends on time. The operators x_i and $p_i = -i\hbar\partial/\partial x_i$ do not change with time. Now we can write

$$\frac{d}{dt}\frac{\langle\psi(t)\mid p_i\psi(t)\rangle}{\langle\psi(t)\mid\psi(t)\rangle} = -\frac{\left\langle\psi(t)\,\middle|\,\frac{\partial V(\vec{x})}{\partial x_i}\psi(t)\right\rangle}{\langle\psi(t)\mid\psi(t)\rangle} \tag{3.68}$$

$$\frac{d}{dt}\frac{\langle\psi(t)\mid x_i\psi(t)\rangle}{\langle\psi(t)\mid\psi(t)\rangle} = \frac{1}{m}\frac{\langle\psi(t)\mid p_i\psi(t)\rangle}{\langle\psi(t)\mid\psi(t)\rangle} \tag{3.69}$$

But

$$\frac{d}{dt}\langle\psi(t)\mid\psi(t)\rangle = 0 \text{ since } \langle\psi(t)\mid\psi(t)\rangle \text{ is constant} \tag{3.70}$$

implies that we cancel the factor

$$\frac{1}{\langle\psi(t)\mid\psi(t)\rangle} \tag{3.71}$$

in these equations. Therefore

$$\frac{d}{dt}\langle\psi(t)\mid p_i\psi(t)\rangle = -\left\langle\psi(t)\,\middle|\,\frac{\partial V(\vec{x})}{\partial x_i}\psi(t)\right\rangle \tag{3.72}$$

$$\frac{d}{dt}\langle\psi(t)\mid x_i\psi(t)\rangle = \frac{1}{m}\langle\psi(t)\mid p_i\psi(t)\rangle \tag{3.73}$$

so that

$$\begin{aligned}
-\left\langle\psi(t)\,\middle|\,\frac{\partial V(\vec{x})}{\partial x_i}\psi(t)\right\rangle &= \frac{d}{dt}\langle\psi(t)\mid p_i\psi(t)\rangle \\
&= \left\langle\frac{\partial\psi}{\partial t}\,\middle|\,p_i\psi\right\rangle + \left\langle\psi\,\middle|\,p_i\frac{\partial\psi}{\partial t}\right\rangle \\
&= -\frac{1}{i\hbar}\langle\theta\psi\mid p_i\psi\rangle + \frac{1}{i\hbar}\langle\psi\mid p_i\theta\psi\rangle \\
&= -\frac{1}{i\hbar}\langle\psi\mid\theta p_i\psi\rangle + \frac{1}{i\hbar}\langle\psi\mid p_i\theta\psi\rangle \\
&= -\frac{1}{i\hbar}\langle\psi\mid[\theta,p_i]\,\psi\rangle = -\frac{1}{i\hbar}\left\langle\psi\,\middle|\,i\hbar\frac{\partial\theta}{\partial x_i}\psi\right\rangle \\
&= -\left\langle\psi\,\middle|\,\frac{\partial\theta}{\partial x_i}\psi\right\rangle
\end{aligned} \tag{3.74}$$

Since the above equation is true for any $\psi(\vec{x},t)$ we have

$$\frac{\partial\theta(\vec{x},\vec{p},t)}{\partial x_i} = \frac{\partial V(\vec{x})}{\partial x_i} \tag{3.75}$$

In a similar manner we can also show the following:

$$\begin{aligned}
\frac{1}{m}\langle\psi(t)\mid p_i\psi(t)\rangle &= \frac{d}{dt}\langle\psi(t)\mid x_i\psi(t)\rangle \\
&= \left\langle\frac{\partial\psi}{\partial t}\,\middle|\, x_i\psi\right\rangle + \left\langle\psi\,\middle|\, x_i\frac{\partial\psi}{\partial t}\right\rangle \\
&= -\frac{1}{i\hbar}\langle\theta\psi\mid x_i\psi\rangle + \frac{1}{i\hbar}\langle\psi\mid x_i\theta\psi\rangle \\
&= -\frac{1}{i\hbar}\langle\psi\mid \theta x_i\psi\rangle + \frac{1}{i\hbar}\langle\psi\mid x_i\theta\psi\rangle \\
&= -\frac{1}{i\hbar}\langle\psi\mid [\theta, x_i]\,\psi\rangle = \frac{1}{i\hbar}\left\langle\psi\,\middle|\, i\hbar\frac{\partial\theta}{\partial p_i}\psi\right\rangle \\
&= \left\langle\psi\,\middle|\,\frac{\partial\theta}{\partial p_i}\psi\right\rangle
\end{aligned} \tag{3.76}$$

Since the above equation is true for any $\psi(\vec{x},t)$ we have

$$\frac{\partial\theta(\vec{x},\vec{p},t)}{\partial p_i} = \frac{p_i}{m} \tag{3.77}$$

We can now determine the operator $\theta(\vec{x},\vec{p},t)$:

$$\frac{\partial\theta(\vec{x},\vec{p},t)}{\partial p_x} = \frac{p_x}{m} \rightarrow \theta(\vec{x},\vec{p},t) = \frac{p_x^2}{2m} + \theta_1(p_y,p_z,x,y,z,t) \tag{3.78}$$

$$\frac{\partial\theta(\vec{x},\vec{p},t)}{\partial p_y} = \frac{\partial\theta_1(\vec{x},\vec{p},t)}{\partial p_y} = \frac{p_y}{m} \rightarrow \theta_1(\vec{x},\vec{p},t) = \frac{p_y^2}{2m} + \theta_2(p_z,x,y,z,t) \tag{3.79}$$

$$\frac{\partial\theta(\vec{x},\vec{p},t)}{\partial p_z} = \frac{\partial\theta_1(\vec{x},\vec{p},t)}{\partial p_z} = \frac{p_z}{m} \rightarrow \theta_2(\vec{x},\vec{p},t) = \frac{p_z^2}{2m} + \theta_3(x,y,z,t) \tag{3.80}$$

$$\frac{\partial\theta(\vec{x},\vec{p},t)}{\partial x_i} = \frac{\partial\theta_3(x,y,z,t)}{\partial x_i} = \frac{\partial V(\vec{x})}{\partial x_i} \rightarrow \theta_3(x,y,z,t) = V(\vec{x}) + c(t) \tag{3.81}$$

where $c(t)$ is an arbitrary function of t; i.e., it is independent of $\vec{x}$ and $\vec{p}$. Therefore,

$$\theta(\vec{x},\vec{p},t) = \frac{\vec{p}\cdot\vec{p}}{2m} + V(\vec{x}) + c(t) \tag{3.82}$$

is the solution of the partial differential equations which $\theta(\vec{x},\vec{p},t)$ must obey. Note that $\theta(\vec{x},\vec{p},t)$ being hermitian implies that $c(t)$ must be a real function of t.

Claim: $c(t)$ has no physical significance and can be chosen to be zero.

Proof: For $c(t)$ any arbitrary function, the wave function obeys

$$\frac{\partial\psi_c(\vec{x},t)}{\partial t} = \frac{1}{i\hbar}\left[\frac{\vec{p}\cdot\vec{p}}{2m} + V(\vec{x}) + c(t)\right]\psi_c(\vec{x},t) \tag{3.83}$$

subject to the initial condition $\psi_c(\vec{x},t_0)=\psi(\vec{x},t_0)$, which is a given square-integrable function. Consider the function $N_c(t)\psi_c(\vec{x},t)$ with

$$N_c(t)=e^{+\frac{i}{\hbar}\int_{t_0}^{t}c(t')dt'} \tag{3.84}$$

where $c(t)$ real implies that $|N_c(t)|=1$. Therefore $N_c(t=t_0)=e^0=1$. This means that $N_c(t)\psi_c(\vec{x},t)$ and $\psi_c(\vec{x},t)$ obey the same initial conditions at $t=t_0$.

Because $N_c(t)$ is just a multiplicative factor independent of $\vec{x}$ (it happens to depend on time), $N_c(t)\psi_c(\vec{x},t)$ and $\psi_c(\vec{x},t)$ determine exactly the same probability distribution and average values.

Thus, we can use $N_c(t)\psi_c(\vec{x},t)$ as the wave function rather than $\psi_c(\vec{x},t)$ and no physical values will be altered.

The differential equation obeyed by $N_c(t)\psi_c(\vec{x},t)$ is

$$\begin{aligned}\frac{\partial(N_c\psi_c)}{\partial t}&=\frac{\partial N_c}{\partial t}\psi_c+N_c\frac{\partial\psi_c}{\partial t}=\frac{i}{\hbar}c(t)N_c\psi_c+\frac{1}{i\hbar}\theta N_c\psi_c\\&=\frac{1}{i\hbar}\left(\theta-c(t)\right)N_c\psi_c=\frac{1}{i\hbar}\left[\frac{\vec{p}\cdot\vec{p}}{2m}+V(\vec{x})\right]N_c\psi_c\end{aligned} \tag{3.85}$$

Letting $N_c(t)\psi_c(\vec{x},t)=\psi(\vec{x},t)$ we have

$$\frac{\partial\psi(\vec{x},t)}{\partial t}=\frac{1}{i\hbar}\left[\frac{\vec{p}\cdot\vec{p}}{2m}+V(\vec{x})\right]\psi(\vec{x},t) \tag{3.86}$$

which proves that no physical values will be altered if we use

$$\theta(\vec{x},\vec{p},t)=\frac{\vec{p}\cdot\vec{p}}{2m}+V(\vec{x}) \tag{3.87}$$

with no $c(t)$ present. Thus,

$$\theta(\vec{x},\vec{p},t)=\frac{\vec{p}\cdot\vec{p}}{2m}+V(\vec{x})=H(\vec{x},\vec{p}) \tag{3.88}$$

It is the Hamiltonian operator!

The partial differential equation just obtained determines the time-development of the wave function between measurements.

Rather than postulate assumptions (a),(b),(c),(d), which went into the above derivation, we will just postulate the result.

3.2.2. Postulate 5: Time Development of the Wave Function

For a particle in a conservative force field, the wave function obeys the *time-dependent Schrodinger equation*:

$$i\hbar\frac{\partial\psi(\vec{x},t)}{\partial t} = H(\vec{x},\vec{p})\psi(\vec{x},t) = \left[\frac{\vec{p}\cdot\vec{p}}{2m} + V(\vec{x})\right]\psi(\vec{x},t)$$
$$= -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{x},t) + V(\vec{x})\psi(\vec{x},t) \tag{3.89}$$

From this equation, one can determine $\psi(\vec{x},t)$ at any time t by knowing $\psi(\vec{x},t_0)$, the wave function at some initial time t_0.

We note the important fact that the wave function's *time-development* is completely determined by the time-dependent Schrodinger equation during periods of time when no measurements are made. While a measurement is being made, the wave function does not obey the time-dependent Schrodinger equation - instead, the wave function emphcollapses to an eigenfunction of the observable being measured. The eigenfunction to which the wave function collapses is, in general, *unpredictable* - only the probabilities for specific results of a measurement can be determined. Contrast this with the completely predictable time-development during periods of time when no measurements are made - a time-development determined by the time-dependent Schrodinger equation.

3.3. Structure of Quantum Theory

3.3.1. Initial preparation of the wave function at t_0

Measuring a complete set of compatible observables at t_0 determines $\psi(\vec{x},t_0)$ immediately after these measurements (up to a multiplicative constant).

Then time development is governed by

$$H\psi = i\hbar\frac{\partial\psi}{\partial t} \tag{3.90}$$

which takes $\psi(\vec{x},t_0)$ (given) into $\psi(\vec{x},t)$ (determined).

Measurement of A at time t (A need not be related to the observables measured

at t_0) gives

$$\wp(a_n,t) = \frac{1}{\langle\psi(t)\mid\psi(t)\rangle}\sum_\alpha \left|c_n^{(\alpha)}(t)\right|^2 = \sum_\alpha \frac{\left\langle\psi(t)\,\middle|\,u_n^{(\alpha)}\right\rangle\left\langle u_n^{(\alpha)}\,\middle|\,\psi(t)\right\rangle}{\langle\psi(t)\mid\psi(t)\rangle} \tag{3.91}$$

$$\tilde{\wp}(a_{c\nu},t_0) = \frac{1}{\langle\psi(t)\mid\psi(t)\rangle}\sum_\beta \left|d_\nu^{(\beta)}\right|^2 = \sum_\beta \frac{\left\langle\psi(t)\,\middle|\,u_{c\nu}^{(\beta)}\right\rangle\left\langle u_{c\nu}^{(\beta)}\,\middle|\,\psi(t)\right\rangle}{\langle\psi(t)\mid\psi(t)\rangle} \tag{3.92}$$

$$\left\langle A^N\right\rangle = \frac{\left\langle\psi(t)\,\middle|\,A^N\psi(t)\right\rangle}{\langle\psi(t)\mid\psi(t)\rangle} \tag{3.93}$$

Immediately after the measurement, the wave function *collapses* to a function which depends on the result of the measurement.

Notice the conceptual difference between the time-dependent Schrodinger equation

$$H\psi = i\hbar\frac{\partial\psi}{\partial t} \tag{3.94}$$

and the time-independent Schrodinger equation $H\psi = E\psi$. The time-dependent Schrodinger equation determines the time-development of any wave function between measurements. The time-independent Schrodinger equation is just one of many eigenvalue equations - it is the eigenvalue equation for energy and determines the possible results of an energy measurement.

The time-dependent Schrodinger equation is motivated by the *correspondence principle - average values obey the classical equations of motion.*

One can reverse our previous arguments and show that the time-dependent Schrodinger equation implies that average values obey the classical equations of motion.

3.3.2. Basic Problem of Quantum Mechanics

Given $\psi(\vec{x},0)$, find $\psi(\vec{x},t)$.

Let $\left\{u_n^{(\alpha)}(\vec{x})\right\}$ be a CON set of eigenfunctions of H ($Hu_n^{(\alpha)} = E_n u_n^{(\alpha)}$). For simplicity of notation, we will assume that the spectrum of H is entirely discrete. Our results generalize in an obvious manner when a continuum is also present.

Now we can expand $\psi(\vec{x},t)$ at fixed time t in terms of a CON set as

$$\psi(\vec{x},t) = \sum_{n,\alpha} c_n^{(\alpha)}(t)u_n^{(\alpha)}(\vec{x}) \tag{3.95}$$

Therefore, we have

$$i\hbar\frac{\partial\psi}{\partial t} = \sum_{n,\alpha} i\hbar\frac{\partial c_n^{(\alpha)}(t)}{\partial t}u_n^{(\alpha)}(\vec{x}) = H\psi$$
$$= \sum_{n,\alpha} c_n^{(\alpha)}(t)Hu_n^{(\alpha)}(\vec{x}) = \sum_{n,\alpha} c_n^{(\alpha)}(t)E_n u_n^{(\alpha)}(\vec{x}) \tag{3.96}$$

The linear independence of the $\left\{u_n^{(\alpha)}(\vec{x})\right\}$ implies that we can equate coefficients in the expansions:

$$i\hbar\frac{\partial c_n^{(\alpha)}(t)}{\partial t} = E_n c_n^{(\alpha)}(t) \text{ for all } \alpha, n \tag{3.97}$$

This equation is easily solved:

$$c_n^{(\alpha)}(t) = c_n^{(\alpha)}(0)e^{-\frac{i}{\hbar}E_n t} \tag{3.98}$$

so that

$$\psi(\vec{x},t) = \sum_{n,\alpha} c_n^{(\alpha)}(0)e^{-\frac{i}{\hbar}E_n t}u_n^{(\alpha)}(\vec{x}) \tag{3.99}$$

This is a **very important result**. It represents the general result for **expansion of an arbitrary wave function in terms of energy eigenfunctions**.

The coefficients $c_n^{(\alpha)}(0)$ can be found from the given $\psi(\vec{x},0)$ since

$$\psi(\vec{x},0) = \sum_{n,\alpha} c_n^{(\alpha)}(0)u_n^{(\alpha)}(\vec{x}) \tag{3.100}$$

so that

$$c_n^{(\alpha)}(0) = \left\langle u_n^{(\alpha)} \,\middle|\, \psi(t=0)\right\rangle \tag{3.101}$$

Therefore, we have determined $\psi(\vec{x},t)$ in terms of $\psi(\vec{x},0)$.

We note that the solution just obtained for $\psi(\vec{x},t)$ can also be obtained by solving the time-dependent Schrodinger equation by the method of *separation of variables*. We have

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V(\vec{x})\psi \tag{3.102}$$

Trying a solution of the form $\psi(\vec{x},t) = U(\vec{x})T(t)$ we get

$$i\hbar\frac{dT}{dt}U = \left(-\frac{\hbar^2}{2m}\nabla^2 U + V(\vec{x})U\right)T$$
$$\Rightarrow i\hbar\frac{1}{T}\frac{dT}{dt} = \frac{1}{U}\left(-\frac{\hbar^2}{2m}\nabla^2 U + V(\vec{x})U\right)$$

We thus have function of t = function of $\vec{x}$. Because $\vec{x}$ and t are independent variables, each side of this equation must equal a constant λ (the separation constant). We then have

$$i\hbar\frac{1}{T}\frac{dT}{dt} = \lambda = \frac{1}{U}\left(-\frac{\hbar^2}{2m}\nabla^2 U + V(\vec{x})U\right) = \frac{1}{U}HU \tag{3.103}$$

or $HU = \lambda U$ so that U must be an energy eigenfunction with energy eigenvalue $\lambda = E$ and

$$i\hbar\frac{dT}{dt} = \lambda T \rightarrow T(t) = T(0)e^{-\frac{i}{\hbar}\lambda t} \tag{3.104}$$

Therefore, for a particular value of E (one of the eigenvalues) we have

$$\psi(\vec{x},t) = T_E(0)e^{-\frac{i}{\hbar}Et}U_E(\vec{x}) \quad (= c_n^{(\alpha)}(0)e^{-\frac{i}{\hbar}E_n t}u_n^{(\alpha)}(\vec{x})) \tag{3.105}$$

which represents a *complete set* when we use all linearly independent solutions for all possible E values. The general solution to the time-dependent Schrodinger equation is obtained by summing over all such particular solutions:

$$\psi(\vec{x},t) = \sum_E T_E(0)e^{-\frac{i}{\hbar}Et}U_E(\vec{x}) = \sum_{n,\alpha} c_n^{(\alpha)}(0)e^{-\frac{i}{\hbar}E_n t}u_n^{(\alpha)}(\vec{x}) \tag{3.106}$$

as obtained earlier.

Some Notes:

(a) Let $\psi(\vec{x},t)$ be an arbitrary wave function. Its expansion in terms of energy eigenfunctions is:

$$\psi(\vec{x},t) = \sum_{n,\alpha} c_n^{(\alpha)}(t)u_n^{(\alpha)}(\vec{x}) \tag{3.107}$$

where

$$c_n^{(\alpha)}(t) = c_n^{(\alpha)}(0)e^{-\frac{i}{\hbar}E_n t} \tag{3.108}$$

The probability of measuring E_n at time t is:

$$\wp(E_n,t) = \frac{\sum_\alpha \left|c_n^{(\alpha)}(t)\right|^2}{\langle\psi(t)\mid\psi(t)\rangle} \tag{3.109}$$

But $\langle\psi(t)\mid\psi(t)\rangle = \langle\psi(0)\mid\psi(0)\rangle$ and $\left|c_n^{(\alpha)}(t)\right| = \left|c_n^{(\alpha)}(0)\right|$. Therefore,

$$\wp(E_n,t) = \frac{\sum_\alpha \left|c_n^{(\alpha)}(0)\right|^2}{\langle\psi(0)\mid\psi(0)\rangle} = \wp(E_n,0) \tag{3.110}$$

Therefore, $\wp(E_n,t)$ *is independent of time* for any wave function (corresponds to energy conservation).

(b) Let $\psi(\vec{x},0) = u_n^{(\alpha)}(\vec{x})$, that is, the particle is in an eigenfunction of energy at $t = 0$. Therefore,

$$\psi(\vec{x},t) = u_n^{(\alpha)}(\vec{x})e^{-\frac{i}{\hbar}E_n t} \tag{3.111}$$

for any time t, that is, we just get multiplication by a phase factor! The particle therefore remains in the *same* eigenfunction of energy for all t if it is initially in an eigenfunction of energy. Eigenfunctions of energy are therefore called *stationary states*. In general, if $\psi(\vec{x},0)$ is an eigenfunction of *some operator other than energy*, then $\psi(\vec{x},t)$ will not remain an eigenfunction of this operator for $t \neq 0$.

3.3.2.1. Properties of Stationary States

In a stationary state we have

$$\psi(\vec{x},t) = u_n^{(\alpha)}(\vec{x})e^{-\frac{i}{\hbar}E_n t} \quad , \quad Hu_n^{(\alpha)} = E_n u_n^{(\alpha)} \tag{3.112}$$

1. The probability density (probability per unit volume) for position measurements is given by

$$\wp(\vec{x},t) = \frac{|\psi(\vec{x},t)|^2}{\langle\psi(t)\mid\psi(t)\rangle} \tag{3.113}$$

and

$$\wp(\vec{x},t) = \frac{\left|u_n^{(\alpha)}(\vec{x})e^{-\frac{i}{\hbar}E_n t}\right|^2}{\langle\psi(t)\mid\psi(t)\rangle} = \frac{\left|u_n^{(\alpha)}(\vec{x})\right|^2}{\langle\psi(0)\mid\psi(0)\rangle} = \frac{|\psi(\vec{x},0)|^2}{\langle\psi(0)\mid\psi(0)\rangle} = \wp(\vec{x},0)$$

Therefore, $\wp(\vec{x},t)$ is independent of time for a stationary state.

2. Let A be any physical observable. For simplicity of notation, we will assume that the spectrum of A is entirely discrete. Let $\left\{v_m^{(\beta)}(\vec{x})\right\}$ be a CON set of eigenfunctions of A:

$$Av_m^{(\beta)}(\vec{x}) = a_m v_m^{(\beta)}(\vec{x}) \tag{3.114}$$

Therefore,

$$\begin{aligned}
&\wp(a_m,t)\\
&= \sum_\beta \frac{\left\langle\psi(t)\,\middle|\,v_m^{(\beta)}\right\rangle\left\langle v_m^{(\beta)}\,\middle|\,\psi(t)\right\rangle}{\langle\psi(t)\mid\psi(t)\rangle} = \sum_\beta \frac{\left\langle u_n^{(\alpha)}e^{-\frac{i}{\hbar}E_n t}\,\middle|\,v_m^{(\beta)}\right\rangle\left\langle v_m^{(\beta)}\,\middle|\,u_n^{(\alpha)}e^{-\frac{i}{\hbar}E_n t}\right\rangle}{\langle\psi(0)\mid\psi(0)\rangle}\\
&= \sum_\beta \frac{\left\langle u_n^{(\alpha)}\,\middle|\,v_m^{(\beta)}\right\rangle\left\langle v_m^{(\beta)}\,\middle|\,u_n^{(\alpha)}\right\rangle e^{\frac{i}{\hbar}E_n t}e^{-\frac{i}{\hbar}E_n t}}{\langle\psi(0)\mid\psi(0)\rangle} = \sum_\beta \frac{\left\langle u_n^{(\alpha)}\,\middle|\,v_m^{(\beta)}\right\rangle\left\langle v_m^{(\beta)}\,\middle|\,u_n^{(\alpha)}\right\rangle}{\langle\psi(t)\mid\psi(t)\rangle}\\
&= \sum_\beta \frac{\left\langle\psi(0)\,\middle|\,v_m^{(\beta)}\right\rangle\left\langle v_m^{(\beta)}\,\middle|\,\psi(0)\right\rangle}{\langle\psi(t)\mid\psi(t)\rangle} = \wp(a_m,0)
\end{aligned}$$

Thus, $\wp(a_m,t)$ is independent of time for a stationary state.

3. Let A be any physical observable. Then

$$\langle A\rangle_t = \frac{\langle\psi(t)\mid A\psi(t)\rangle}{\langle\psi(t)\mid\psi(t)\rangle} = \frac{\left\langle u_n^{(\alpha)} e^{-\frac{i}{\hbar}E_n t}\,\middle|\, A u_n^{(\alpha)} e^{-\frac{i}{\hbar}E_n t}\right\rangle}{\langle\psi(0)\mid\psi(0)\rangle}$$
$$= \frac{\left\langle u_n^{(\alpha)}\,\middle|\, A u_n^{(\alpha)}\right\rangle}{\langle\psi(0)\mid\psi(0)\rangle} = \frac{\langle\psi(0)\mid A\psi(0)\rangle}{\langle\psi(0)\mid\psi(0)\rangle} = \langle A\rangle_{t=0}$$

Therefore, $\langle A\rangle$ is independent of time for a stationary state.

3.3.2.2. Example of a Non-Stationary State

Let $\psi(\vec{x},0)$ be a linear combination of two non-degenerate energy eigenfunctions

$$\psi(\vec{x},0) = c_1 u_1(\vec{x}) + c_2 u_2(\vec{x}) \tag{3.115}$$

where

$$Hu_i = E_i u_i \text{ for } i = 1,2, E_2 > E_1\ ,\ \ \langle u_i\mid u_j\rangle = \delta_{ij} \text{ for } i = 1,2 \text{ (ON)} \tag{3.116}$$

We have the energy level diagram as shown in Figure 3.1 below.

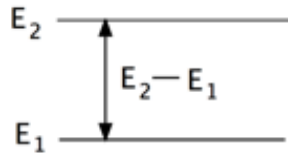


Figure 3.1: Energy Levels

Therefore,

$$\psi(\vec{x},t) = c_1 u_1(\vec{x}) e^{-\frac{iE_1 t}{\hbar}} + c_2 u_2(\vec{x}) e^{-\frac{iE_2 t}{\hbar}} \tag{3.117}$$

with

$$\langle\psi(t)\mid\psi(t)\rangle = \langle\psi(0)\mid\psi(0)\rangle = |c_1|^2 + |c_2|^2 \tag{3.118}$$

and

$$\wp(E_1,t) = \frac{|c_1|^2}{|c_1|^2 + |c_2|^2} \quad , \quad \wp(E_2,t) = \frac{|c_2|^2}{|c_1|^2 + |c_2|^2} \tag{3.119}$$

independent of t.

Let A be any physical observable, and let us calculate the time dependence of

$\langle A \rangle$ for the above state.

$$\begin{aligned}
\langle A \rangle &= \frac{\langle \psi(t) \mid A\psi(t) \rangle}{\langle \psi(t) \mid \psi(t) \rangle} \\
&= \frac{\left\langle c_1 u_1(\vec{x}) e^{-\frac{iE_1 t}{\hbar}} + c_2 u_2(\vec{x}) e^{-\frac{iE_2 t}{\hbar}} \;\middle|\; A\left(c_1 u_1(\vec{x}) e^{-\frac{iE_1 t}{\hbar}} + c_2 u_2(\vec{x}) e^{-\frac{iE_2 t}{\hbar}} \right) \right\rangle}{|c_1|^2 + |c_2|^2} \\
&= \frac{1}{|c_1|^2 + |c_2|^2} \left(\begin{array}{l} |c_1|^2 \langle u_1 \mid Au_1 \rangle + |c_2|^2 \langle u_2 \mid Au_2 \rangle \\ \quad + c_2^* c_1 e^{\frac{i(E_2 - E_1)t}{\hbar}} \langle u_2 \mid Au_1 \rangle + c_1^* c_2 e^{-\frac{i(E_2 - E_1)t}{\hbar}} \langle u_1 \mid Au_2 \rangle \end{array} \right) \\
&= \frac{1}{|c_1|^2 + |c_2|^2} \left(\begin{array}{l} |c_1|^2 \langle u_1 \mid Au_1 \rangle + |c_2|^2 \langle u_2 \mid Au_2 \rangle \\ \quad + c_2^* c_1 e^{\frac{i(E_2 - E_1)t}{\hbar}} \langle u_2 \mid Au_1 \rangle + c_1^* c_2 e^{-\frac{i(E_2 - E_1)t}{\hbar}} \langle Au_2 \mid u_1 \rangle^* \end{array} \right) \\
&= \frac{1}{|c_1|^2 + |c_2|^2} \left(\begin{array}{l} |c_1|^2 \langle u_1 \mid Au_1 \rangle + |c_2|^2 \langle u_2 \mid Au_2 \rangle \\ \quad + c_2^* c_1 e^{\frac{i(E_2 - E_1)t}{\hbar}} \langle u_2 \mid Au_1 \rangle + c_1^* c_2 e^{-\frac{i(E_2 - E_1)t}{\hbar}} \langle u_2 \mid Au_1 \rangle^* \end{array} \right)
\end{aligned}$$

Now let

$$R = \frac{|c_1|^2 \langle u_1 \mid Au_1 \rangle + |c_2|^2 \langle u_2 \mid Au_2 \rangle}{|c_1|^2 + |c_2|^2} \tag{3.120}$$

(this is a *real* number (because A is hermitian)) and

$$Z = \frac{c_2^* c_1 \langle u_2 \mid Au_1 \rangle}{|c_1|^2 + |c_2|^2} = |Z| e^{i\xi} \tag{3.121}$$

which is a complex number. Therefore,

$$\begin{aligned}
\langle A \rangle &= R + Z e^{\frac{i(E_2 - E_1)t}{\hbar}} + Z^* e^{-\frac{i(E_2 - E_1)t}{\hbar}} \\
&= R + |Z| \left[e^{i\left[\frac{(E_2 - E_1)t}{\hbar} + \xi\right]} + e^{-i\left[\frac{(E_2 - E_1)t}{\hbar} + \xi\right]} \right] \\
&= R + 2|Z| \cos\left[\frac{(E_2 - E_1)t}{\hbar} + \xi \right]
\end{aligned} \tag{3.122}$$

so that $\langle A \rangle$ oscillates in time with a frequency $\omega = (E_2 - E_1)/\hbar$ when $|Z| \neq 0$, which requires $\langle u_2 \mid Au_1 \rangle \neq 0$.

If $A = \vec{x}$ (position operator), then $\langle \vec{x} \rangle$ is harmonic in time with frequency $\omega = (E_2 - E_1)/\hbar$. If the particle is charged (for example, an electron), then its average position will oscillate harmonically in time and the particle will therefore radiate at angular frequency $\omega = (E_2 - E_1)/\hbar$ when $c_2^* c_1 \langle u_2 \mid Au_1 \rangle \neq 0$. Suppose an electron in an atom makes a *transition* from energy level E_2 to energy level E_1. We will show later in this chapter that the wave function for such an electron is a linear combination of u_2 and u_1 with neither c_2 or c_1 zero. Thus, the electron will radiate at angular frequency ω such that $\hbar\omega = (E_2 - E_1)$ when $\langle u_2 \mid \vec{x} u_1 \rangle \neq 0$.This requirement for the radiation to occur is known as a *selection rule* - it is a condition on the states u_2 and u_1 for a radiative transition to be

possible.

Of course, the electron does not radiate forever as it goes from level E_2 to level E_1. We will show later in this chapter that c_2 *eventually becomes zero* so that the electron is eventually in the lower energy state completely and no radiation is emitted thereafter (the transition is then over). If we assume one photon is emitted during the transition, energy conservation implies $E_{1\,photon} = E_2 - E_1 = \hbar\omega$ where ω = angular frequency of the radiation. We therefore obtain the Einstein relation $E_{photon} = \hbar\omega$!

3.4. Free Particle in One Dimension (motion along the x-axis)

We have

$$H = \frac{p_{xop}^2}{2m} \tag{3.123}$$

We will use p to denote the eigenvalues of the operator p_{xop}.

Now, $[H, p_{xop}] = 0$ implies that there exists a CON set of simultaneous eigenfunctions of H and p_{xop}. The eigenfunctions of p_{xop} are (from earlier)

$$u_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{px}{\hbar}} \quad , \quad p \in [-\infty, +\infty] \tag{3.124}$$

Thus, $\{u_p(x)\}$ is a CON set of simultaneous eigenfunctions of H and p_{xop}.

Suppose we are given $\psi(\vec{x}, 0)$. The problem is then to find $\psi(\vec{x}, t)$ for all t. We may expand $\psi(\vec{x}, t)$ in terms of $\{u_p(x)\}$:

$$\psi(x,t) = \int_{-\infty}^{\infty} dp\, \tilde{\psi}(p,t) u_p(x) \tag{3.125}$$

where the $\tilde{\psi}(p,t)$ are expansion coefficients which depend on the time at which the expansion is made.

Because $u_p(x)$ is an energy eigenfunction, the time dependence of $\tilde{\psi}(p,t)$ is given by

$$\tilde{\psi}(p,t) = \tilde{\psi}(p,0) e^{-i\frac{p^2 t}{2m\hbar}} \quad , \quad E = \frac{p^2}{2m} \tag{3.126}$$

Therefore,

$$\psi(x,t) = \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi\hbar}} \tilde{\psi}(p,0) e^{i\left(\frac{px}{\hbar} - \frac{p^2 t}{2m\hbar}\right)} \tag{3.127}$$

$\tilde{\psi}(p,0)$ may be expressed in terms of the given $\psi(x,0)$ as

$$\psi(x,0) = \int_{-\infty}^{\infty} dp\, \tilde{\psi}(p,0) u_p(x) \tag{3.128}$$

so that

$$\begin{aligned} \langle u_{p'} \mid \psi(t=0)\rangle &= \int_{-\infty}^{\infty} dp \tilde{\psi}(p,0) \langle u_{p'} \mid u_p\rangle \\ &= \int_{-\infty}^{\infty} dp \tilde{\psi}(p,0)\delta(p'-p) = \tilde{\psi}(p',0) \end{aligned} \tag{3.129}$$

Thus,

$$\tilde{\psi}(p,0) = \langle u_p \mid \psi(t=0)\rangle = \int_{-\infty}^{\infty} dx\, u_p^*(x)\psi(x,0) \tag{3.130}$$

that is,

$$\tilde{\psi}(p,0) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\hbar}}\, e^{-i\frac{px}{\hbar}} \psi(x,0) \tag{3.131}$$

Thus, given $\psi(x,0)$ we can calculate $\tilde{\psi}(p,0)$ and then $\psi(x,t)$.

The probability distribution of momentum measurements is given by:

$$\tilde{\wp}(p,t) = \frac{\langle \psi(t) \mid u_p\rangle \langle u_p \mid \psi(t)\rangle}{\langle \psi(t) \mid \psi(t)\rangle} \tag{3.132}$$

where

$$\begin{aligned} \langle u_p \mid \psi(t)\rangle &= \tilde{\psi}(p,t) = \tilde{\psi}(p,0) e^{-i\frac{p^2 t}{2m\hbar}} \\ &= \tilde{\psi}(p,0) \times \text{ (a phase factor)} \end{aligned} \tag{3.133}$$

Therefore,

$$\tilde{\wp}(p,t) = \frac{\left|\tilde{\psi}(p,t)\right|^2}{\langle \psi(t) \mid \psi(t)\rangle} = \frac{\left|\tilde{\psi}(p,0)\right|^2}{\langle \psi(t) \mid \psi(t)\rangle} = \tilde{\wp}(p,0) \tag{3.134}$$

For a free particle, the momentum probability distribution does not change with time. This is momentum conservation for a particle with no forces acting on it. In general, the spatial probability distribution changes with time.

Now,

$$\psi(x,t) = \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi\hbar}} \tilde{\psi}(p,0) e^{i\left(\frac{px}{\hbar} - \frac{p^2 t}{2m\hbar}\right)} \tag{3.135}$$

where

$$e^{i\left(\frac{px}{\hbar}-\frac{p^2t}{2m\hbar}\right)} = e^{i(kx-\omega t)} = \text{ plane wave with } k = \frac{p}{\hbar} \text{ and } \omega = \frac{p^2}{2m\hbar} \tag{3.136}$$

$\psi(x,t)$ is a *superposition of plane waves* and is called a *wave packet.*

For each plane wave:

$$\frac{2\pi}{\lambda} = k = \frac{p}{\hbar} \Rightarrow \lambda = \frac{2\pi\hbar}{p} = \frac{h}{p} \tag{3.137}$$

$$2\pi\nu = \omega = \frac{p^2}{2m\hbar} \Rightarrow \nu = \frac{p^2}{4\pi m\hbar} = \frac{p^2}{2mh} \tag{3.138}$$

The planes of constant phase move at the phase velocity

$$v_{phase} = \lambda\nu = \frac{p}{2m} \tag{3.139}$$

The phase velocity has a different value for each p in the superposition. The factor 1/2 in the expression

$$v_{phase} = \frac{p}{2m} \tag{3.140}$$

may seem surprising because, for classical particles,

$$v_{classical} = \frac{p_{classical}}{m} \tag{3.141}$$

However, one must remember that the *entire* wave packet $\psi(x,t)$ describes the particle. The pertinent quantity is the so-called *group velocity of the wave packet*:

$$v_{group} = \frac{d}{dt}\langle x\rangle = \left\langle \frac{p}{m} \right\rangle \tag{3.142}$$

where the averages are for the entire wave packet. The group velocity characterizes the entire wave function and is the quantity that corresponds to $v_{classical}$.

Often, one would like to estimate the behavior of $\psi(x,t)$ without explicitly doing the integral over the plane waves. The following very general method of approximation is useful for such estimates.

3.4.1. The Method of Stationary Phase

Let

$$\psi(x,t) = \int_{-\infty}^{\infty} dp\, g(p,x,t) \tag{3.143}$$

where $g(p,x,t)$ is a complex function such that

$$g(p,x,t) = G(p,x,t)e^{i\gamma(p,x,t)} \tag{3.144}$$

with

$$0 \le G(p,x,t) = \text{ real amplitude of } g(p,x,t)$$
$$\gamma(p,x,t) = \text{ phase angle of } g(p,x,t)$$

Therefore,

$$\psi(x,t) = \int_{-\infty}^{\infty} dp\, G(p,x,t) e^{i\gamma(p,x,t)} \tag{3.145}$$

Now we assume that $G(p,x,t)$ is sharply peaked at $p = p_0$ and is appreciable only in a small range Δp about p_0 as shown in Figure 3.2 below.

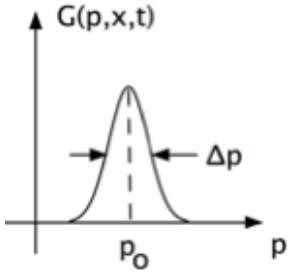


Figure 3.2: Weight Function

We assume that Δp and p_0 do not depend on x and t. However, the value of G at p_0 and the detailed behavior of G depend on x and t.

(a) Estimate of of (x,t) values for which $|\psi(x,t)|$ is a maximum

For given x and t, $\psi(x,t) \approx 0$ if $\gamma(p,x,t)$ changes quite a bit as p varies over the Δp range (for such a case, $\cos\gamma(p,x,t)$ and $\sin\gamma(p,x,t)$ oscillate a great deal over Δp and the integral ≈ 0 because of cancellations - recall that $G(p,x,t) \ge 0$.

$|\psi(x,t)|$ will be a maximum if $\gamma(p,x,t)$ changes a negligible amount over the Δp range (for such a case, the entire integrand does not change sign over Δp and there are no cancellations). Therefore we want

$$\left[\frac{d\gamma(p,x,t)}{dp}\right]_{p=p_0} = 0 \tag{3.146}$$

as the condition for (x,t) values for which $|\psi(x,t)|$ is a maximum. This just says that the integrand's phase is stationary at p_0.

Estimate of (x,t) values for which $|\psi(x,t)|$ is appreciable

$|\psi(x,t)|$ will be appreciable, that is, non-negligible, for all (x,t) values for which

$e^{i\gamma(p,x,t)}$ does not vary over more than one cycle in the Δp range. If $e^{i\gamma(p,x,t)}$ varied over much more than one cycle in the Δp range, the integral would be ≈ 0 because of cancellations. Therefore, for appreciable or non-negligible $|\psi(x,t)|$ we must have

$$|[\text{change in } \gamma(p,x,t) \text{ over } \Delta p]| = \Delta p \left[\frac{d\gamma(p,x,t)}{dp}\right]_{p=p_0} \leq 2\pi \tag{3.147}$$

Comment: $\psi(x,t)$ is certainly non-negligible when $|\psi(x,t)|$ is a maximum. This is consistent with the above conditions because $|\psi(x,t)|$ is a maximum when

$$\left[\frac{d\gamma(p,x,t)}{dp}\right]_{p=p_0} = 0 \tag{3.148}$$

and this clearly satisfies the condition for $\psi(x,t)$ to be non-negligible.

3.4.2. Application to a Free-Particle Wave Packet

We have

$$\psi(x,t) = \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi\hbar}} \tilde{\psi}(p,0) e^{i\left(\frac{px}{\hbar} - \frac{p^2 t}{2m\hbar}\right)} \tag{3.149}$$

Let $\tilde{\psi}(p,0) = \left|\tilde{\psi}(p,0)\right| e^{i\alpha(p)/\hbar}$ be non-negligible in a Δp range about $p = p_0$. For convenience, the phase of $\tilde{\psi}(p,0)$ is written as $\alpha(p)/\hbar$. Δp measures the spread in the momentum probability distribution. We have

$$\psi(x,t) = \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi\hbar}} \left|\tilde{\psi}(p,0)\right| e^{i\left(\frac{px}{\hbar} - \frac{p^2 t}{2m\hbar} + \frac{\alpha(p)}{\hbar}\right)} \tag{3.150}$$

We have separated the integrand into an amplitude and a phase factor. The values of (x,t) for which $|\psi(x,t)|$ is a maximum are given by the stationary phase condition

$$\frac{d}{dp}\left(\frac{px}{\hbar} - \frac{p^2 t}{2m\hbar} + \frac{\alpha(p)}{\hbar}\right)_{p=p_0} = \frac{x}{\hbar} - \frac{pt}{m\hbar} + \frac{1}{\hbar}\frac{d\alpha(p)}{dp} = 0$$

Therefore, $\psi(x,t)$ is peaked at $x = x_{peak}(t)$ where

$$x_{peak}(t) = \frac{p_0 t}{m} - \left[\frac{d\alpha(p)}{dp}\right]_{p=p_0} \tag{3.151}$$

that is, the peak of the wave packet moves at constant velocity

$$v_{packet} = \frac{p_0}{m} \tag{3.152}$$

Notice that the phase angle of $\tilde{\psi}(p,0)$ determines the position of the peak at $t=0$. $\psi(x,t)$ is appreciable at all (x,t) satisfying

$$\Delta p \left| \frac{d}{dp}\left(\frac{px}{\hbar} - \frac{p^2 t}{2m\hbar} + \frac{\alpha(p)}{\hbar} \right)_{p=p_0} \right| \leq 2\pi$$

$$\Delta p \left| \left(\frac{x}{\hbar} - \frac{p_0 t}{m\hbar} + \frac{1}{\hbar}\left[\frac{d\alpha(p)}{dp} \right]_{p=p_0} \right) \right| \leq 2\pi$$

$$\Delta p \, |x - x_{peak}(t)| \leq 2\pi\hbar$$

or we must have

$$|x - x_{peak}(t)| \leq \frac{2\pi\hbar}{\Delta p} = \frac{h}{\Delta p} \tag{3.153}$$

for $\psi(x,t)$ appreciable as shown in Figure 3.3 below.

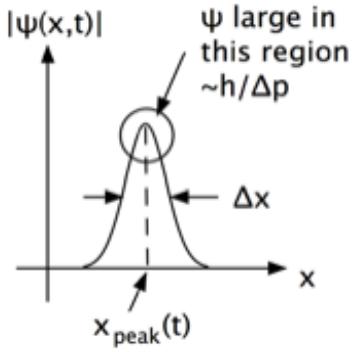


Figure 3.3: $\psi(x,t)$ appreciable

The maximum value of $|x - x_{peak}(t)|$ (with x such that $\psi(x,t)$ is appreciable) is $\approx h/\Delta p$. But Δx, the *spread* of $\psi(x,t)$ is not less (see figure) than $\max|x - x_{peak}(t)|$ for $\psi(x,t)$ appreciable. Therefore, $\Delta x \geq h/\Delta p$, which is consistent with uncertainty principle.

3.5. Constants of the Motion

The time-development of the wave function is determined by the time-dependent Schrodinger equation:

$$H\psi = i\hbar \frac{\partial \psi}{\partial t} \tag{3.154}$$

Let $A = A(\vec{x}, \vec{p})$ be the hermitian operator corresponding to some physical quantity. We will assume that this operator does not change with time (A is independent of t).

The average value of A,

$$\langle A \rangle = \frac{\langle \psi(t) \mid A\psi(t) \rangle}{\langle \psi(t) \mid \psi(t) \rangle} \tag{3.155}$$

depends on time through the time dependence of $\psi(x,t)$. Recall that $\langle \psi(t) \mid \psi(t) \rangle = \langle \psi(0) \mid \psi(0) \rangle$ is independent of time. Thus,

$$\begin{aligned}
\frac{d}{dt}\langle A \rangle &= \frac{1}{\langle \psi(t) \mid \psi(t) \rangle} \frac{d}{dt} \left(\langle \psi(t) \mid A\psi(t) \rangle \right) \\
&= \frac{1}{\langle \psi(t) \mid \psi(t) \rangle} \left(\left\langle \frac{\partial \psi}{\partial t} \,\middle|\, A\psi \right\rangle + \left\langle \psi \,\middle|\, A\frac{\partial \psi}{\partial t} \right\rangle \right) \\
&= \frac{1}{\langle \psi(t) \mid \psi(t) \rangle} \left(\left\langle \frac{1}{i\hbar} H\psi \,\middle|\, A\psi \right\rangle + \left\langle \psi \,\middle|\, A\frac{1}{i\hbar} H\psi \right\rangle \right) \\
&= \frac{1}{\langle \psi(t) \mid \psi(t) \rangle} \frac{1}{i\hbar} \left(-\langle H\psi \mid A\psi \rangle + \langle \psi \mid AH\psi \rangle \right) \\
&= \frac{1}{\langle \psi(t) \mid \psi(t) \rangle} \frac{1}{i\hbar} \left(-\langle \psi \mid HA\psi \rangle + \langle \psi \mid AH\psi \rangle \right) \\
&= \frac{1}{\langle \psi(t) \mid \psi(t) \rangle} \left\langle \psi \,\middle|\, \frac{1}{i\hbar} [A,H]\, \psi \right\rangle
\end{aligned} \tag{3.156}$$

or

$$\begin{aligned}
\frac{d}{dt}\langle A \rangle &= \left\langle \frac{1}{i\hbar} [A,H] \right\rangle \\
\frac{d}{dt}\langle \psi(t) \mid A\psi(t) \rangle &= \left\langle \psi(t) \,\middle|\, \frac{1}{i\hbar} [A,H]\, \psi(t) \right\rangle
\end{aligned} \tag{3.157}$$

Definition: The physical observable A is *conserved*, that is, A is a *constant of the motion*, if

$$\frac{d}{dt}\langle A \rangle = 0 \text{ for any } \psi(\vec{x},t) \tag{3.158}$$

Recall that $d\langle B \rangle / dt = 0$ for *any* observable B if the average value is taken in a *stationary state*. B is conserved if $d\langle B \rangle / dt = 0$ for all possible non-stationary states as well.

3.5.0.1. Notes

1. A is conserved if $[A,H] = 0$, which follows immediately from the definition and the preceding results.

2. A is conserved if A and H have a CON set of simultaneous eigenfunctions. This follows from (1) and the fact that commutativity is equivalent to compatibility.

3. If A is conserved, then the probability distribution of measurements of A ($\wp(a_n,t)$ and $\wp(a_{c\nu},t)$) is constant in time for any $\psi(\vec{x},t)$. Recall that the probability distribution of measurements for any observable is constant in

time for a stationary state.

Proof: A and H possess a CON set of simultaneous eigenfunctions $\left\{u_{nm}^{(\alpha)}(\vec{x})\right\}$. For simplicity of notation, we assume that the spectra are entirely discrete. Then

$$Au_{nm}^{(\alpha)}(\vec{x}) = a_n u_{nm}^{(\alpha)}(\vec{x})$$
$$Hu_{nm}^{(\alpha)}(\vec{x}) = E_m u_{nm}^{(\alpha)}(\vec{x})$$

and

$$\psi(\vec{x},t) = \sum_{nm\alpha} \underbrace{c_{nm}^{(\alpha)}(0)e^{-i\frac{E_m t}{\hbar}}}_{c_{nm}^{(\alpha)}(t)} u_{nm}^{(\alpha)}(\vec{x}) \tag{3.159}$$

Thus,

$$\wp(a_n,t) = \frac{\left|c_{nm}^{(\alpha)}(t)\right|^2}{\langle\psi(t)\mid\psi(t)\rangle} = \frac{\left|c_{nm}^{(\alpha)}(0)\right|^2}{\langle\psi(0)\mid\psi(0)\rangle} = \wp(a_n,0) \tag{3.160}$$

4. Let A be conserved. If $\psi(\vec{x},0)$ is an eigenfunction of A with eigenvalue a_n, then $\psi(\vec{x},t)$ remains an eigenfunction of A with eigenvalue a_n for all time. This follows immediately from note (3) and the fact that $\wp(a_n,t) = 1$ if $\psi(\vec{x},t) =$ an eigenfunction of A with eigenvalue a_n.

3.5.0.2. Example

Particle in a conservative force field

$$H = \frac{\vec{p}\cdot\vec{p}}{2m} + V(\vec{x}) \tag{3.161}$$

$$[H,H] = 0 \Rightarrow H \text{ conserved (energy conservation)} \tag{3.162}$$

3.5.0.3. Example

Free particle (no forces present)

$$H = \frac{\vec{p}\cdot\vec{p}}{2m} \tag{3.163}$$

$$[p_i,H] = 0 \Rightarrow p_i \text{ conserved (linear momentum conservation)} \tag{3.164}$$

3.5.0.4. Example

Particle in a central force field

$$H = \frac{\vec{p}\cdot\vec{p}}{2m} + V(r) \text{ where } r = |\vec{x}| \tag{3.165}$$

Consider $L_z = xp_y - yp_x$. We have

$$\begin{aligned}
[L_z, H] &= \left[xp_y - yp_x, \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} + V(r)\right] \\
&= \left[xp_y, \frac{p_x^2}{2m}\right] + [xp_y, V(r)] - \left[yp_x, \frac{p_y^2}{2m}\right] \\
&\qquad - [yp_x, V(r)] + \text{othertermswhicharezero} \\
&= \frac{1}{2m}\left[x, p_x^2\right] p_y + x\,[p_y, V(r)] \\
&\qquad - \frac{1}{2m}\left[y, p_y^2\right] p_x - y\,[p_x, V(r)] \\
&= \frac{1}{2m}(i\hbar\frac{p_x}{m})p_y + x(-i\hbar\frac{\partial V}{\partial y}) \\
&\qquad - \frac{1}{2m}(i\hbar\frac{p_y}{m})p_x - y(-i\hbar\frac{\partial V}{\partial x}) \\
&= i\hbar x(y\frac{\partial V}{\partial x} - x\frac{\partial V}{\partial y}) = i\hbar x(y\frac{\partial r}{\partial x} - x\frac{\partial r}{\partial y})\frac{\partial V}{\partial r} \\
&= i\hbar x(y\frac{x}{r} - x\frac{y}{r})\frac{\partial V}{\partial r} = 0
\end{aligned}$$

Thus, $[L_z, H] = 0$. Because

$$H = \frac{\vec{p}\cdot\vec{p}}{2m} + V(r) \tag{3.166}$$

is unchanged when z and x are interchanged or when z and y are interchanged, we conclude that $[L_x, H] = 0$ and $[L_y, H] = 0$. Therefore, $[L_z, H] = 0$ or L_z is conserved (angular momentum conservation for a central force).

We now consider a particular (solvable)physical system in great detail.

3.6. Harmonic Oscillator in One Dimension

We have

$$-\frac{dV(x)}{dx} = F_x = -kx \quad , \quad k > 0 \quad , \quad V(x) = \frac{1}{2}kx^2 \tag{3.167}$$

Therefore,

$$H = \frac{p_x^2}{2m} + \frac{1}{2}kx^2 \tag{3.168}$$

Classical

$$\frac{d^2x}{dt^2} = -\frac{k}{m}x \Rightarrow x = A\sin\omega t + B\cos\omega t \quad , \quad \omega = \sqrt{\frac{k}{m}} \tag{3.169}$$

Let $x = 0$ and $dx/dt = v_0$ at $t = 0$. Then $B = 0$ and $A = v_0/\omega$ so that

$$x = \frac{v_0}{\omega} \sin \omega t \tag{3.170}$$

The classical motion is therefore bounded $x \in [-x_{\max}, +x_{\max}]$ where $x_{\max} = A = v_0/\omega$. We therefore expect the spectrum of H to be entirely discrete when we do the quantum mechanical problem.

Quantum Mechanical: We have

$$\frac{d}{dt} \langle x \rangle = \frac{1}{i\hbar} \langle [x, H] \rangle = \frac{1}{i2m\hbar} \left\langle \left[x, p_x^2\right] \right\rangle = \frac{1}{i2m\hbar} \frac{i\hbar}{m} \langle p_x \rangle = \frac{1}{m} \langle p_x \rangle \tag{3.171}$$

$$\frac{d}{dt} \langle p_x \rangle = \frac{1}{i\hbar} \langle [p_x, H] \rangle = \frac{1}{i\hbar} \frac{1}{2} k \left\langle \left[p_x, x^2\right] \right\rangle = \frac{1}{i\hbar} \frac{1}{2} (-i\hbar) k^2 \langle x \rangle = -k \langle x \rangle \tag{3.172}$$

The time dependence of $\langle x \rangle$ is easily found:

$$\frac{d^2}{dt^2} \langle x \rangle = \frac{1}{m} \frac{d}{dt} \langle p_x \rangle = -\frac{k}{m} \langle x \rangle \tag{3.173}$$

Therefore

$$\langle x \rangle = A \sin \omega t + B \cos \omega t \text{ with } \omega = \sqrt{\frac{k}{m}} \tag{3.174}$$

so that $\langle x \rangle$ follows the classical trajectory!

Let us now look for the stationary states of the harmonic oscillator. These are the energy eigenfunctions and are important for two reasons:

1. The corresponding energy eigenvalues are the only possible results from an energy measurement.

2. The time dependence of any $\psi(x, t)$ describing a particle in the presence of a harmonic oscillator force can be obtained easily.

We will find the energy eigenfunctions and eigenvalues by two very different methods:

(a) Differential equation method

(b) Operator algebra method

Let us express the Hamiltonian in terms of the classical (angular) frequency $\omega = \sqrt{k/m}$:

$$H = \frac{p_x^2}{2m} + \frac{1}{2} m\omega^2 x^2 \quad , \quad H\phi(x) = E\phi(x) \tag{3.175}$$

3.6.1. Differential Equation Method

We have

$$H\phi(x) = E\phi(x) \Rightarrow -\frac{\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2\phi(x) = E\phi(x) \tag{3.176}$$

We solve the differential equation for $\phi(x)$ with E an arbitrary constant and find allowed values of E by requiring that $\phi(x)$ not become infinite as $|x| \to \infty$. This will give us the entire spectrum of H - discrete and continuum parts.

Step 1: Introduce dimensionless variables and parameters.

$$\begin{aligned} &-\frac{\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2\phi(x) = E\phi(x) \\ &\Rightarrow \frac{1}{\left(\frac{m\omega}{\hbar}\right)}\frac{d^2\phi(x)}{dx^2} - \frac{m\omega}{\hbar}x^2\phi(x) = -\frac{2mE}{\hbar^2}\phi(x) \end{aligned}$$

Define

$$y = \sqrt{\frac{m\omega}{\hbar}}x \text{ and } \varepsilon = \frac{2E}{\hbar\omega} \tag{3.177}$$

(both dimensionless). Therefore, we get

$$\frac{d^2\phi}{dy^2} + (\varepsilon - y^2)\phi = 0 \tag{3.178}$$

Step 2: Factor out the asymptotic ($y \to \pm\infty$) behavior of ϕ. Let $y \to \infty$. Then $\varepsilon - y^2 \approx -y^2$ so that we have the equation

$$\frac{d^2\phi}{dy^2} - y^2\phi = 0 \tag{3.179}$$

As can be easily seen by direct substitution, this asymptotic equation is solved by

$$\phi = y^\alpha e^{\pm\frac{1}{2}y^2} \tag{3.180}$$

for arbitrary constant α. But ϕ cannot be infinite as $y \to \infty$. Therefore, the asymptotic solution

$$y^\alpha e^{+\frac{1}{2}y^2} \tag{3.181}$$

must be discarded. Therefore, asymptotically the solution is

$$\phi = y^\alpha e^{-\frac{1}{2}y^2} \tag{3.182}$$

We now try to find an *exact* solution of the form

$$\phi(x) = \phi\left(\sqrt{\frac{m\omega}{\hbar}}x\right) = e^{-\frac{1}{2}y^2}F(y) \tag{3.183}$$

This form is motivated by the form of the asymptotic solution. The equation which $F(y)$ obeys is obtained by substituting this form into

$$\frac{d^2\phi}{dy^2} + (\varepsilon - y^2)\phi = 0 \tag{3.184}$$

We have

$$\frac{d\phi}{dy} = -ye^{-\frac{1}{2}y^2}F + e^{-\frac{1}{2}y^2}\frac{dF}{dy} \tag{3.185}$$

$$\frac{d^2\phi}{dy^2} = -e^{-\frac{1}{2}y^2}F + y^2e^{-\frac{1}{2}y^2}F - ye^{-\frac{1}{2}y^2}\frac{dF}{dy} - ye^{-\frac{1}{2}y^2}\frac{dF}{dy} + e^{-\frac{1}{2}y^2}\frac{d^2F}{dy^2} \tag{3.186}$$

so that the equation for $F(y)$ becomes

$$\frac{d^2F}{dy^2} - 2y\frac{dF}{dy} + (\varepsilon - 1)F = 0 \tag{3.187}$$

which is Hermite's differential equation. **Step 3**: Solve Hermite's differential equation by the power series method Taylor where we expand $F(y)$ about $y = 0$. Let

$$F(y) = \sum_{k=0}^{\infty} A_k y^k \tag{3.188}$$

and substitute into the differential equation. We have

$$0 = \underbrace{\sum_{k=0}^{\infty} k(k-1)A_k y^{k-2}}_{\substack{\text{Series begins at } k=2. \\ \text{Relabeling index } (k\to k+2) \\ \to \sum_{k=0}^{\infty}(k+2)(k+1)A_{k+2}y^k}} \underbrace{-2y\sum_{k=0}^{\infty} kA_k y^{k-1}}_{\sum_{k=0}^{\infty} 2kA_k y^k} + (\varepsilon - 1)\sum_{k=0}^{\infty} A_k y^k \tag{3.189}$$

or

$$0 = \sum_{k=0}^{\infty} y^k \underbrace{\{(k+2)(k+1)A_{k+2} - 2kA_k + (\varepsilon - 1)A_k\}}_{\text{Each of these coefficients must therefore be zero}} \text{ for all y} \tag{3.190}$$

Therefore

$$A_{k+2} = \frac{(2k - \varepsilon + 1)}{(k+2)(k+1)}A_k \text{ for } k = 0, 1, 2, 3, ... \tag{3.191}$$

this is called a *recursion* relation. Using the recursion relation

$$A_0 \text{ given } \Rightarrow A_2, A_4, A_6, ... \text{ all determined}$$
$$A_1 \text{ given } \Rightarrow A_3, A_5, A_7, ... \text{ all determined}$$

A_0 and A_1 are arbitrary. These are the two arbitrary constants which always appear in the most general solution of a second-order differential equation. Thus,

$$F(y) = \underbrace{\sum_{k=0,2,4,6,....} A_k y^k}_{\substack{= F_{even}(y) \\ \text{(determined by } A_0\text{)}}} + \underbrace{\sum_{k=1,3,5,....} A_k y^k}_{\substack{= F_{odd}(y) \\ \text{(determined by } A_1\text{)}}} \tag{3.192}$$

Note: If $A_N = 0$ for some N , then $A_{N+2} = A_{N+4} = A_{N+6} = ... = 0$.

Step 4: $F(y)$ given above solves Hermite's differential equation for any given value of ε. The *allowed values* of

$$E = \varepsilon \frac{\hbar\omega}{2} \tag{3.193}$$

are determined by requiring that ϕ not become infinite as $y \to \infty$. Now

$$\phi(x) = \phi\left(\sqrt{\frac{m\omega}{\hbar}}x\right) = e^{-\frac{1}{2}y^2} F(y)$$

(i) If $F(y)$ is a polynomial of finite degree (the series *terminates* after some term), then $\phi(x)$ asymptotically goes as

$$e^{-\frac{1}{2}y^2}\left[y^{\text{finite power}}\right] \to 0 \tag{3.194}$$

This is an acceptable $\phi(x)$.

(ii) Suppose the series for $F(y)$ does not terminate. Then as $y \to \infty$, the terms with large k dominate in

$$F(y) = \sum_{k=0}^{\infty} A_k y^k \tag{3.195}$$

For $k \to \infty$

$$\frac{A_{k+2}}{A_k} = \frac{(2k - \varepsilon + 1)}{(k+2)(k+1)} \underset{k\to\infty}{\to} \frac{2k}{k^2} = \frac{2}{k} \tag{3.196}$$

Therefore,

$$F_{even}(y) = \sum_{k=0,2,4,..} A_k y^k \Rightarrow \frac{A_{k+2}}{A_k} \underset{k\to\infty}{\to} \frac{2}{k}$$

$$F_{odd}(y) = \sum_{k=1,3,5,....} A_k y^k \Rightarrow \frac{A_{k+2}}{A_k} \underset{k\to\infty}{\to} \frac{2}{k}$$

But,

$$e^{+y^2} = \sum_{n=0}^{\infty} \frac{y^{2n}}{n!} = \sum_{k=0,2,4,..} \frac{y^k}{\left(\frac{k}{2}\right)!}$$

$$\to \sum_{\substack{\text{large even} \\ k}} B_k y^k \text{with} \frac{B_{k+2}}{B_k} = \frac{1/\left(\frac{k+2}{2}\right)!}{1/\left(\frac{k}{2}\right)!} = \frac{1}{\frac{k}{2}+1} \approx \frac{2}{k}$$

and

$$ye^{+y^2} = \sum_{n=0}^{\infty} \frac{y^{2n+1}}{n!} = \sum_{k=1,3,5,..} \frac{y^k}{\left(\frac{k-1}{2}\right)!}$$

$$\rightarrow \sum_{\substack{\text{large odd} \\ k}} C_k y^k \text{with} \frac{C_{k+2}}{C_k} = \frac{1/\left(\frac{k+1}{2}\right)!}{1/\left(\frac{k-1}{2}\right)!} = \frac{1}{\frac{k+1}{2}} \approx \frac{2}{k}$$

Therefore, as $y \rightarrow \infty$

$$F_{even}(y) \rightarrow e^{+y^2} \quad , \quad F_{odd}(y) \rightarrow ye^{+y^2} \tag{3.197}$$

if the series does not terminate. Therefore,

$$\phi = e^{-\frac{1}{2}y^2} F(y) \Rightarrow \phi_{even} \rightarrow e^{+\frac{1}{2}y^2} \text{ and } \phi_{odd} \rightarrow ye^{+\frac{1}{2}y^2} \tag{3.198}$$

These solutions diverge as $y \rightarrow \infty$ and therefore are unacceptable.

Conclusion: $F(y)$ must be a polynomial of finite degree, that is, the series for $F(y)$ must terminate after some term! This gives us the allow values of ε. We have

$$A_{k+2} = \frac{(2k - \varepsilon + 1)}{(k+2)(k+1)} A_k \tag{3.199}$$

Therefore, F_{even} terminates if $A_0 = 0$ ($\rightarrow F_{even} \equiv 0$) *or* $2N_1 - \varepsilon + 1 = 0$ for some even N_1. Therefore

$$F_{even} = A_0 + A_2 y^2 + ... + A_{N_1} y^{N_1} \tag{3.200}$$

Therefore, F_{odd} terminates if $A_1 = 0$ ($\rightarrow F_{odd} \equiv 0$) *or* $2N_2 - \varepsilon + 1 = 0$ for some odd N_2. Therefore

$$F_{odd} = A_1 + A_3 y^2 + ... + A_{N_2} y^{N_2} \tag{3.201}$$

Now $F = F_{even} + F_{odd}$. Therefore F terminates if both F_{even} *and* F_{odd} terminate.

This means we need

$$2N_1 - \varepsilon + 1 = 0, \text{ even } N_1 \text{ AND } 2N_2 - \varepsilon + 1 = 0, \text{ odd } N_2 \tag{3.202}$$

which CANNOT be satisfied simultaneously. Therefore

(1) $A_0 = 0$ and $2N_2 - \varepsilon + 1 = 0$ for some odd $N_2 \Rightarrow \varepsilon = 2N_2 + 1$
(2) $A_1 = 0$ and $2N_1 - \varepsilon + 1 = 0$ for some even $N_1 \Rightarrow \varepsilon = 2N_1 + 1$

The allowed values of ε are therefore

$$\varepsilon_N = 2N + 1 \quad , \quad N = 0, 1, 2, 3, ... \tag{3.203}$$

and

$$\varepsilon_N = \frac{2E_N}{\hbar\omega} \rightarrow E_N = \frac{\hbar\omega}{2}(2N + 1) \text{ for } N = 0, 1, 2, 3, ... \tag{3.204}$$

The corresponding $F_N(y)$ is obtained from

$$F_N(y) = \sum_{k=0}^{\infty} A_k^{(N)} y^k \tag{3.205}$$

where

$$A_{k+2}^{(N)} = \frac{(2k - \varepsilon_N + 1)}{(k+2)(k+1)} A_k^{(N)} = \frac{2(k-N)}{(k+2)(k+1)} A_k^{(N)}$$
$$A_{odd\,k}^{(even\,N)} = 0 = A_{even\,k}^{(odd\,N)}$$

Therefore,

N **even**:

$$F_N(y) = A_0^{(N)} \left\{ \begin{array}{l} 1 + y^2 \frac{2(0-N)}{2!} + y^4 \frac{2^2(0-N)(2-N)}{4!} \\ \qquad + y^6 \frac{2^3(0-N)(2-N)(4-N)}{6!} + \ldots + y^N \, term \end{array} \right\} \tag{3.206}$$

N **odd**:

$$F_N(y) = A_1^{(N)} \left\{ \begin{array}{l} y + y^3 \frac{2(1-N)}{3!} + y^5 \frac{2^2(1-N)(3-N)}{5!} \\ \qquad + y^7 \frac{2^3(1-N)(3-N)(5-N)}{7!} + \ldots + y^N \, term \end{array} \right\} \tag{3.207}$$

The energy eigenfunctions are

$$\phi_N(x) = e^{-\frac{1}{2}y^2} F_N(y) \tag{3.208}$$

where

$$y = \sqrt{\frac{m\omega}{\hbar}} x \tag{3.209}$$

Then

$$H\phi_N = E_N \phi_N \text{ with } E_N = \hbar\omega(N + 1/2) \quad , \quad N = 0, 1, 2, 3, ... \tag{3.210}$$

Notes

1. The energy spectrum is entirely discrete and there is no degeneracy.

2. $F_N(y)$ is a polynomial in y of degree N. N even means only even powers of y occur and N odd means only odd powers of y occur.

3. $F_N(y)$ obeys the differential equation

$$\frac{d^2F_N}{dy^2} - 2y\frac{dF_N}{dy} + 2NF_N = 0$$

which is Hermite's differential equation.

4. $F_N(y) = H_N(y)$ = Hermite polynomial of order N, when the arbitrary constants A_0 and A_1 are chosen such that the coefficient of y^N is 2^N.

   Examples

   $H_0(y) = A_0^{(N=0)}\{1\}$: y^0 coefficient is $2^0 = 1$ so that $A_0^{(N=0)} = 1$ and thus $H_0(y) = 1$.

   $H_1(y) = A_1^{(N=1)}\{y\}$: y^1 coefficient is $2^1 = 2$ so that $A_1^{(N=1)} = 2$ and thus $H_1(y) = 2y$.

   $H_2(y) = A_0^(N=2)\left\{1 + y^2\frac{2(-2)}{2!}\right\} = A_0^{(N=2)}\left\{1 - 2y^2\right\}$: y^2 coefficient is $2^2 = 4$ so that $A_0^{(N=2)} = -2$ and thus $H_2(y) = 4y^2 - 2$.

   Note that the Hermite polynomials are real functions of y.

5. The normalized eigenfunctions of H are

$$u_N(x) = C_N H_N(y) e^{-\frac{1}{2}y^2} \tag{3.211}$$

   where $|C_N|$ is determined from $\langle u_N \,|\, u_N\rangle = 1$. We have

$$1 = \langle u_N \mid u_N\rangle = \int_{-\infty}^{\infty} dx u_N^*(x) u_N(x) = |C_N|^2 \int_{-\infty}^{\infty} dx \left[H_N(y)\right]^2 e^{-y^2}$$

$$y = \sqrt{\frac{m\omega}{\hbar}}x \Rightarrow dy = \sqrt{\frac{m\omega}{\hbar}}dx \Rightarrow 1 = |C_N|^2\sqrt{\frac{\hbar}{m\omega}}\int_{-\infty}^{\infty} dy \left[H_N(y)\right]^2 e^{-y^2}$$

6. $\{u_N(x)\}_{N=0,1,2,\ldots}$ is a CON set with $\langle u_{N'} \,|\, u_N\rangle = \delta'_N{}^N$

$$\delta_{N'N} = \langle u_{N'} \mid u_N\rangle = \int_{-\infty}^{\infty} dx C_{N'}^* H_{N'}(y) e^{-\frac{1}{2}y^2} C_N H_N(y) e^{-\frac{1}{2}y^2}$$

$$= \sqrt{\frac{\hbar}{m\omega}} C_{N'}^* C_N \int_{-\infty}^{\infty} dy H_{N'}(y) H_N(y) e^{-y^2}$$

   In particular,

$$\int_{-\infty}^{\infty} dy H_{N'}(y) H_N(y) e^{-y^2} = 0 \tag{3.212}$$

   for $N' \neq N$. Thus, the Hermite polynomials are orthogonal with respect to the *weighting factor* e^{-y^2}.

7. $E_N = \hbar\omega(N + 1/2)$

(a) $E_0 = \hbar\omega/2$ = *ground state energy.* Classically, the oscillator could stay at $x = 0$ with zero velocity, which would be the minimum energy state (energy = 0). Quantum mechanically, the uncertainty principle implies that the oscillator cannot be precisely at $x = 0$ with p_x *precisely* zero. Thus, the minimum energy > 0.

(b) $E_{N+1} - E_N = \hbar\omega$ independent of N. The energy levels are *evenly spaced.*

8. **Ground State ($N = 0$):**

$$u_0(x) = C_0 H_0(y) e^{-\frac{1}{2}y^2} = C_0 e^{-\frac{1}{2}y^2} \quad , \quad y = \sqrt{\frac{m\omega}{\hbar}}x \tag{3.213}$$

C_0 is found as in note (5):

$$\begin{aligned} 1 &= |C_0|^2 \sqrt{\frac{\hbar}{m\omega}} \int_{-\infty}^{\infty} dy \left[H_0(y)\right]^2 e^{-y^2} \\ &= |C_0|^2 \sqrt{\frac{\hbar}{m\omega}} \int_{-\infty}^{\infty} dy e^{-y^2} = |C_0|^2 \sqrt{\frac{\hbar}{m\omega}}\sqrt{\pi} \\ &\Rightarrow |C_0|^2 = \sqrt{\frac{m\omega}{\pi\hbar}} \end{aligned} \tag{3.214}$$

Choosing C_0 to be a positive real number, we have

$$u_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} \tag{3.215}$$

Let $\psi(x,0) = u_0(x) \Rightarrow \psi(x,t) = u_0(x)e^{-i\frac{E_0 t}{\hbar}} = u_0(x)e^{-i\frac{\omega t}{2}}$ for a particle in the ground state for all t. Therefore,

$$\wp(x,t) = \frac{|\psi(x,t)|^2}{\langle\psi(t) \mid \psi(t)\rangle} = |u_0(x)|^2 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\frac{m\omega}{\hbar}x^2} \tag{3.216}$$

This is independent of time, as expected for a stationary state. Classically, x_{max} occurs when $p_x = 0$ (a turning point). Therefore,

$$E = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2 = \frac{1}{2}m\omega^2 x_{\max}^2 \Rightarrow x_{\max}^2 = \frac{2E}{m\omega^2} \tag{3.217}$$

For $E = E_0 = \hbar\omega/2$ we have $x_{\max}^2 = \hbar/m\omega$. Therefore,

$$\wp(x,t) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\left(\frac{x}{x_{\max}}\right)^2} \tag{3.218}$$

for the ground state as shown in Figure 3.4 below.

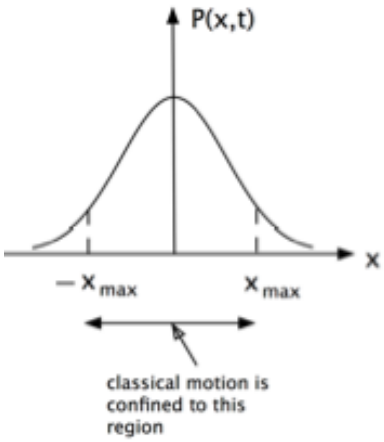


Figure 3.4: Probability Function

Now the classical motion is confined to the region $x \in [-x_{\max}, +x_{\max}]$. Notice that there is a non-zero probability to find the particle outside the classically allowed region! This may seem strange because $x > x_{\max} \Rightarrow V(x) > E_{N=0} \Rightarrow KE < 0$!

However, if a measurement tells us that the particle is *not* in the classical region (shine light over the classical region and look for the particle), then the wave function will collapse to the wave function shown in Figure 3.5 below (measurement is made at t_0).

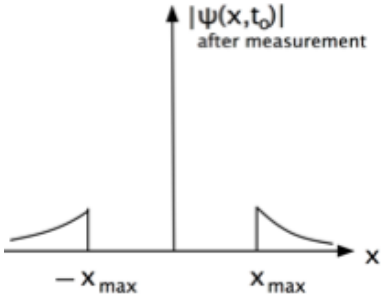


Figure 3.5: Wave Function After Measurement

This is no longer an eigenfunction of energy. Therefore, if the particle is known to be somewhere outside the classical region, the particle does not have a definite energy ($\Delta E \neq 0$) and the statement $V(x) > E_{N=0}$ is no longer applicable.

9. Let $\psi(x, 0)$ be arbitrarily given. It need not be an energy eigenfunction

of H. What is $\psi(x,t)$ for a harmonic oscillator?

$$\begin{aligned}\psi(x,t) &= \sum_{N=0}^{\infty} C_N(0) e^{-i\frac{E_N t}{\hbar}} u_N(x) \\ &= e^{-i\frac{\omega t}{2}} \sum_{N=0}^{\infty} C_N(0) e^{-iN\omega t} u_N(x)\end{aligned} \tag{3.219}$$

where $E_N = \hbar\omega(N + 1/2)$ and the $C_N(0)$ are determined from

$$\begin{aligned}\psi(x,0) &= \sum_{N=0}^{\infty} C_N(0) u_N(x) \Rightarrow C_N(0) \\ &= \langle u_N \mid \psi(t=0)\rangle = \int_{-\infty}^{\infty} dx u_N^*(x)\psi(x,0)\end{aligned} \tag{3.220}$$

3.6.2. Algebraic Method

Given

$$H = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2 \tag{3.221}$$

where x and p_x are hermitian operators satisfying $[x, p_x] = i\hbar$. We will now solve the energy eigenvalue problem $H\phi_E = E\phi_E$ by using only

(1) the hermiticity of x and p_x

and

(2) the above commutation relation

We will not need the explicit representation

$$p_x = \frac{\hbar}{i}\frac{\partial}{\partial x} \tag{3.222}$$

required by working in the $x - p$ representations.

Because H is a sum of a p_x^2 and an x^2 term, we will try to write H as the product of two factors, each of which is linear in x and p_x. We have

$$\begin{aligned}\left(\sqrt{\frac{m\omega^2}{2}}x - i\sqrt{\frac{1}{2m}}p_x\right)\left(\sqrt{\frac{m\omega^2}{2}}x + i\sqrt{\frac{1}{2m}}p_x\right) &= \frac{m\omega^2}{2}x^2 + \frac{1}{2m}p_x^2 + i\frac{\omega}{2}xp_x - i\frac{\omega}{2}p_x x \\ &= H + i\frac{\omega}{2}[x, p_x] = H - \frac{\hbar\omega}{2}\end{aligned} \tag{3.223}$$

where we must be careful to preserve the ordering of the non-commuting operators x and p_x. Therefore

$$\begin{aligned} H &= \left(\sqrt{\frac{m\omega^2}{2}}x - i\sqrt{\frac{1}{2m}}p_x\right)\left(\sqrt{\frac{m\omega^2}{2}}x + i\sqrt{\frac{1}{2m}}p_x\right) + \frac{\hbar\omega}{2} \\ &= \hbar\omega\left[\left(\sqrt{\frac{m\omega}{2\hbar}}x - i\sqrt{\frac{1}{2m\hbar\omega}}p_x\right)\left(\sqrt{\frac{m\omega}{2\hbar}}x + i\sqrt{\frac{1}{2m\hbar\omega}}p_x\right) + \frac{1}{2}\right] \end{aligned} \tag{3.224}$$

We now define a new operator

$$a = \sqrt{\frac{m\omega}{2\hbar}}x + i\sqrt{\frac{1}{2m\hbar\omega}}p_x \tag{3.225}$$

Because x and p_x are are hermitian, we have

$$a^+ = \sqrt{\frac{m\omega}{2\hbar}}x - i\sqrt{\frac{1}{2m\hbar\omega}}p_x \tag{3.226}$$

The Hamiltonian then becomes the *simple* expression

$$H = \hbar\omega(a^+a + 1/2) \tag{3.227}$$

The following commutators will be important in our discussion:

$$\begin{aligned} [a, a^+] &= \left[\sqrt{\frac{m\omega}{2\hbar}}x + i\sqrt{\frac{1}{2m\hbar\omega}}p_x, \sqrt{\frac{m\omega}{2\hbar}}x - i\sqrt{\frac{1}{2m\hbar\omega}}p_x\right] \\ &= \frac{i}{2\hbar}[p_x, x] - \frac{i}{2\hbar}[x, p_x] = \frac{i}{2\hbar}(-i\hbar) - \frac{i}{2\hbar}(i\hbar) = 1 \end{aligned} \tag{3.228}$$

or $[a, a^+] = 1$.

$$\begin{aligned} [a, H] &= [a, \hbar\omega(a^+a + 1/2)] = \hbar\omega\,[a, a^+a] \\ &= \hbar\omega\,(aa^+a - a^+aa) = \hbar\omega\,((a^+a + 1)a - a^+aa) = \hbar\omega\,a \end{aligned} \tag{3.229}$$

or $[a, H] = \hbar\omega\,a$.

$$\begin{aligned} [a^+, H] &= [a^+, \hbar\omega(a^+a + 1/2)] = \hbar\omega\,[a^+, a^+a] \\ &= \hbar\omega\,(a^+a^+a - a^+aa^+) = \hbar\omega\,(a^+a^+a - a^+(a^+a + 1)) = -\hbar\omega\,a^+ \end{aligned} \tag{3.230}$$

or $[a^+, H] = -\hbar\omega\,a^+$.

These commutation relations imply the following:

1. $E \geq \hbar\omega/2$ with equality if $a\phi_E = 0$

   Proof: we have

$$\begin{aligned} 0 \leq \langle a\phi_E \mid a\phi_E\rangle = \langle \phi_E \mid a^+a\phi_E\rangle &= \left\langle \phi_E \,\middle|\, \left(\frac{H}{\hbar\omega} - \frac{1}{2}\right)\phi_E \right\rangle \\ &= \left(\frac{E}{\hbar\omega} - \frac{1}{2}\right)\langle \phi_E \mid \phi_E\rangle \end{aligned} \tag{3.231}$$

But $\langle \phi_E \mid \phi_E \rangle > 0$ (ϕ_E not identically zero). Therefore,

$$\left(\frac{E}{\hbar\omega} - \frac{1}{2}\right) \geq 0 \Rightarrow E \geq \frac{\hbar\omega}{2} \text{ with equality if } a\phi_E = 0 \tag{3.232}$$

2. $a^+\phi_E \neq 0$ for any E

   Proof: we have

$$\begin{aligned}\langle a^+\phi_E \mid a^+\phi_E \rangle &= \langle \phi_E \mid aa^+\phi_E \rangle = \langle \phi_E \mid (1 + a^+a)\phi_E \rangle \\ &= \left\langle \phi_E \,\middle|\, \left(\frac{H}{\hbar\omega} + \frac{1}{2}\right)\phi_E \right\rangle = \left(\frac{E}{\hbar\omega} + \frac{1}{2}\right)\langle \phi_E \mid \phi_E \rangle \end{aligned} \tag{3.233}$$

   Now

$$\begin{aligned}&\left(\frac{E}{\hbar\omega} + \frac{1}{2}\right) \geq 1 \quad , \quad \langle \phi_E \mid \phi_E \rangle > 0 \\ &\Rightarrow \langle a^+\phi_E \mid a^+\phi_E \rangle \neq 0, \text{thatis} a^+\phi_E \neq 0\end{aligned}$$

3. $a^+\phi_E$ is an energy eigenfunction ($a^+\phi_E \neq 0$) of H with eigenvalue $E + \hbar\omega$

   Proof: we have

$$\begin{aligned}H(a^+\phi_E) &= \left([H, a^+] + a^+H\right)\phi_E \\ &= \left(\hbar\omega a^+ + a^+E\right)\phi_E = (E + \hbar\omega)(a^+\phi_E)\end{aligned}$$

4. $a\phi_E = 0$ or $a\phi_E$ is an energy eigenfunction ($a\phi_E \neq 0$) of H with eigenvalue $E - \hbar\omega$

   Proof: we have

$$\begin{aligned}H(a\phi_E) &= \left([H, a] + aH\right)\phi_E \\ &= \left(-\hbar\omega a + aE\right)\phi_E = (E - \hbar\omega)(a^+\phi_E)\end{aligned} \tag{3.234}$$

   If $a\phi_E \neq 0$, then this equation implies that $a\phi_E$ is an energy eigenfunction of H.

Note: Because a^+ increases the eigenvalue E by an increment $\hbar\omega$ (it *creates* added energy $\hbar\omega$), a^+ is called a *raising operator* or a *creation operator*. Because a decreases the eigenvalue E by an increment $\hbar\omega$ (it *annihilates* added energy $\hbar\omega$), a is called a *lowering operator* or a *annihilation operator*.

Given a specific ϕ_E, we can form the sequences:

$$\underbrace{\phi_E}_{E}\ ,\ \underbrace{a\phi_E}_{E-\hbar\omega}\ ,\ \underbrace{a^2\phi_E}_{E-3\hbar\omega}\ ,\ \underbrace{a^3\phi_E}_{E-5\hbar\omega}\ ,\ \text{.....}$$

$$\underbrace{\phi_E}_{E}\ ,\ \underbrace{a^+\phi_E}_{E+\hbar\omega}\ ,\ \underbrace{(a^+)^2\phi_E}_{E+3\hbar\omega}\ ,\ \underbrace{(a^+)^3\phi_E}_{E+5\hbar\omega}\ ,\ \text{.....}$$

But the energy eigenvalues must be $\geq \hbar\omega/2$. Therefore, the first of the above sequences $(E, E-\hbar\omega, E-2\hbar\omega, E-3\hbar\omega, ...)$ must terminate (otherwise, we would eventually obtain eigenvalues less than $\hbar\omega/2$. This termination occurs if there exists an n $(0, 1, 2, ...)$ such that $a^n\phi_E$ is an energy eigenfunction (and therefore non-zero) with eigenvalue $E - n\hbar\omega$ and

$$a^{n+1}\phi_E = 0\ ,\ a^{n+2}\phi_E = 0\ ,\ a^{n+3}\phi_E = 0\ ,\ .... \tag{3.235}$$

Result (1) above then implies that

$$E - n\hbar\omega = \frac{\hbar\omega}{2} \Rightarrow E = \hbar\omega(n + 1/2) \tag{3.236}$$

This shows that if one is given an eigenvalue E, then it can be written $E = \hbar\omega(n + 1/2)$ for some non-negative integer n. It remains to be shown that $\hbar\omega(N + 1/2)$ for any $N = 0, 1, 2, ...$ is an eigenvalue. But this is easy since from above we have

$$E = \hbar\omega(n + 1/2) \tag{3.237}$$

for some non-negative integer n. Forming the two sequences above, we find that

$$\hbar\omega(n - 1/2), \hbar\omega(n - 3/2), ..., \frac{\hbar\omega}{2} \tag{3.238}$$

and

$$\hbar\omega(n + 3/2), \hbar\omega(n + 5/2), \hbar\omega(n + 7/2), ... \tag{3.239}$$

are also allowed energy eigenvalues. Thus,

$$E_N = \hbar\omega(N + 1/2) \text{with} N = 0, 1, 2, ... \tag{3.240}$$

yields the entire spectrum of H. The spectrum has now been obtained without using the explicit representation

$$p_x = \frac{\hbar}{i}\frac{\partial}{\partial x} \tag{3.241}$$

Let $\phi_E(x) = u_N(x)$ with $\langle u_{N'} \mid u_N \rangle = \delta_{N'N}$.

Claim: All the energy eigenvalues are non-degenerate if the $N = 0$ eigenvalue $(E_0 = \hbar\omega/2)$ is non-degenerate.

Proof: It is sufficient to show the following: If E_N for some $N > 0$ is degenerate, then E_{N-1} is also degenerate, that is, E_{N-1} non-degenerate implies that E_N is non-degenerate.

If E_N is degenerate, one can find at least two orthogonal eigenfunctions $(u_N^{(1)}\ and\ u_N^{(2)})$ with eigenvalue E_N and $\left\langle u_N^{(1)} \,\middle|\, u_N^{(2)} \right\rangle = 0$. However,

$$\left\langle u_N^{(1)} \,\middle|\, a^+ a u_N^{(2)} \right\rangle = \left\langle u_N^{(1)} \,\middle|\, \left(\frac{H}{\hbar\omega} - \frac{1}{2}\right) u_N^{(2)} \right\rangle = \left(\frac{E_N}{\hbar\omega} - \frac{1}{2}\right) \underbrace{\left\langle u_N^{(1)} \,\middle|\, u_N^{(2)} \right\rangle}_{=0} = 0$$

Therefore $0 = \left\langle u_N^{(1)} \,\middle|\, a^+ a u_N^{(2)} \right\rangle = \left\langle a u_N^{(1)} \,\middle|\, a u_N^{(2)} \right\rangle$. But $N > 0$ implies that $E_N > \hbar\omega/2$ which implies $a u_N^{(1)} \neq 0$ and $a u_N^{(2)} \neq 0$. Therefore, $a u_N^{(1)}$ and $a u_N^{(2)}$ are orthogonal eigenfunctions (not identically zero) corresponding to the eigenvalue E_{N-1}, which is therefore degenerate.

Let us show by explicit construction that $E_{N=0} = \hbar\omega/2$ is non-degenerate. We can then conclude that the entire spectrum of H is *non-degenerate*.

Ground State: $N = 0$, $E_0 = \hbar\omega/2$. We have

$$E_0 = \frac{\hbar\omega}{2} \Leftrightarrow a u_0 = 0 \tag{3.242}$$

which gives all eigenfunctions for $N = 0$. Now

$$a = \sqrt{\frac{m\omega}{2\hbar}} x + \frac{i}{\sqrt{2m\hbar\omega}} p_x = \sqrt{\frac{\hbar}{2m\omega}} \left(\frac{d}{dx} + \frac{m\omega}{\hbar} x \right) \tag{3.243}$$

using

$$p_x = \frac{\hbar}{i} \frac{d}{dx} \tag{3.244}$$

Therefore,

$$\sqrt{\frac{\hbar}{2m\omega}} \left(\frac{d}{dx} + \frac{m\omega}{\hbar} x \right) u_0 = 0 \Rightarrow \left(\frac{d}{dx} + \frac{m\omega}{\hbar} x \right) u_0 = 0 \tag{3.245}$$

so that

$$u_0(x) = C_0 e^{-\frac{m\omega}{2\hbar} x^2} \text{ where } C_0 = \text{ any constant} \tag{3.246}$$

All eigenfunctions for $N = 0$ have this form. Thus, the $N = 0$ level is non-degenerate. This implies that the entire spectrum of H is non-degenerate. Now from an earlier result

$$\langle u_0 \mid u_0 \rangle = 1 \Rightarrow |C_0| = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \tag{3.247}$$

Choosing C_0 to be positive real we have

$$u_0(x) = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-\frac{m\omega}{2\hbar} x^2} \tag{3.248}$$

One can easily obtain any energy state (u_N for $N > 0$) by applying the raising operator a^+ a sufficient number of times to the ground state.

Note: $a^+ u_N$ has energy $E_N + \hbar\omega = E_{N+1}$ where u_N has energy $E_N = \hbar\omega(N + 1/2)$. But E_{N+1} is non-degenerate. Therefore, $a^+ u_N = A_N u_{N+1}$ where A_N is

some constant. $|A_N|$ can be determined from the fact that u_N and u_{N+1} are normalized.

$$\langle a^+ u_N \mid a^+ u_N \rangle = |A_N|^2 \underbrace{\langle u_{N+1} \mid u_{N+1} \rangle}_{=1} = |A_N|^2 \tag{3.249}$$

$$\begin{aligned} \langle u_N \mid a a^+ u_N \rangle &= \langle u_N \mid ([a, a^+] + a^+ a)\, u_N \rangle \\ &= \left\langle u_N \,\middle|\, \left(\frac{H}{\hbar\omega} + \frac{1}{2}\right) u_N \right\rangle \\ &= (N+1) \underbrace{\langle u_N \mid u_N \rangle}_{=1} = |A_N|^2 \end{aligned} \tag{3.250}$$

so that

$$|A_N| = \sqrt{N+1} \Rightarrow a^+ u_N = \sqrt{N+1} u_{N+1} \tag{3.251}$$

which specifies u_{N+1} in terms of u_N. Therefore,

$$a a^+ u_N = \sqrt{N+1} a u_{N+1} \tag{3.252}$$

and

$$\begin{aligned} ([a, a^+] + a^+ a)\, u_N &= \left(\frac{H}{\hbar\omega} + \frac{1}{2}\right) u_N = \left(\frac{E_N}{\hbar\omega} + \frac{1}{2}\right) \\ &= (N+1) u_N = \sqrt{N+1} a u_{N+1} \end{aligned} \tag{3.253}$$

so that

$$a u_{N+1} = \sqrt{N+1} u_N \Rightarrow a u_N = \sqrt{N} u_{N-1} \tag{3.254}$$

and, in particular, $a u_0 = 0$.

Note that $a^+ a u_N = \sqrt{N} a^+ u_{N-1} = \sqrt{N}\sqrt{N} u_N = N u_N$ so that u_N is also an eigenfunction of $a^+ a$ (which only differs from H by an additive constant).

We can now find $u_N(x)$ in terms of the ground state $u_0(x)$. We use

$$a^+ u_N = \sqrt{N+1} u_{N+1} \Rightarrow a^+ u_{N-1} = \sqrt{N} u_N \tag{3.255}$$

Thus,

$$\begin{aligned} u_N &= \frac{1}{\sqrt{N}} a^+ u_{N-1} = \frac{1}{\sqrt{N}} a^+ \left(\frac{1}{\sqrt{N-1}} a^+ u_{N-2}\right) \\ &= \frac{1}{\sqrt{N}} a^+ \left(\frac{1}{\sqrt{N-1}} a^+ \left(\frac{1}{\sqrt{N-2}} a^+ u_{N-3}\right)\right) = \ldots\ldots \end{aligned}$$

or

$$u_N = \frac{1}{\sqrt{N!}} (a^+)^N u_0 \tag{3.256}$$

Now

$$a^+ = \sqrt{\frac{m\omega}{2\hbar}} x - \frac{i}{\sqrt{2m\hbar\omega}} p_x$$

so that

$$u_N = \frac{1}{\sqrt{N!}}\left(\sqrt{\frac{m\omega}{2\hbar}}x - \frac{i}{\sqrt{2m\hbar\omega}}p_x\right)^N u_0$$
$$= \frac{1}{\sqrt{N!}}\left(\sqrt{\frac{m\omega}{2\hbar}}x - \sqrt{\frac{\hbar}{2m\omega}}\frac{d}{dx}\right)^N \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$

Now, as earlier, let

$$y = \sqrt{\frac{m\omega}{\hbar}}x \tag{3.257}$$

(a dimensionless variable). Therefore,

$$u_N(x) = \frac{1}{\sqrt{N!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{2^{N/2}}\left(y - \frac{d}{dy}\right)^N e^{-\frac{1}{2}y^2} \tag{3.258}$$

which is an explicit formula for u_N.

Note:

$$\left(y - \frac{d}{dy}\right)^N e^{-\frac{1}{2}y^2} = \underbrace{\left(y - \frac{d}{dy}\right)\left(y - \frac{d}{dy}\right).....\left(y - \frac{d}{dy}\right)}_{\substack{N \text{ factors - each } \frac{d}{dy} \text{ acts on everything which} \\ \text{appears to the right o it}}} e^{-\frac{1}{2}y^2}$$
$$= e^{-\frac{1}{2}y^2}\,(\text{polynomial of degree } N) \tag{3.259}$$

The coefficient of y^N in this polynomial is 2^N.

Proof: To obtain y^N a factor of y must come from *each* $(y - d/dy)$ term. For each term, the y can come from *one* of two places (from y or from $-d(e^{-\frac{1}{2}y^2})/dy$. There are therefore, 2^N possible ways to obtain y^N.

We can use this result for $u_N(x)$ to obtain an explicit expression for the Hermite polynomials $H_N(y)$. From the differential equation method we found that

$$u_N(x) = C_N H_N(y) e^{-\frac{1}{2}y^2} \tag{3.260}$$

Comparing our two expressions for $u_N(x)$

$$C_N H_N(y) e^{-\frac{1}{2}y^2} = \frac{1}{\sqrt{N!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{2^{N/2}}\left(y - \frac{d}{dy}\right)^N e^{-\frac{1}{2}y^2} \tag{3.261}$$

We can avoid doing the integral $\langle u_N \mid u_N\rangle = 1$ to evaluate C_N by recalling that $H_N(y)$ = polynomial of degree N with 2^N as the coefficient of y^N. But

$$\left(y - \frac{d}{dy}\right)^N e^{-\frac{1}{2}y^2} = e^{-\frac{1}{2}y^2} \tag{3.262}$$

(polynomial of degree N with 2^N as the coefficient of y^N). Therefore,

$$H_N(y) = e^{+\frac{1}{2}y^2}\left(y - \frac{d}{dy}\right)^N e^{-\frac{1}{2}y^2} \tag{3.263}$$

and

$$u_N(x) = \frac{1}{\sqrt{N!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{2^{N/2}}H_N(y)e^{-\frac{1}{2}y^2} \tag{3.264}$$

Comment on Parity: $u_N(x)$ is an even function of x for N even and an odd function of x for N odd (because $H_N(y)$ has this property). Thus, the eigenfunctions of H are either even or odd functions. We could have anticipated this result from the following discussion.

The parity operator Π is defined by its action on the wave function:

$$\Pi\psi(\vec{x},t) = \psi(-\vec{x},t) \tag{3.265}$$

The parity operator Π is linear and hermitian. Since

$$\Pi^2\psi(\vec{x},t) = \Pi\psi(-\vec{x},t) = \psi(\vec{x},t) \tag{3.266}$$

we have

$$\Pi^2 = I \tag{3.267}$$

and since its eigenvalue equation

$$\Pi\psi = \lambda\psi \tag{3.268}$$

implies

$$\Pi^2\psi = \lambda\Pi\psi = \lambda^2\psi = I\psi = \psi \Rightarrow \lambda^2 = 1 \rightarrow \lambda = \pm 1$$

or the eigenvalues of Π are ± 1. We then have

$$\Pi\psi_{even}(\vec{x},t) = \psi_{even}(-\vec{x},t) = \psi_{even}(\vec{x},t) \tag{3.269}$$

$$\Pi\psi_{odd}(\vec{x},t) = \psi_{odd}(-\vec{x},t) = -\psi_{odd}(\vec{x},t) \tag{3.270}$$

so that any even function of $\vec{x}$ is an eigenfunction of Π with eigenvalue +1 and any odd function of $\vec{x}$ is an eigenfunction of Π with eigenvalue −1.

Let us apply this result to the one-dimensional harmonic oscillator:

$$\begin{aligned}\Pi H\psi(x,t) &= \Pi\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2\right]\psi(x,t)\\ &= \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2\right]\psi(-x,t)\\ &= H\Pi\psi(x,t)\end{aligned}$$

so that (since $\psi(x,t)$ is arbitrary)

$$\Pi H = H\Pi \Rightarrow [\Pi, H] = 0 \tag{3.271}$$

Therefore, we can find a CON set of simultaneous eigenfunctions of H and Π. But the eigenfunctions of H are non-degenerate, and therefore, each $u_N(x)$ is an eigenfunction of Π also. This means that each $u_N(x)$ obeys $\Pi u_N(x) = \pm u_N(x)$ or that each $u_N(x)$ is either an even function of x or an odd function of x.

3.6.3. Use of Raising and Lowering Operators

One can compute inner products of the form $\langle u_{N'} \mid A(x,p_x)u_N\rangle$ *without* doing any cumbersome integrals. Now

$$a = \sqrt{\frac{m\omega}{2\hbar}}x + \frac{i}{\sqrt{2m\hbar\omega}}p_x \text{ and } a^+ = \sqrt{\frac{m\omega}{2\hbar}}x - \frac{i}{\sqrt{2m\hbar\omega}}p_x$$

imply that

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^+) \text{ and } p_x = \frac{1}{i}\sqrt{\frac{m\hbar\omega}{2}}(a - a^+) \tag{3.272}$$

Thus, $A(x,p_x)$ can be expressed in terms of the raising and lowering operators, where

$$au_N = \sqrt{N}u_{N-1} \text{ and } a^+u_N = \sqrt{N+1}u_{N+1} \tag{3.273}$$

Example: Consider the stationary state

$$\psi(x,t) = u_N(x)e^{-i\frac{E_N t}{\hbar}} \tag{3.274}$$

We have

$$\langle\psi(t) \mid \psi(t)\rangle = 1 \tag{3.275}$$

and

$$\begin{aligned}\langle x\rangle = \langle\psi(t) \mid x\psi(t)\rangle &= \left\langle u_N e^{-i\frac{E_N t}{\hbar}} \,\middle|\, xu_N e^{-i\frac{E_N t}{\hbar}}\right\rangle = \langle u_N \mid xu_N\rangle \\ &= \sqrt{\frac{\hbar}{2m\omega}}\,\langle u_N \mid (a+a^+)u_N\rangle = \sqrt{\frac{\hbar}{2m\omega}}\,(\langle u_N \mid au_N\rangle + \langle u_N \mid a^+u_N\rangle) \\ &= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{N}\underbrace{\langle u_N \mid u_{N-1}\rangle}_{=0} + \sqrt{N+1}\underbrace{\langle u_N \mid u_{N+1}\rangle}_{=0}\right) = 0\end{aligned}$$

so that $\langle x \rangle = 0$ for the given stationary state. Now

$$\begin{aligned}
\langle x^2 \rangle &= \left\langle \psi(t) \,\middle|\, x^2 \psi(t) \right\rangle = \left\langle u_N e^{-i\frac{E_N t}{\hbar}} \,\middle|\, x^2 u_N e^{-i\frac{E_N t}{\hbar}} \right\rangle = \langle u_N \,|\, x^2 u_N \rangle \\
&= \frac{\hbar}{2m\omega} \left\langle u_N \,\middle|\, (a+a^+)^2 u_N \right\rangle = \frac{\hbar}{2m\omega} \langle u_N \,|\, (aa + aa^+ + a^+a + a^+a^+) u_N \rangle \\
&= \frac{\hbar}{2m\omega} \left[\begin{array}{l} \left(\sqrt{N}\sqrt{N-1}\right) \underbrace{\langle u_N \,|\, u_{N-2} \rangle}_{=0} + \left(\sqrt{N+1}\sqrt{N+1}\right) \underbrace{\langle u_N \,|\, u_N \rangle}_{=1} \\ \quad + \left(\sqrt{N}\sqrt{N}\right) \underbrace{\langle u_N \,|\, u_N \rangle}_{=1} + \left(\sqrt{N+1}\sqrt{N+2}\right) \underbrace{\langle u_N \,|\, u_{N+2} \rangle}_{=0} \end{array} \right] \\
&= \frac{\hbar}{m\omega} \left(N + \frac{1}{2} \right) = \frac{E_N}{m\omega^2}
\end{aligned} \tag{3.276}$$

Therefore,

$$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2 = \frac{E_N}{m\omega^2} \Rightarrow \Delta x = \sqrt{\frac{E_N}{m\omega^2}} \tag{3.277}$$

It is quite reasonable for Δx to increase with E_N. Classically,

$$E = \frac{1}{2} m\omega^2 x_{\max}^2 \tag{3.278}$$

Therefore,

$$x_{\max} = \sqrt{\frac{2E}{m\omega^2}} \tag{3.279}$$

which increases with E. Quantum mechanically, one has $\langle x \rangle = 0$ with a spread in positions of the order of x_{max}.

Example: Consider the non-stationary state

$$\psi(x,0) = \frac{1}{\sqrt{3}} u_0(x) + \sqrt{\frac{2}{3}} u_1(x) \tag{3.280}$$

We use $H u_N = E_N u_N$, $E_N = \hbar\omega(N + 1/2)$, $\langle u_{N'} \,|\, u_N \rangle = \delta_{N'N}$. These two wave functions are shown in Figure 3.6 below.

$$u_0(x) \propto e^{-\frac{m\omega}{2\hbar}x^2} \qquad\qquad u_1(x) \propto x e^{-\frac{m\omega}{2\hbar}x^2} \tag{3.281}$$

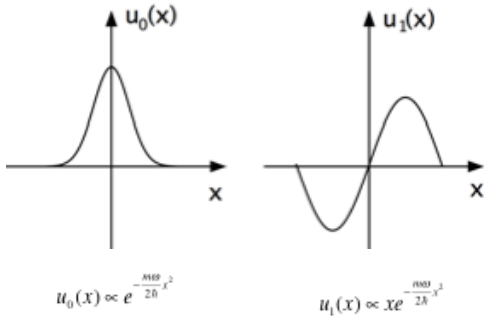


Figure 3.6: Two wave functions making up the state

Therefore,

$$\psi(x,t) = \frac{1}{\sqrt{3}}u_0(x)e^{-i\frac{\omega t}{2}} + \sqrt{\frac{2}{3}}u_1(x)e^{-i\frac{3\omega t}{2}} \tag{3.282}$$

so that

$$\begin{aligned}
&\langle\psi(t) \mid \psi(t)\rangle = \frac{1}{3} + \frac{2}{3} = 1 \\
&\wp(E_0 = 3\hbar\omega/2, t) = \frac{2}{3} \quad , \quad \wp(E_{N>1}, t) = 0 \\
&\langle H\rangle = \langle\psi(t) \mid H\psi(t)\rangle = \sum_{N=0}^{\infty} \wp(E_N, t)E_N = \frac{1}{3}\left(\frac{\hbar\omega}{2}\right) + \frac{2}{3}\left(\frac{3\hbar\omega}{2}\right) = \frac{7\hbar\omega}{6}
\end{aligned}$$

and

$$\begin{aligned}
\langle x\rangle &= \left\langle \begin{array}{c} \frac{1}{\sqrt{3}}u_0(x)e^{-i\frac{\omega t}{2}} \\ +\sqrt{\frac{2}{3}}u_1(x)e^{-i\frac{3\omega t}{2}} \end{array} \middle| \, x\left(\begin{array}{c} \frac{1}{\sqrt{3}}u_0(x)e^{-i\frac{\omega t}{2}} \\ +\sqrt{\frac{2}{3}}u_1(x)e^{-i\frac{3\omega t}{2}} \end{array} \right) \right\rangle \\
&= \frac{1}{3}\langle u_0(x) \mid xu_0(x)\rangle + \frac{2}{3}\langle u_0(x) \mid xu_1(x)\rangle \\
&\quad + \frac{\sqrt{2}}{3}e^{i\omega t}\langle u_1(x) \mid xu_0(x)\rangle + \frac{\sqrt{2}}{3}e^{-i\omega t}\langle u_0(x) \mid xu_1(x)\rangle
\end{aligned}$$

We must calculate $\langle u_{N'} \mid xu_N\rangle$.

$$\begin{aligned}
\langle u_{N'} \mid xu_N\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\langle u_{N'} \mid (a + a^+)u_N\rangle \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left(\langle u_{N'} \mid au_N\rangle + \langle u_{N'} \mid a^+u_N\rangle\right) \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{N}\langle u_{N'} \mid u_{N-1}\rangle + \sqrt{N+1}\langle u_{N'} \mid u_{N+1}\rangle\right) \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{N}\delta_{N',N-1} + \sqrt{N+1}\delta_{N',N+1}\right)
\end{aligned} \tag{3.283}$$

This gives

$$\langle x \rangle = 0 + 0 + \sqrt{\frac{\hbar}{2m\omega}} \frac{\sqrt{2}}{3} \left(e^{i\omega t} + e^{-i\omega t} \right) = \frac{2}{3} \sqrt{\frac{\hbar}{m\omega}} \cos \omega t \tag{3.284}$$

We have the probability distribution as shown in Figure 3.7 below.

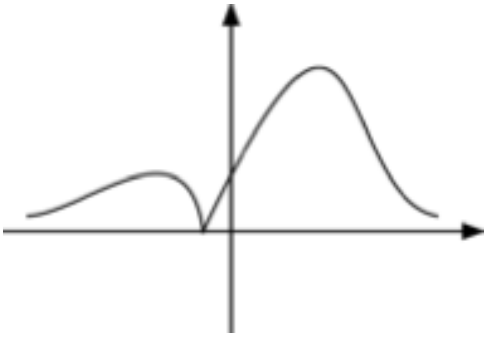


Figure 3.7: Probability distribution

Now an energy measurement is made at $t = 0$ and the value $\hbar\omega/2$ is obtained. The wave function collapses to

$$\psi'(x,0) = \frac{1}{\sqrt{3}} u_0(x) \tag{3.285}$$

and we now have the probability distribution as shown in Figure 3.8 below.

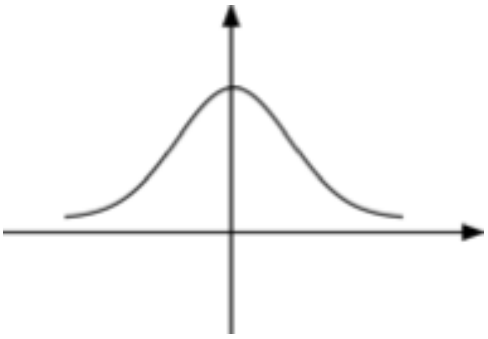


Figure 3.8: Probability distribution

Immediately after the energy measurement, a position measurement indicates

that the particle is not on the negative portion of the $x-$axis at $t = 0$ (for example, one shines light on the region $x < 0$ at $t = 0$ and does not see the particle). The wave function then collapses to $\psi''(x,0)$. To calculate this new wave function, one must expand $\psi'(x,0)$ in terms of position eigenfunctions.

We have $xv_X(x) = Xv_X(x)$, where X = constant eigenvalue of position or

$$(x - X)v_X(x) = 0 \tag{3.286}$$

This implies that $v_X(x) \sim \delta(x - X)$ is the position eigenfunction where

$$\langle v_{X'} \mid v_X \rangle = \int_{-\infty}^{\infty} dx\delta(x - X')\delta(x - X) = \delta(X' - X) \tag{3.287}$$

and

$$\psi'(x,0) = \int_{-\infty}^{\infty} dXC_X v_X(x) \tag{3.288}$$

which is an expansion in terms of CON set $\{v_X(x)\}$ with

$$C_X = \langle v_X \mid \psi'(t = 0) \rangle = \int_{-\infty}^{\infty} dx\delta(x - X)\psi'(x,0) = \psi'(X,0) \tag{3.289}$$

Because the position measurement indicates that the particle is *not* in the $x < 0$ region, the wave function collapses to

$$\psi''(x,0) = \int_{0}^{\infty} dXC_X v_X(x) \tag{3.290}$$

which is the part of the wave function with position eigenfunctions for $X > 0$. Therefore,

$$\psi''(x,0) = \int_{0}^{\infty} dX\psi'(X,0)\delta(x - X) = \begin{cases} 0 & \text{for } x < 0 \\ \psi'(x,0) & \text{for } x > 0 \end{cases} \tag{3.291}$$

where

$$\psi'(x,0) = \frac{1}{\sqrt{3}}u_0(x) \tag{3.292}$$

We get the probability distribution shown in Figure 3.9 below.

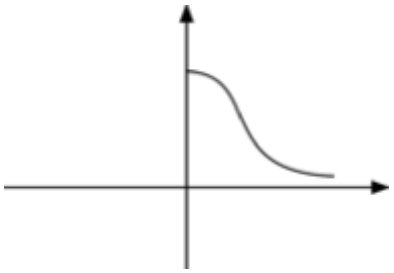


Figure 3.9: After the position measurement

A position measurement just collapses the wave function to zero in those regions where the particle is known not to be!

Note that

$$\begin{aligned}\langle \psi''(t=0) \mid \psi''(t=0) \rangle &= \int_{-\infty}^{\infty} dx \psi''^*(x,0)\psi''(x,0) \\ &= \int_0^{\infty} dx \psi'^*(x,0)\psi'(x,0) = \frac{1}{3}\int_0^{\infty} dx u_0^*(x)u_0(x) \\ &= \frac{1}{3}\left(\frac{1}{2}\int_{-\infty}^{\infty} dx u_0^*(x)u_0(x)\right) = \frac{1}{6}\langle u_0 \mid u_0 \rangle = \frac{1}{6}\end{aligned}$$

$\psi''(x,0)$ is no longer an eigenfunction of energy. The probability of now measuring the energy to be $E_0 = \hbar\omega/2$ is given by

$$\begin{aligned}\wp''(E_0 = \hbar\omega/2, 0) &= \frac{\langle \psi''(t=0) \mid u_0 \rangle \langle u_0 \mid \psi''(t=0) \rangle}{\langle \psi''(t=0) \mid \psi''(t=0) \rangle} = \frac{1}{1/6}\left|\int_{-\infty}^{\infty} dx u_0^*(x)\psi''(x,0)\right|^2 \\ &= 6\left|\int_0^{\infty} dx u_0^*(x)\psi'(x,0)\right|^2 = 6\left|\int_0^{\infty} dx u_0^*(x)\frac{1}{\sqrt{3}}u_0(x)\right|^2 \\ &= 2\left|\frac{1}{2}\int_{-\infty}^{\infty} dx u_0^*(x)u_0(x)\right|^2 = 2\frac{1}{4}(1) = \frac{1}{2}\end{aligned}$$

Suppose that we make no measurements after the wave function has collapsed to $\psi''(x,0)$. The wave function will then develop in time under the action of the harmonic oscillator force. Let us find $\psi''(x,\tau/2)$ where $\tau = 2\pi/omega$ is the

classical period of the oscillator. We have

$$\psi''(x,0) = \sum_{N=0}^{\infty} C_N u_N(x) \tag{3.293}$$

$$\Rightarrow \psi''(x,t) = \sum_{N=0}^{\infty} C_N u_N(x) e^{-i\frac{E_N t}{\hbar}} = e^{-i\frac{\omega t}{2}} \sum_{N=0}^{\infty} C_N u_N(x) e^{-iN\omega t} \tag{3.294}$$

and

$$\begin{aligned} C_N &= \langle u_N \mid \psi''(t=0)\rangle = \int_{-\infty}^{\infty} dx u_N^*(x)\psi''(x,0) \\ &= \int_0^{\infty} dx u_N^*(x)\psi'(x,0) = \frac{1}{\sqrt{3}}\int_0^{\infty} dx u_N^*(x)u_0(x) \end{aligned} \tag{3.295}$$

This is very complicated in general (we cannot use orthogonality since that requires the integration range $[-\infty,+\infty]$. We can do the following however.

For N even we can write

$$C_N = \frac{1}{\sqrt{3}}\int_0^{\infty} dx u_N^*(x)u_0(x) = \frac{1}{\sqrt{3}}\frac{1}{2}\int_{-\infty}^{\infty} dx u_N^*(x)u_0(x) = \frac{1}{2\sqrt{3}}\delta_{N0} \tag{3.296}$$

so that $C_0 = 1/2\sqrt{3}$ and for all other even N the C_N are zero. We will not need an explicit formula for odd N values of C_N.

We then have

$$\psi''(x,t) = e^{-i\frac{\omega t}{2}} \sum_{N=0}^{\infty} C_N u_N(x) e^{-iN\omega t} = e^{-i\frac{\omega t}{2}}\left[C_0 u_0 + \sum_{N=1,3,5,....} C_N u_N(x) e^{-iN\omega t}\right] \tag{3.297}$$

$$\begin{aligned} \psi''(x,\tau/2) &= e^{-i\frac{\pi}{2}}\left[\frac{1}{2\sqrt{3}}u_0 + \sum_{N=1,3,5,....} C_N u_N(x) \underbrace{e^{-iN\pi}}_{=1 \text{for odd} N}\right] \\ &= -i\left[\frac{1}{\sqrt{3}}u_0 - \left(\frac{1}{2\sqrt{3}}u_0 + \sum_{N=1,3,5,....} C_N u_N(x)\right)\right] \\ &= -i\left[\frac{1}{\sqrt{3}}u_0 - \underbrace{\left(C_0 u_0 + \sum_{N=1,3,5,....} C_N u_N(x)\right)}_{\psi''(x,0)}\right] = -i\left[\frac{1}{\sqrt{3}}u_0 - \psi''(x,0)\right] \end{aligned} \tag{3.298}$$

Therefore,

$$\psi''(x,\tau/2) = -i\left[\frac{i}{\sqrt{3}}u_0 - \psi''(x,0)\right] = \begin{cases} \frac{i}{\sqrt{3}}u_0 & \text{for } x < 0 \\ 0 & \text{for } x > 0 \end{cases} \tag{3.299}$$

Therefore at $\tau/2$, the probability distribution has *oscillated* to the $x < 0$ region as shown in Figure 3.10 below.

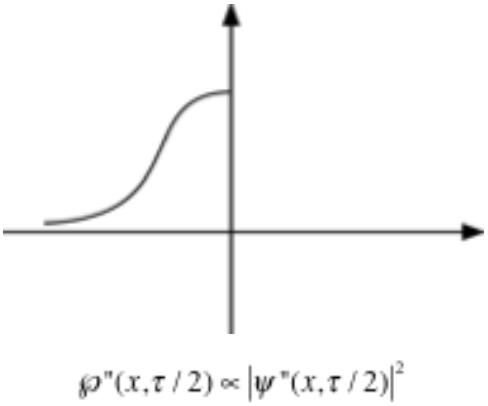


Figure 3.10: After the position measurement

as we might expect for an oscillator!

We now discuss *general potential functions.*

3.7. General Potential Functions

Consider a particle with potential energy $V(\vec{x})$ so that

$$H = \frac{\vec{p}\cdot\vec{p}}{2m} + V(\vec{x}) = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x}) \tag{3.300}$$

The particle is completely described by a wave function $\psi(\vec{x},t)$, where $\langle\psi(t) \mid \psi(t)\rangle$ is finite and non-zero and where the time-development of the wave function between measurements is determined by the time-dependent Schrodinger equation

$$H\psi(\vec{x},t) = i\hbar\frac{\partial\psi(\vec{x},t)}{\partial t} \tag{3.301}$$

To study the behavior of such a particle, one begins by finding the energy eigenfunctions and eigenvalues:

$\left\{u_n^{(\alpha)}(x), u_{c\nu}^{(\alpha)}(x)\right\}$ - CON set of eigenfunctions of H

$Hu_n^{(\alpha)}(x) = E_n u_n^{(\alpha)}(x)$ - discrete part of the spectrum

$Hu_{c\nu}^{(\alpha)}(x) = E_{c\nu}u_{c\nu}^{(\alpha)}(x)$ - continuum part of the spectrum

Knowledge of $\left\{u_n^{(\alpha)}(x), u_{c\nu}^{(\alpha)}(x), E_n, E_{c\nu}\right\}$ not only gives the possible results of an energy measurement but also gives a simple expression for the time-dependence of any wave function for the particle:

$$\psi(\vec{x},t) = \sum_{n\alpha} c_n^{(\alpha)} u_n^{(\alpha)}(x) e^{-i\frac{E_n t}{\hbar}} + \int d\nu \sum_{\beta} d_\nu^{(\beta)} u_{c\nu}^{(\beta)}(x) e^{-i\frac{E_{c\nu} t}{\hbar}} \tag{3.302}$$

where

$$c_n^{(\alpha)} = \left\langle u_n^{(\alpha)} \,\middle|\, \psi(t=0) \right\rangle \text{ and } d_\nu^{(\beta)} = \left\langle u_{c\nu}^{(\beta)}(x) \,\middle|\, \psi(t=0) \right\rangle \tag{3.303}$$

This explicitly gives $\psi(\vec{x},t)$ in terms of $\psi(\vec{x},0)$.

Let us first consider a particle constrained to move along the $x-$axis (one-dimensional problem). We have already discussed the one-dimensional harmonic oscillator. Now, we want to discuss a particle whose potential energy is given by:

$$V(x) = \begin{cases} V_L(constant) & \text{for } x < x_L \\ V_R(constant) & \text{for } x > x_R \\ V(x)(arbitrary) & \text{for } x_L < x < x_R \end{cases} \tag{3.304}$$

as shown in Figure 3.11 below.

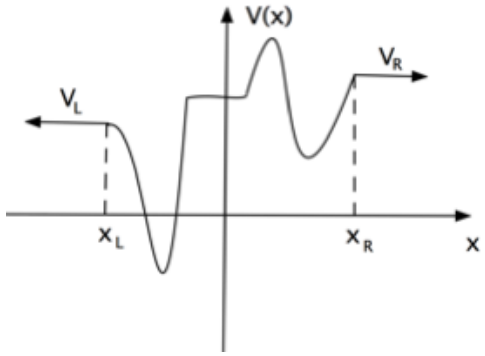


Figure 3.11: General Potential Function

We have the energy eigenfunction/eigenvalue equation:

$$H\phi = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi + V(\vec{x})\phi = E\phi \tag{3.305}$$

$$\Rightarrow \frac{d^2\phi(x)}{dx^2} = \frac{2m}{\hbar^2}\left(V(x) - E\right)\phi(x) \tag{3.306}$$

3.7.1. Method for Solving this Eigenvalue Equation

1. Solve the differential equation with E any arbitrary constant.

2. Determine the allowed values of E by requiring that the solution ϕ does not become infinite as $|x| \to \infty$. This is a necessary condition for ϕ to be an acceptable energy eigenfunction - the inner product of ϕ with almost every square-integrable function must be finite. For some values of E, the solution to the differential equation will become infinite as $|x| \to \infty$. Such a solution is not an acceptable energy eigenfunction and, therefore, the corresponding value of E is not an allowed eigenvalue.

Notes:

(a) The given differential equation implies that ϕ *and* $d\phi/dx$ *must be continuous in regions where* $V(x)$ *is finite* (however, $V(x)$ need not be continuous in such regions). These are necessary conditions for $d^2\phi(x)/dx^2$ to be finite, where the given differential equation implies that $d^2\phi(x)/dx^2$ must be finite for finite $V(x)$ and finite E.

More General Discussion (from Chapter 2)

Since $\phi(x)$ is physically related to a probability amplitude and hence to a measurable probability, we *assume* that $\phi(x)$ is continuous.

Using this fact, we can determine the general continuity properties of $d\phi(x)/dx$. The continuity property at a particular point, say $x = x_0$, is derived as follows:

$$\int_{x_0-\varepsilon}^{x_0+\varepsilon} \frac{d^2\phi(x)}{dx^2}dx = \int_{x_0-\varepsilon}^{x_0+\varepsilon} d\left(\frac{d\phi(x)}{dx}\right)$$

$$= -\frac{2m}{\hbar^2}\left[E\int_{x_0-\varepsilon}^{x_0+\varepsilon}\phi(x)dx - \int_{x_0-\varepsilon}^{x_0+\varepsilon}V(x)\phi(x)dx\right]$$

Taking the limit as $\varepsilon \to 0$

$$\lim_{\varepsilon\to 0}\left(\left.\frac{d\phi(x)}{dx}\right|_{x=x_0+\varepsilon} - \left.\frac{d\phi(x)}{dx}\right|_{x=x_0-\varepsilon}\right)$$

$$= -\frac{2m}{\hbar^2}\left[E\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon}\phi(x)dx - \lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon}V(x)\phi(x)dx\right]$$

or

$$\Delta\left(\frac{d\phi(x)}{dx}\right) = \frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon}V(x)\phi(x)dx \tag{3.307}$$

where we have used the continuity of $\phi(x)$ to set

$$\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon}\phi(x)dx = 0$$

This make it clear that whether or not $d\phi(x)/dx$ has a discontinuity depends directly on the potential energy function.

If $V(x)$ is continuous at $x = x_0$ (harmonic oscillator example), i.e.,

$$\lim_{\varepsilon\to 0}\left[V(x_0+\varepsilon) - V(x_0-\varepsilon)\right] = 0 \tag{3.308}$$

then

$$\Delta\left(\frac{d\phi(x)}{dx}\right) = \frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon} V(x)\phi(x)dx = 0 \tag{3.309}$$

and $d\phi(x)/dx$ is continuous.

If $V(x)$ has a finite discontinuity (jump) at $x = x_0$ (finite square well and square barrier examples later), i.e.,

$$\lim_{\varepsilon\to 0}\left[V(x_0+\varepsilon) - V(x_0-\varepsilon)\right] = finite \tag{3.310}$$

and $d\phi(x)/dx$ is continuous.

Finally, if $V(x)$ has an infinite jump at $x = x_0$ (infinite square well and delta-function examples later), then we have two choices

(a) if the potential is infinite over an extended range of x (the infinite well), then we must force $\phi(x) = 0$ in that region and use only the continuity of $\phi(x)$ as a boundary condition at the edge of the region

(b) if the potential is infinite at a single point, i.e., $V(x) = \delta(x-x_0)$, then

$$\begin{aligned}\Delta\left(\frac{d\phi(x)}{dx}\right) &= \frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon} V(x)\phi(x)dx \\ &= \frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon} \delta(x-x_0)\phi(x)dx \\ &= \frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\phi(x_0) = \frac{2m}{\hbar^2}\phi(x_0)\end{aligned} \tag{3.311}$$

and, thus,$d\phi(x)/dx$ is discontinuous.

We will use these rules later.

(b) Because $V(x)$ is a real function of x and because the allowed values of E must be real (they are eigenvalues of the hermitian operator H), Reϕ and Imϕ obey the same differential equation as does $\phi = \text{Re}\phi + i\text{Im}\phi$, i.e.,

$$\frac{d^2\left(\text{Re}\phi + i\text{Im}\phi\right)}{dx^2} = \frac{2m}{\hbar^2}\left(V(x) - E\right)\left(\text{Re}\phi + i\text{Im}\phi\right)$$

implies that

$$\frac{d^2}{dx^2}\left\{\begin{array}{c}\mathrm{Re}\phi\\ \mathrm{Im}\phi\end{array}\right\} = \frac{2m}{\hbar^2}\left(V(x)-E\right)\left\{\begin{array}{c}\mathrm{Re}\phi\\ \mathrm{Im}\phi\end{array}\right\}$$

(c) In any region where $V(x) > E$, $\{\mathrm{Re}\phi, \mathrm{Im}\phi\}$ and $d^2\{\mathrm{Re}\phi, \mathrm{Im}\phi\}/dx^2$ have the *same* sign. Thus, $\{\mathrm{Re}\phi, \mathrm{Im}\phi\}$ must be concave upward if $\{\mathrm{Re}\phi, \mathrm{Im}\phi\}$ is positive and concave downward if $\{\mathrm{Re}\phi, \mathrm{Im}\phi\}$ is negative - $\{\mathrm{Re}\phi, \mathrm{Im}\phi\}$ must curve away from the x-axis (non-oscillatory) as shown in Figure 3.12 below.

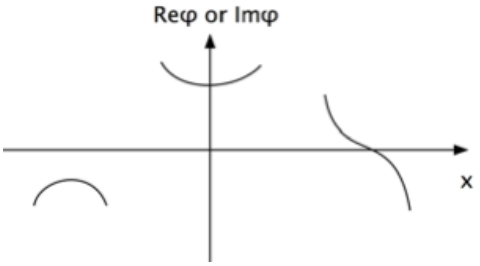


Figure 3.12: Behavior for $V(x) > E$

Note that $V(x) > E$ is the classically forbidden region where the kinetic energy would be negative.

In any region where $V(x) < E$, $\{\mathrm{Re}\phi, \mathrm{Im}\phi\}$ and $d^2\{\mathrm{Re}\phi, \mathrm{Im}\phi\}/dx^2$ have the *opposite* signs. Thus, $\{\mathrm{Re}\phi, \mathrm{Im}\phi\}$ must be concave upward if $\{\mathrm{Re}\phi, \mathrm{Im}\phi\}$ is negative and concave downward if $\{\mathrm{Re}\phi, \mathrm{Im}\phi\}$ is positive - $\{\mathrm{Re}\phi, \mathrm{Im}\phi\}$ must curve toward the x-axis (oscillatory) as shown ib Figure 3.13 below.

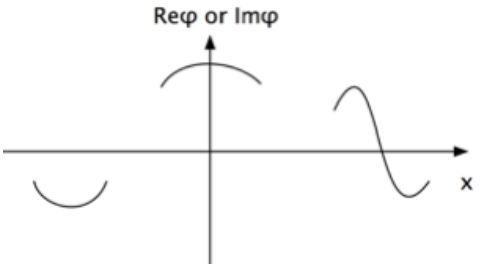


Figure 3.13: Behavior for $V(x) < E$

Note that $V(x) < E$ is the classically allowed region where the kinetic energy would be positive.

(d) If $V(x)$ is equal to some constant value V_0 in a region, then $phi(x)$ can easily be found in that region:

$$E > V_0 \ \ (oscillatory)$$

$$\frac{d^2\phi(x)}{dx^2} = \underbrace{\frac{2m}{\hbar^2}(V_0 - E)}_{-k^2\ (negative)}\phi(x) \quad , \quad k = +\sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

$$\phi(x) = Ae^{ikx} + Be^{-ikx} = C\sin kx + D\cos kx$$

$$E < V_0 \ \ (non - oscillatory)$$

$$\frac{d^2\phi(x)}{dx^2} = \underbrace{\frac{2m}{\hbar^2}(V_0 - E)}_{+k^2\ (positive)}\phi(x) \quad , \quad k = +\sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

$$\phi(x) = Ae^{kx} + Be^{-kx} = C\sinh kx + D\cosh kx$$

$$E = V_0$$

$$\frac{d^2\phi(x)}{dx^2} = \underbrace{\frac{2m}{\hbar^2}(V_0 - E)}_{=0}\phi(x)$$

$$\phi(x) = Ax + B$$

Let us now consider *some properties of the spectrum* of H when the potential energy $V(x)$ has the general form given earlier

$$V(x) = \begin{cases} V_L(constant) & \text{for } x < x_L \\ V_R(constant) & \text{for } x > x_R \\ V(x)(arbitrary) & \text{for } x_L < x < x_R \end{cases}$$

For definiteness, let $V_L \leq V_R$. For any constant E, the differential equation for $\phi(x)$ has *two linearly independent solutions* (because the differential equation is second order). However, the extra condition that $\phi(x)$ not become infinite as $|x| \to \infty$ may limit the number of acceptable solutions for that E - for a given E, there may exist two linearly independent acceptable solutions, only one linearly independent acceptable solution, or no non-zero acceptable solution.

For $E > V_R \geq V_L$ we have

$$x < x_L \Rightarrow V(x) = V_L$$

$$\Rightarrow \phi(x) = Ae^{ik_L x} + Be^{-ik_L x} \text{ where } k_L = +\sqrt{\frac{2m}{\hbar^2}(E - V_L)} \tag{3.312}$$

$$x > x_R \Rightarrow V(x) = V_R$$

$$\Rightarrow \phi(x) = Ce^{ik_R x} + De^{-ik_R x} \text{ where } k_R = +\sqrt{\frac{2m}{\hbar^2}(E - V_R)} \tag{3.313}$$

That the given differential equation has two linearly independent solutions means that $\phi(x)$, $x \in (-\infty, +\infty)$ has two arbitrary constants. Choose these constants to be C and D. Then $A(C, D)$ and $B(C, D)$ will be functions of C and D, which are found by solving the differential equation. The extra condition, $\phi(x)$ does not become infinite as $|x| \to \infty$ puts no restrictions on the solutions we have written. Thus, C and D can still be arbitrary. Therefore, there exists an acceptable $\phi(x)$ for any $E > V_R \geq V_L$ and it depends on two arbitrary constants - there is 2-fold degeneracy for any $E > V_R \geq V_L$. The corresponding eigenfunctions are clearly non-normalizable (*continuum* eigenfunctions).

For $V_R > E > V_L$ we have

$$x < x_L \Rightarrow V(x) = V_L$$

$$\Rightarrow \phi(x) = Ae^{k_L x} + Be^{-k_L x} \quad \text{where} \quad k_L = +\sqrt{\frac{2m}{\hbar^2}(V_L - E)} \tag{3.314}$$

$$x > x_R \Rightarrow V(x) = V_R$$

$$\Rightarrow \phi(x) = Ce^{k_R x} + De^{-k_R x} \quad \text{where} \quad k_R = +\sqrt{\frac{2m}{\hbar^2}(V_R - E)} \tag{3.315}$$

Choose C and D as the two arbitrary constants which enter into the solution of the given second-order differential equation. $A(C, D)$ and $B(C, D)$ will be functions of C and D. The extra condition, $\phi(x)$ does not become infinite as $|x| \to \infty$ requires that $C = 0$ *and* $B = 0$. If a non-trivial, acceptable solution to the differential equation exists, then D must be able to take on any arbitrary value. This follows from the fact that the given differential equation is homogeneous: if $\phi(x)$ is an acceptable solution, then any constant times $\phi(x)$ is also an acceptable solution. Thus, $C = 0$ *and* $B(C = 0, D) = 0$ with D arbitrary can be satisfied. These would correspond to the allowed values of E, and the corresponding eigenfunctions would be non-degenerate (one arbitrary constant D) and normalizable since $|\phi(x)|$ decreases exponentially as $x \to \pm\infty$, which implies that $\langle \phi \mid \phi \rangle$ is finite. Whether or not these allowed values of E exist depends on the $V(x)$ considered.

Note: E is not allowed if $E < V(x)$ for *all* $x \in (-\infty, +\infty)$.

Proof: We have

$$\frac{d^2}{dx^2}\left\{\begin{array}{c}\mathrm{Re}\phi\\ \mathrm{Im}\phi\end{array}\right\} = \underbrace{\frac{2m}{\hbar^2}\left(V(x)-E\right)}_{positive\,for\,all\,x}\left\{\begin{array}{c}\mathrm{Re}\phi\\ \mathrm{Im}\phi\end{array}\right\} \tag{3.316}$$

Therefore, $d^2\{\mathrm{Re}\phi,\mathrm{Im}\phi\}/dx^2$ and $\{\mathrm{Re}\phi,\mathrm{Im}\phi\}$ have the same sign for all x, which implies that $\{\mathrm{Re}\phi,\mathrm{Im}\phi\}$ always curves away from the x–axis. The acceptable solutions have

$$E < V_L \Rightarrow \left\{\begin{array}{c}\mathrm{Re}\phi\\ \mathrm{Im}\phi\end{array}\right\} \quad and \quad \phi(x) \propto e^{k_L x} \quad for \quad x < x_L \tag{3.317}$$

$$E < V_R \Rightarrow \left\{\begin{array}{c}\mathrm{Re}\phi\\ \mathrm{Im}\phi\end{array}\right\} \quad and \quad \phi(x) \propto e^{-k_R x} \quad for \quad x > x_R \tag{3.318}$$

As can be seen from Figure 3.14 below, it is clearly impossible to join the 2 parts of $\{\mathrm{Re}\phi,\mathrm{Im}\phi\}$ at x_R such that the function is continuous and has a continuous first derivative. Thus, such values of E are unacceptable. For an allowed value of E, it is therefore necessary to have some region of x in which $E > V(x)$.

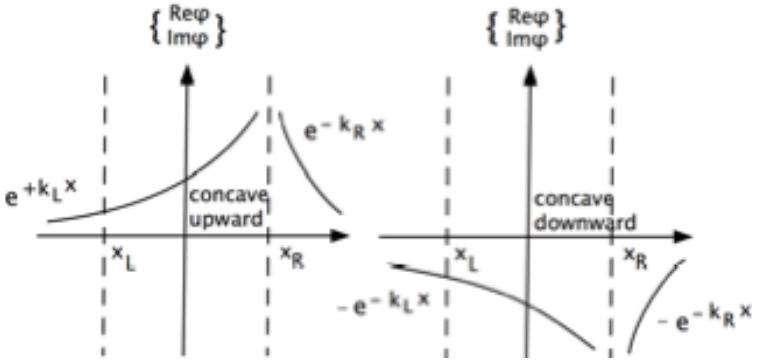


Figure 3.14: Impossible to join

Summary: (these degeneracy statements apply only to one-dimensional motion along a straight line)

$E > V_R \geq V_L$

All such E values are allowed.
Each E is 2–*fold degenerate*
$\phi(x)$ is oscillatory for $x < x_L$ and for $x > xR$
$\phi(x)$ is non-normalizable (*continuum*)

$V_R > E > V_L$

All such E values are allowed.
Each E is *non-degenerate*
$\phi(x)$ is oscillatory for $x < x_L$ and exponentially decreasing for $x > xR$
$\phi(x)$ is non-normalizable (*continuum*)

$E < V_L \leq V_R$

Only certain E values are allowed(it is possible for no E values to be allowed in this range)
Each E is *non-degenerate*
$\phi(x)$ is exponentially decreasing for $x < x_L$ and for $x > xR$
$\phi(x)$ is is normalizable (*discrete*)
Eigenfunctions in this energy range are called *bound states*

Examples: Examples are shown in Figures 3.15 and 3.16 below.

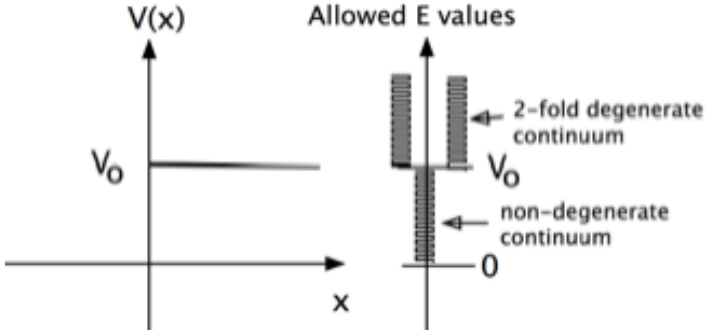


Figure 3.15: Example #1

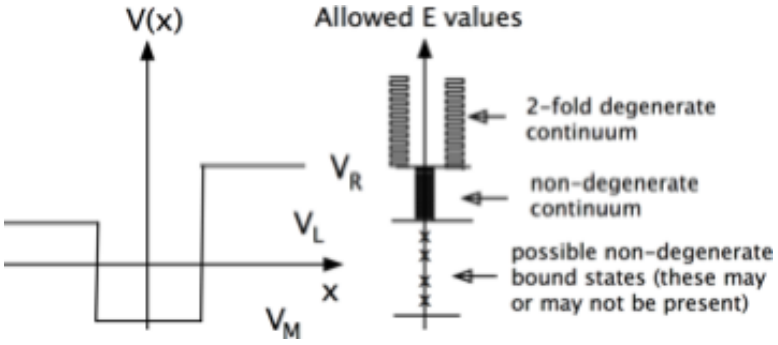


Figure 3.16: Example #2

Piecewise Constant Potential Energies

In one-dimension these are particularly simple to analyze. Consider the potential shown in Figure 3.17 below.

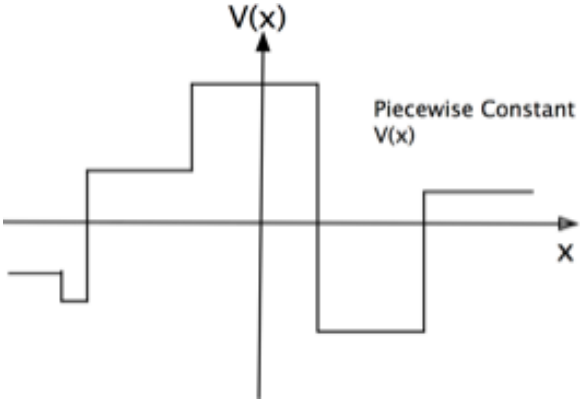


Figure 3.17: Piecewise Constant Potential Energy

Given the differential equation

$$\frac{d^2\phi(x)}{dx^2} = \frac{2m}{\hbar^2}\left(V(x) - E\right)\phi(x) \tag{3.319}$$

we have the following *method*:

1. Solve the differential equation with E any arbitrary constant. This is most easily accomplished as follows:

   (a) Solve the differential equation in each region for which $V(x)$ is a constant (discussed earlier). Special case: $\phi = 0$ in a region where $V(x) = \infty$.

(b) Match the solutions across each boundary: ϕ and $d\phi/dx$ are continuous. Special case: only ϕ is continuous across a boundary with an infinite jump in $V(x)$.

2. Determine the allowed values of E by requiring that the solution ϕ to not become infinite as $|x| \to \infty$.

The following example will illustrate the method. We consider the potential function shown in Figure 3.18 below.

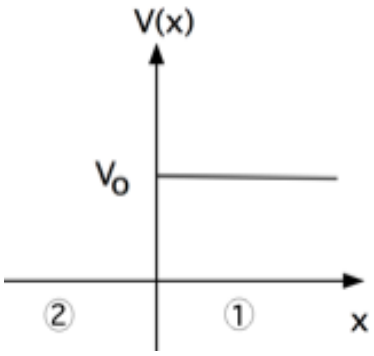


Figure 3.18: Step Function Potential - Infinite Barrier

Our general results completely determine the spectrum (see earlier discussion). However, let us calculate it explicitly.

We have $F_x = -dV/dx = 0$ except at $x = 0$. Classically, $E < 0$ is not allowed. $0 < E < V_0$ has unbound motion confined to $x < 0$. $E > V_0$ has unbound motion over the entire $x-$axis.

$$E < 0$$

$$x < 0 \Rightarrow \phi = \phi_2 = Ae^{k_2 x} + Be^{-k_2 x} \tag{3.320}$$

$$x > 0 \Rightarrow \phi = \phi_1 = Ce^{k_1 x} + De^{-k_1 x} \tag{3.321}$$

where

$$k_2 = \sqrt{-\frac{2mE}{\hbar^2}} \text{ and } k_1 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \tag{3.322}$$

ϕ must not become infinite as $|x| \to \infty$, which implies that $B = C = 0$ so that

$$\phi_{2'} = Ae^{k_2 x} \text{and} \phi_1 = De^{-k_1 x} \tag{3.323}$$

Then

$$\phi_1(0) = \phi_2(0) \Rightarrow D = A$$

$$\frac{d\phi_1(0)}{dx} = \frac{d\phi_2(0)}{dx} \Rightarrow -k_1 D = k_2 A \Rightarrow -k_1 = k_2$$

which is impossible. Therefore, there are *no allowed values* for $E < 0$.

$$0 < E < V_0$$

$$x < 0 \Rightarrow \phi = \phi_2 = Ae^{ik_2 x} + Be^{-ik_2 x} \tag{3.324}$$

$$x > 0 \Rightarrow \phi = \phi_1 = Ce^{k_1 x} + De^{-k_1 x} \tag{3.325}$$

where

$$k_2 = \sqrt{\frac{2mE}{\hbar^2}} \text{ and } k_1 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \tag{3.326}$$

ϕ must not become infinite as $|x| \to \infty$, which implies that $C = 0$ so that

$$\phi_2 = Ae^{ik_2 x} + Be^{-ik_2 x} \text{ and } \phi_1 = De^{-k_1 x} \tag{3.327}$$

Then

$$\phi_1(0) = \phi_2(0) \Rightarrow D = A + B$$

$$\frac{d\phi_1(0)}{dx} = \frac{d\phi_2(0)}{dx} \Rightarrow -k_1 D = ik_2 A - ik_2 B$$

These two equations determine A and B in terms of D, which is arbitrary. This is possible for any E. Therefore, all E values for $0 < E < V_0$ are allowed and they are non-degenerate (one arbitrary constant D).

$$E > V_0$$

$$x < 0 \Rightarrow \phi = \phi_2 = Ae^{ik_2 x} + Be^{-ik_2 x} \tag{3.328}$$

$$x > 0 \Rightarrow \phi = \phi_1 = Ce^{ik_1 x} + De^{-ik_1 x} \tag{3.329}$$

where

$$k_2 = \sqrt{\frac{2mE}{\hbar^2}} \text{ and } k_1 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}} \tag{3.330}$$

ϕ must not become infinite as $|x| \to \infty$ places no restrictions on A, B, C, D. Then

$$\phi_1(0) = \phi_2(0) \Rightarrow C + D = A + B$$

$$\frac{d\phi_1(0)}{dx} = \frac{d\phi_2(0)}{dx} \Rightarrow -ik_1(C - D) = ik_2(A - B)$$

These two equations determine A and B in terms of C and D, which are both arbitrary. This is possible for any E. Therefore, all E values for $E > V_0$ are allowed and there is 2–fold degeneracy (two arbitrary constants C and D).

These results agree with our analysis of the general $V(x)$.

Notice that the potential energy just considered has some physical significance:

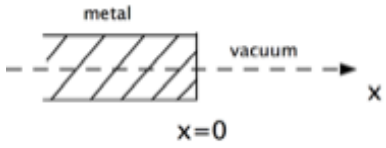


Figure 3.19: End of a wire

(a) Consider an electron constrained to move along the $x-$axis. See Figure 3.19 above.

The electron has no force acting on it when it is in the vacuum region. Furthermore, the electron is essentially free in its motion through the metal. However, an energy V_0 (the metal's *work function*) is needed for the electron to leave the metal's surface and enter the vacuum region. Thus,

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } x > 0 \end{cases} \tag{3.331}$$

as in the example above.

(b) Consider an electron constrained to move along the $x-$axis. The electron moves within 2 conducting cylindrical tubes which are separated by a small gap and which are maintained at different potentials (the $x > 0$ tube is at electrical potential $-\Phi$ with respect to the $x > 0$ tube). See Figure 3.20 below.

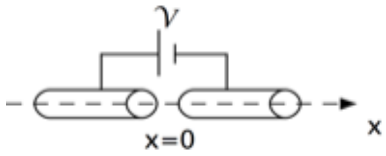


Figure 3.20: Gap between tubes

The potential energy is

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } x > 0 \end{cases} \tag{3.332}$$

where $V_0 = -e\Phi$ where e = the electron's charge. Again, this is the same as in the example above.

3.7.2. Symmetrical Potential Well (finite depth)

We consider the potential energy function shown in Figure 3.21 below:

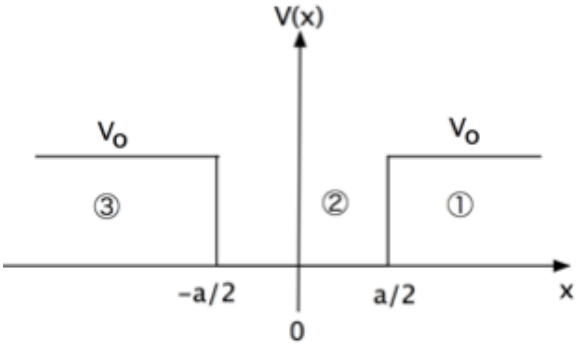


Figure 3.21: Finite square well

so that

$$V(x) = \begin{cases} V_0 & \text{for } x > a/2 \\ 0 & \text{for } -a/2 < x < a/2 \\ V_0 & \text{for } x < -a/2 \end{cases} \tag{3.333}$$

The energy spectrum has a 2–fold degenerate continuum for all $E > V_0$. There are no energy eigenvalues for $E < 0$. The *question* is whether or not there are *bound states* in the region $0 < E < V_0$.

Note: We have $V(x) = V(-x)$. Recall that the *parity operator* Π is defined by $\Pi f(x) = f(-x)$. The eigenvalues of Π are ± 1 and the corresponding eigenfunctions are (even, odd) functions of x.

Notice also that $[\Pi, H] = 0$.

Proof: We have

$$\begin{aligned} \Pi H f(x) &= \Pi \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \right) f(x) \\ &= \left(-\frac{\hbar^2}{2m}\frac{d^2}{d(-x)^2} + V(-x) \right) f(-x) \\ &= \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \right) \Pi f(x) \end{aligned}$$

so that $\Pi H f(x) = H \Pi f(x)$ for any $f(x)$ or $[\Pi, H] = 0$.

Thus, we can find a CON set of simultaneous eigenfunctions of Π and H - each eigenfunction in this set will be either an even function of x or an odd function of x. This observation will simplify our calculation - we need to match ϕ and $d\phi/dx$ at $x = a/2$ only. An even or odd function of x will then automatically have ϕ and $d\phi/dx$ at $x = -a/2$.

$0 < E < V_0$: we define

$$k_2 = \sqrt{\frac{2mE}{\hbar^2}} \text{ and } k_1 = k_3 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \tag{3.334}$$

ϕ_{even}: we have

$$x > a/2 \Rightarrow \phi = \phi_1 = \underbrace{Ae^{+k_1 x}}_{\substack{A=0 \text{ for } \phi \\ \text{not infinite} \\ \text{as } |x| \to \infty}} + Be^{-k_1 x} \tag{3.335}$$

$$-a/2 < x < a/2 \Rightarrow \phi = \phi_2 = \underbrace{C \sin k_2 x}_{\substack{C=0 \text{ for an} \\ \text{even function}}} + D \cos k_2 x \tag{3.336}$$

$$\phi_1(a/2) = \phi_2(a/2) \Rightarrow Be^{-k_1 a/2} = D \cos \frac{k_2 a}{2} \tag{3.337}$$

$$\frac{d\phi_1(a/2)}{dx} = \frac{d\phi_2(a/2)}{dx} \Rightarrow -k_1 Be^{-k_1 a/2} = -k_2 D \sin \frac{k_2 a}{2} \tag{3.338}$$

Therefore, $B, D \neq 0$ implies that we can divide (3.338) by (3.337) and get

$$k_1 = k_2 \tan \frac{k_2 a}{2} \tag{3.339}$$

E must obey the above transcendental equation for ϕ_{even} to be an eigenfunction.

ϕ_{odd}: we have

$$x > a/2 \Rightarrow \phi = \phi_1 = \underbrace{Ae^{+k_1 x}}_{\substack{A=0 \text{ for } \phi \\ \text{not infinite} \\ \text{as } |x| \to \infty}} + Be^{-k_1 x} \tag{3.340}$$

$$-a/2 < x < a/2 \Rightarrow \phi = \phi_2 = C \sin k_2 x + \underbrace{D \cos k_2 x}_{\substack{D=0 \text{ for an} \\ \text{odd function}}} \tag{3.341}$$

$$\phi_1(a/2) = \phi_2(a/2) \Rightarrow Be^{-k_1 a/2} = C \sin \frac{k_2 a}{2} \tag{3.342}$$

$$\frac{d\phi_1(a/2)}{dx} = \frac{d\phi_2(a/2)}{dx} \Rightarrow -k_1 Be^{-k_1 a/2} = k_2 C \cos \frac{k_2 a}{2} \tag{3.343}$$

Therefore, $B, C \neq 0$ implies that we can divide (3.343) by (3.342) and get

$$-k_1 = k_2 \cot \frac{k_2 a}{2} \tag{3.344}$$

E must obey the above transcendental equation for ϕ_{odd} to be an eigenfunction.

Therefore we have

$$\phi_{even}: \quad k_1 \frac{a}{2} = k_2 \frac{a}{2} \tan \frac{k_2 a}{2} \tag{3.345}$$

$$\phi_{odd}: \quad -k_1 \frac{a}{2} = k_2 \frac{a}{2} \cot \frac{k_2 a}{2} \tag{3.346}$$

We let

$$\eta = k_2 \frac{a}{2} = \sqrt{\frac{2mE}{\hbar^2}} \frac{a}{2} \tag{3.347}$$

and then

$$k_1 \frac{a}{2} = \frac{a}{2} \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} = \sqrt{\Gamma - \eta^2} \tag{3.348}$$

where

$$\Gamma = \frac{mV_0 a^2}{2\hbar^2} \tag{3.349}$$

Thus,

$$\phi_{even}: \quad \sqrt{\Gamma - \eta^2} = \eta \tan \eta \tag{3.350}$$

$$\phi_{odd}: \quad \sqrt{\Gamma - \eta^2} = -\eta \cot \eta \tag{3.351}$$

These equations determine the allowed values of E for the two types of solutions. We can solve these transcendental equations graphically. We plot $y = \eta \tan \eta$ and $y = -\eta \cot \eta$. The intersections of these curves with the curve $y = \sqrt{\Gamma - \eta^2}$ yields the allowed values of

$$\eta = \sqrt{\frac{2mE}{\hbar^2}} \frac{a}{2} \tag{3.352}$$

and thus the allowed E values for the even and odd solutions. Now $E < V_0 \Rightarrow \eta^2 < \Gamma$ so that $y = +\sqrt{\Gamma - \eta^2}$ is one quadrant of a circle of radius Γ. Note also that η is always positive. The graphical solutionis shown in Figure 3.22 below.

Comments:

1. There always exists at least one bound state for the symmetric potential well, regardless of the value of Γ. Asymmetric wells need not have any bound states.

2. The bound state energies are indeed discrete (separated).

3. Γ finite implies that there are a finite number of bound states.

4. Let $V_0 \to \infty$ (a fixed). Therefore, $\Gamma \to \infty$ and the circle $y = +\sqrt{\Gamma - \eta^2}$ has an infinite radius. In this case, the circle intersects $y = \eta \tan \eta$ and $y = -\eta \cot \eta$ at the asymptotes (dotted vertical lines in Figure 3.22). Thus, the allowed values of η are

   $$\frac{\pi}{2}, \pi, \frac{3\pi}{2}, 2\pi, \frac{5\pi}{2}, 3\pi, \frac{7\pi}{2}, ...$$

   (infinite number of bound states). Therefore,

   $$\eta = \sqrt{\frac{2mE}{\hbar^2}} \frac{a}{2} = n \frac{\pi}{2} \Rightarrow E = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \tag{3.353}$$

   which agrees with our earlier result for the potential well with impenetrable walls(infinite square well).

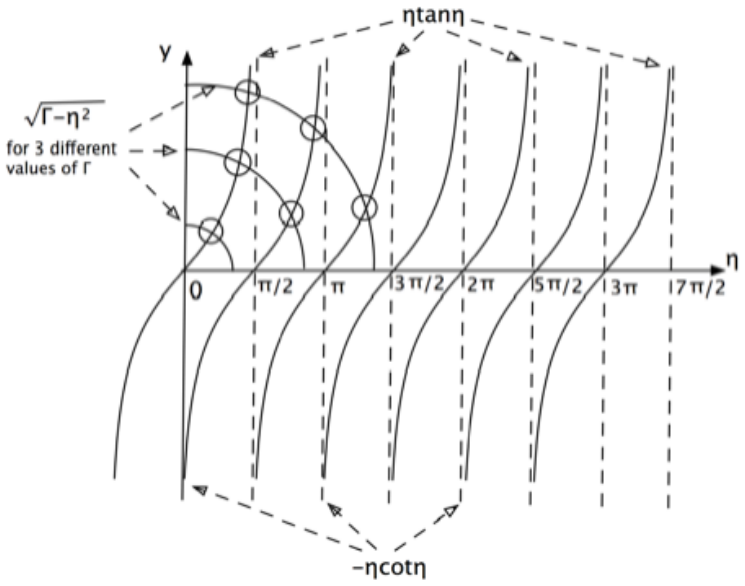


Figure 3.22: Graphical Solution

5. Let N be the number of bound states present. We then have

$$(N-1)\frac{\pi}{2} < \sqrt{\Gamma} < N\frac{\pi}{2} \tag{3.354}$$

is the condition for exactly N bound states to exist. Note that the number of bound states present depends on the combination V_0a^2 - a wide and shallow well can have as many bound states as a narrow and deep well.

6. The ground state is an even function of x. The first excited state (if it exists) is an odd function of x. The second excited state (if it exists) is an even function of x. Obviously, this alternation between even and odd functions of x continues to hold for all bound states.

7. The ground state is always present for $0 < E < V_0$. We have, for the ground state

$$k_2\frac{a}{2} = \sqrt{\frac{2mE}{\hbar^2}}\frac{a}{2} = \eta < \frac{\pi}{2} \Rightarrow E_0 = \frac{\pi^2\hbar^2}{2ma^2} \tag{3.355}$$

and

$$x < -a/2 \Rightarrow \phi = \phi_3 \propto e^{+k_1x} \tag{3.356}$$

$$-a/2 < x < a/2 \Rightarrow \phi = \phi_2 \propto \cos k_2x \tag{3.357}$$

$$x > a/2 \Rightarrow \phi = \phi_1 \propto e^{-k_1x} \tag{3.358}$$

Therefore, ϕ has no zeroes. The wave function is shown in Figure 3.23:

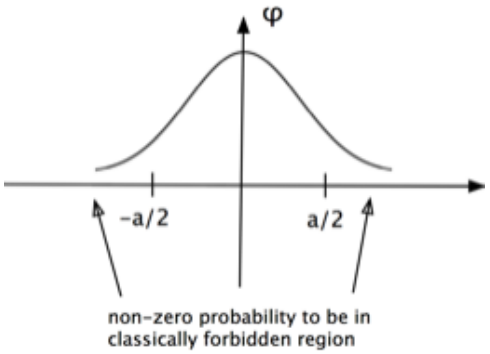


Figure 3.23: Ground state wave function

3.8. General One-Dimensional Motion

We again consider the potential

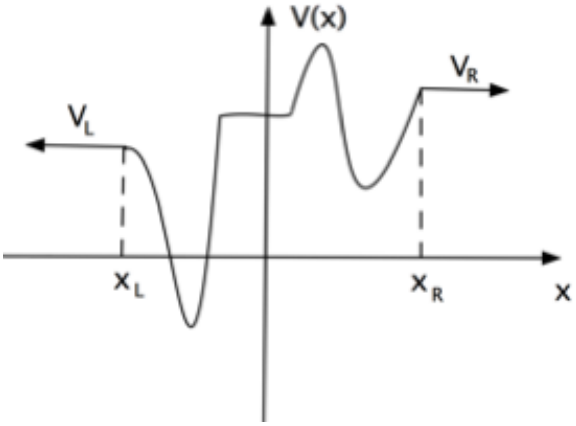


Figure 3.24: General potential function

with

$$V(x) = \begin{cases} V_L(constant) & \text{for } x < x_L \\ V(x)(arbitrary) & \text{for } x_L < x < x_R \\ V_R(constant) & \text{for } x > x_R \end{cases} \tag{3.359}$$

and we choose $V_R > V_L$ for definiteness. We found earlier that

$E > V_R > V_L$ - 2 - fold degenerate continuum (3.360)

$V_R > E > V_L$ - non - degenerate continuum (3.361)

$V_R > V_L > E$ - non - degenerate discrete states (if they exist) (3.362)

The following eigenfunctions of H form a CON set, where the constants $A_L^{(\alpha)}, B_L^{(\alpha)}, A_R^{(\alpha)}, B_R^{(\alpha)}$ and A_L, B_L, A_R, B_R depend on E.

$E > V_R > V_L$: $u_{CE}^{(1)}(x)$ with $\alpha = 1, 2$ are 2 linearly independent eigenfunctions with same E (subscript C stands for continuum). With

$$k_L = \sqrt{\frac{2m}{\hbar^2}(E - V_L)} \text{ and } k_R = \sqrt{\frac{2m}{\hbar^2}(E - V_R)} \tag{3.363}$$

we have

$$u_{CE}^{(1)}(x) = \begin{cases} A_L^{(1)} e^{ik_L x} + B_L^{(1)} e^{-ik_L x} & \text{for } x < x_L \\ A_R^{(1)} e^{ik_R x} & \text{for } x > x_R \\ \text{complicated} & \text{for } x_L < x < x_R \end{cases} \tag{3.364}$$

$$u_{CE}^{(2)}(x) = \begin{cases} B_L^{(2)} e^{-ik_L x} & \text{for } x < x_L \\ A_R^{(2)} e^{ik_R x} + B_R^{(2)} e^{-ik_R x} & \text{for } x > x_R \\ \text{complicated} & \text{for } x_L < x < x_R \end{cases} \tag{3.365}$$

These particular linearly independent eigenfunctions have a simple interpretation (see Figure 3.25 and Figure 3.26 below).

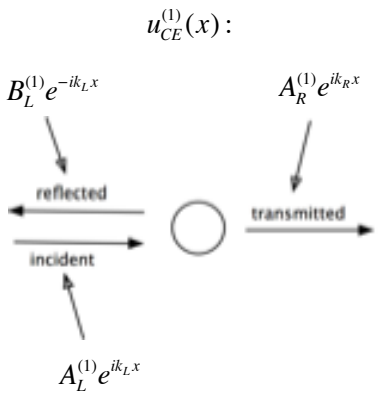


Figure 3.25: $u_{CE}^{(1)}(x)$

and

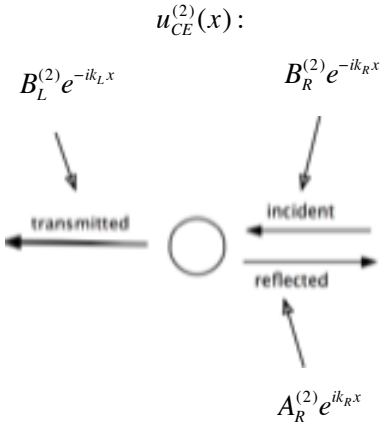


Figure 3.26: $u_{CE}^{(2)}(x)$

$V_R > E > V_L : u_{CE}(x)$ - no degeneracy. With

$$k_L = \sqrt{\frac{2m}{\hbar^2}(E - V_L)} \text{ and } k_R = \sqrt{\frac{2m}{\hbar^2}(V_R - E)} \tag{3.366}$$

we have

$$u_{CE}(x) = \begin{cases} A_L e^{ik_L x} + B_L e^{-ik_L x} & \text{for } x < x_L \\ B_R e^{-k_R x} & \text{for } x > x_R \\ \text{complicated} & \text{for } x_L < x < x_R \end{cases} \tag{3.367}$$

This eigenfunction has a simple interpretation (see Figure 3.27 below).

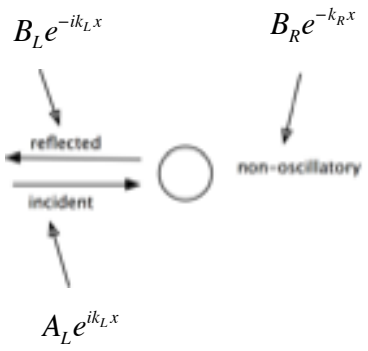


Figure 3.27: $u_{CE}(x)$

$V_R > E > V_L : u_{CE}(x)$ - non-degenerate bound states (E_n). With

$$k_L = \sqrt{\frac{2m}{\hbar^2}(V_L - E)} \text{ and } k_R = \sqrt{\frac{2m}{\hbar^2}(V_R - E)} \tag{3.368}$$

we have

$$u_n(x) = \begin{cases} A_L e^{k_L x} & \text{for } x < x_L \\ B_R e^{-k_R x} & \text{for } x > x_R \\ \text{complicated} & \text{for } x_L < x < x_R \end{cases} \tag{3.369}$$

This eigenfunction has a simple interpretation (see Figure 3.28 below).

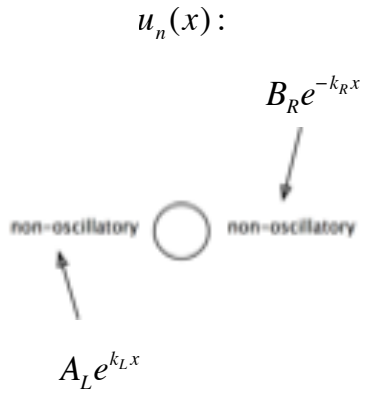


Figure 3.28: $u_n(x)$

Note: Solving the time-independent Schrodinger equation for all x will relate the A and B coefficients appearing in a given eigenfunction.

Normalization: The following normalizations are chosen:

$$\begin{aligned} &\langle u_{n'} \mid u_n \rangle = \delta_{n'n} \\ &\langle u_{CE'} \mid u_{CE} \rangle = \delta(E' - E) \\ &\left\langle u^{(\alpha)}_{CE'} \,\middle|\, u^{(\alpha)}_{CE} \right\rangle = \delta(E' - E) \end{aligned} \tag{3.370}$$

that is, the continuum eigenfunctions are chosen to be normalized to δ–functions of the energy.

Let $\psi(x,t)$ be the wave function for a particle ($\psi(x,t)$ must be normalizable). Now

$$\psi(x,t) = u_n(x) e^{-i\frac{E_n t}{\hbar}} \tag{3.371}$$

is a possible wave function for a bound state (we must have $\langle \psi(t) \mid \psi(t) \rangle = 1$).

However,

$$\psi(x,t) = \left\{ \begin{array}{c} u_{CE}(x) \\ u_{CE}^{(\alpha)}(x) \end{array} \right\} e^{-i\frac{Et}{\hbar}} \tag{3.372}$$

is *not* a possible wave function because u_{CE} and $u_{CE}^{(\alpha)}$ are not normalizable.

Consider, however, the wave function constructed as follows:

$$\psi(x,t) = \frac{1}{\sqrt{\Delta}} \int_{E_0}^{E_0+\Delta} dE \left\{ \begin{array}{c} u_{CE}(x) \\ u_{CE}^{(\alpha)}(x) \end{array} \right\} e^{-i\frac{Et}{\hbar}} \tag{3.373}$$

where we assume that Δ is small. For u_{CE} we have $V_R > E_0 > V_L$ and for $u_{CE}^{(\alpha)}$ we have $E_0 > V_R > V_L$. The integral corresponds to equal weighting of the energies in the range $[E_0, E_0 + \Delta]$.

This $\psi(x,t)$ (using u_{CE}, $u_{CE}^{(1)}$ or $u_{CE}^{(2)}$) is normalizable and therefore a possible wave function. Considering u_{CE} for definiteness, we have

$$\begin{aligned}
\langle \psi(t) \mid \psi(t) \rangle &= \int_{-\infty}^{\infty} dx \frac{1}{\sqrt{\Delta}} \int_{E_0}^{E_0+\Delta} dE\, u_{CE}^*(x) e^{+i\frac{Et}{\hbar}} \frac{1}{\sqrt{\Delta}} \int_{E_0}^{E_0+\Delta} dE'\, u_{CE'}(x) e^{-i\frac{E't}{\hbar}} \\
&= \frac{1}{\Delta} \int_{E_0}^{E_0+\Delta} dE\, e^{+i\frac{Et}{\hbar}} \int_{E_0}^{E_0+\Delta} dE'\, e^{-i\frac{E't}{\hbar}} \int_{-\infty}^{\infty} dx u_{CE}^*(x) u_{CE'}(x) \\
&= \frac{1}{\Delta} \int_{E_0}^{E_0+\Delta} dE\, e^{+i\frac{Et}{\hbar}} \int_{E_0}^{E_0+\Delta} dE'\, e^{-i\frac{E't}{\hbar}} \langle u_{CE} \mid u_{CE'} \rangle \\
&= \frac{1}{\Delta} \int_{E_0}^{E_0+\Delta} dE\, e^{+i\frac{Et}{\hbar}} \int_{E_0}^{E_0+\Delta} dE'\, e^{-i\frac{E't}{\hbar}} \delta(E' - E) \\
&= \frac{1}{\Delta} \int_{E_0}^{E_0+\Delta} dE\, e^{+i\frac{Et}{\hbar}} e^{-i\frac{Et}{\hbar}} = \frac{1}{\Delta} \int_{E_0}^{E_0+\Delta} dE = \frac{\Delta}{\Delta} = 1
\end{aligned}$$

for all time.

Of course, there are other possible wave functions. However, these particular wave functions have a simple physical significance and can be prepared experimentally (as we will shortly see).

Note: We have

$$\lim_{t\to\pm\infty} \underbrace{\frac{1}{\sqrt{\Delta}} \int_{E_0}^{E_0+\Delta} dE \left\{ \begin{array}{c} u_{CE}(x) \\ u_{CE}^{(\alpha)}(x) \end{array} \right\} e^{-i\frac{Et}{\hbar}}}_{\psi(x,t)} = 0 \text{ for any } x \tag{3.374}$$

The reason for obtaining zero is that

$$e^{-i\frac{Et}{\hbar}} = \cos\frac{Et}{\hbar} - i\sin\frac{Et}{\hbar} \tag{3.375}$$

oscillates very rapidly as E varies over $[E_0, E_0+\Delta]$ when t is infinite. These oscillations of the integrand as we integrate from E_0 to $E_0+\Delta$ lead to alternating positive and negative values which cancel. In addition, $\langle\psi(t)\,|\,\psi(t)\rangle = 1$ or all t (including $t \to \pm\infty$). Thus, in some sense, $\psi(x, t = \pm\infty)$ must be non-zero somewhere. The only possibility is $\lim_{t\to\pm\infty}\psi(x,t) \neq 0$ when $|x| \to \infty$. Thus, this $\psi(x,t)$ represents an *unbound state* - the only place there is a non-zero probability of finding the particle when $t \to \pm\infty$ is $|x| \to \infty$. Now for definiteness, let us consider $u^{(1)}_{CE}$. We have

$$\psi(x,t) = \frac{1}{\sqrt{\Delta}}\int_{E_0}^{E_0+\Delta} dE\, u^{(1)}_{CE}(x)e^{-i\frac{Et}{\hbar}} \quad , \quad E_0 > V_R > V_L \tag{3.376}$$

For $x < x_L$:

$$\psi(x,t) = \frac{1}{\sqrt{\Delta}}\int_{E_0}^{E_0+\Delta} dE\,\left\{A^{(1)}_L(E)e^{ik_Lx} + B^{(1)}_L(E)e^{-ik_Lx}\right\}e^{-i\frac{Et}{\hbar}} \tag{3.377}$$

For $x > x_R$:

$$\psi(x,t) = \frac{1}{\sqrt{\Delta}}\int_{E_0}^{E_0+\Delta} dE\,\left\{A^{(1)}_R e^{ik_Rx}\right\}e^{-i\frac{Et}{\hbar}} \tag{3.378}$$

For $x_L < x < x_R$, $\psi(x,t)$ is complicated and depends on the detailed form of $V(x)$.

Now define the following functions (the earlier Figure motivates these definitions):

$$\psi_{incident}(x,t) = \frac{1}{\sqrt{\Delta}}\int_{E_0}^{E_0+\Delta} dE\,\left\{A^{(1)}_L(E)e^{ik_Lx}\right\}e^{-i\frac{Et}{\hbar}} \tag{3.379}$$

$$\psi_{reflected}(x,t) = \frac{1}{\sqrt{\Delta}}\int_{E_0}^{E_0+\Delta} dE\,\left\{B^{(1)}_L(E)e^{-ik_Lx}\right\}e^{-i\frac{Et}{\hbar}} \tag{3.380}$$

$$\psi_{transmitted}(x,t) = \frac{1}{\sqrt{\Delta}}\int_{E_0}^{E_0+\Delta} dE\,\left\{A^{(1)}_R e^{ik_Rx}\right\}e^{-i\frac{Et}{\hbar}} \tag{3.381}$$

We let the above equations define the functions $\psi_{inc}, \psi_{refl}, \psi_{trans}$ for all x and t.

Then, for $x < x_L$, $\psi(x,t) = \psi_{inc}(x,t) + \psi_{refl}(x,t)$ and for $x > x_R$, $\psi(x,t) = \psi_{trans}(x,t)$. Now let

$$A_L^{(1)} = \left|A_L^{(1)}\right| e^{i\alpha_L^{(1)}}, \;\; B_L^{(1)} = \left|B_L^{(1)}\right| e^{i\beta_L^{(1)}}, \;\; A_R^{(1)} = \left|A_R^{(1)}\right| e^{i\alpha_R^{(1)}} \tag{3.382}$$

so that

$$\psi_{inc}(x,t) = \frac{1}{\sqrt{\Delta}} \int_{E_0}^{E_0+\Delta} dE \left|A_L^{(1)}(E)\right| e^{i\left[\alpha_L^{(1)}(E)+k_L x - \frac{Et}{\hbar}\right]} \tag{3.383}$$

$$\psi_{refl}(x,t) = \frac{1}{\sqrt{\Delta}} \int_{E_0}^{E_0+\Delta} dE \left|B_L^{(1)}(E)\right| e^{i\left[\beta_L^{(1)}(E)-k_L x - \frac{Et}{\hbar}\right]} \tag{3.384}$$

$$\psi_{trans}(x,t) = \frac{1}{\sqrt{\Delta}} \int_{E_0}^{E_0+\Delta} dE \left|A_R^{(1)}(E)\right| e^{i\left[\alpha_R^{(1)}(E)+k_R x - \frac{Et}{\hbar}\right]} \tag{3.385}$$

Using the method of stationary phase we discussed earlier we have

$$\psi_{inc}(x,t) \neq 0 \text{ for } \frac{d}{dE}\left[\alpha_L^{(1)}(E) + k_L x - \frac{Et}{\hbar}\right]_{E_0} \approx 0 \tag{3.386}$$

$$\psi_{refl}(x,t) \neq 0 \text{ for } \frac{d}{dE}\left[\beta_L^{(1)}(E) - k_L x - \frac{Et}{\hbar}\right]_{E_0} \approx 0 \tag{3.387}$$

$$\psi_{trans}(x,t) \neq 0 \text{ for } \frac{d}{dE}\left[\alpha_R^{(1)}(E) + k_R x - \frac{Et}{\hbar}\right]_{E_0} \approx 0 \tag{3.388}$$

Now

$$k_{L,R} = \sqrt{\frac{2m}{\hbar^2}(E - V_{L,R})} \tag{3.389}$$

so that

$$\frac{dk_{L,R}}{dE} = \frac{m/\hbar^2}{\sqrt{\frac{2m}{\hbar^2}(E-V_{L,R})}} = \frac{1}{\hbar}\frac{m}{\hbar k_{L,R}} \tag{3.390}$$

Now let

$$p_{L,R} = \hbar k_{L,R} \text{ and } v_{L,R} = \frac{\hbar k_{L,R}}{m} = \frac{p_{L,R}}{m} \tag{3.391}$$

so that

$$\frac{dk_{L,R}}{dE} = \frac{1}{\hbar v_{L,R}} \tag{3.392}$$

Also define

$$v_{L0} = (v_L)_{E=E_0} \text{ and } v_{R0} = (v_R)_{E=E_0} \tag{3.393}$$

Thus,

$$\psi_{inc}(x,t) \neq 0 \text{for} \left[\frac{d\alpha_L^{(1)}}{dE} + \frac{1}{\hbar v_L}x - \frac{t}{\hbar}\right]_{E_0} \approx 0 \tag{3.394}$$

that is, for

$$x \approx v_{L0}\left[t - \hbar\left(\frac{d\alpha_L^{(1)}}{dE}\right)_{E_0}\right] \tag{3.395}$$

or the associated *particle* moves in the $+x$ direction with speed v_{L0}.

Similarly,

$$\psi_{refl}(x,t) \neq 0 \text{ for } \left[\frac{d\beta_L^{(1)}}{dE} - \frac{1}{\hbar v_L}x - \frac{t}{\hbar}\right]_{E_0} \approx 0 \tag{3.396}$$

that is, for

$$x \approx -v_{L0}\left[t - \hbar\left(\frac{d\beta_L^{(1)}}{dE}\right)_{E_0}\right] \tag{3.397}$$

or the *particle* moves in the $-x$ direction with speed v_{L0}.

Finally,

$$\psi_{trans}(x,t) \neq 0 \text{ for } \left[\frac{d\alpha_R^{(1)}}{dE} + \frac{1}{\hbar v_R}x - \frac{t}{\hbar}\right]_{E_0} \approx 0 \tag{3.398}$$

that is, for

$$x \approx v_{R0}\left[t - \hbar\left(\frac{d\alpha_R^{(1)}}{dE}\right)_{E_0}\right] \tag{3.399}$$

or the *particle* moves in the $+x$ direction with speed v_{L0}.

3.8.1. Physical Significance of form of $\psi(x,t)$

(a) The wave function has energy approximately equal to E_0 with a small spread Δ.

(b) Let $t \to -\infty$. Then

$$\psi_{inc} \neq 0 \text{ for } x \to -\infty$$
$$\psi_{refl} \neq 0 \text{ for } x \to +\infty$$
$$\psi_{trans} \neq 0 \text{ for } x \to -\infty$$

which implies that

$$\text{for } x < x_L \quad \psi(x,t) = \psi_{inc}(x,t) + \psi_{refl}(x,t) \underset{t\to-\infty}{\to} \psi_{inc}(x,t)$$
$$\text{for } x > x_R \quad \psi(x,t) = \psi_{trans}(x,t) \underset{t\to-\infty}{\to} 0$$

Thus, $\lim_{t\to-\infty}\psi(x,t)$ is a *localized* wave function located far to the left of x_L and traveling to the right at speed v_{L0} (the incident wave).

(c) Let $t \to +\infty$. Then

$$\psi_{inc} \neq 0 \text{ for } x \to +\infty$$
$$\psi_{refl} \neq 0 \text{ for } x \to -\infty$$
$$\psi_{trans} \neq 0 \text{ for } x \to +\infty$$

which implies that

$$\text{for } x < x_L \quad \psi(x,t) = \psi_{inc}(x,t) + \psi_{refl}(x,t) \underset{t\to+\infty}{\to} \psi_{refl}(x,t)$$
$$\text{for } x > x_R \quad \psi(x,t) = \psi_{inc}(x,t) + \psi_{refl}(x,t) \underset{t\to+\infty}{\to} \psi_{refl}(x,t)$$

Thus, $\lim_{t\to+\infty} \psi(x,t)$ is two *localized* wave functions one located far to the left of x_L and traveling to the left at speed v_{L0} (the reflected wave) and the other located far to the right of x_R and traveling to the left at speed v_{R0} (the transmitted wave).

As noted earlier, $\lim_{t\to\pm\infty} \psi(x,t) = 0$ for $x_L < x < x_R$. Figure 3.29 below shows $\psi(x,t)$ for $t \to \pm\infty$.

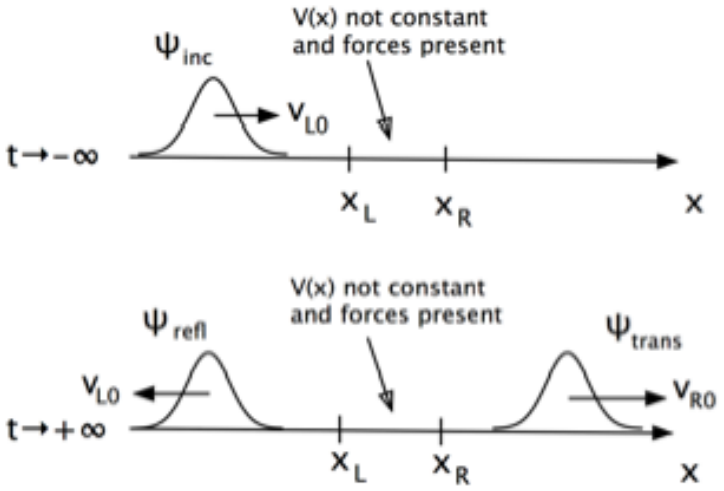


Figure 3.29: Wave Packet Evolution

The particle *does not* break into 2 particles when it reaches the region $[x_L, x_R]$. Rather, the particle, incident from the left at $t \to -\infty$, can be found at $x = +\infty$ or at $x = -\infty$ when $t \to +\infty$; ψ_{trans} determines the probability of transmission to $x = +\infty$ while ψ_{refl} determines the probability of reflection back to $x = -\infty$.

The **transmission coefficient** $\mathfrak{I}$ = the probability of finding the particle at $x = +\infty$ $(x > x_R)$ as $t \to +\infty$.

The **reflection coefficient** $\mathfrak{R}$ = the probability of finding the particle at $x = -\infty$ $(x < x_L)$ as $t \to +\infty$.

$$\mathfrak{I} = \frac{\int_{x_R}^{\infty} dx \psi^*(x,t)\psi(x,t)}{\langle \psi(t) \mid \psi(t) \rangle} \quad , \quad \mathfrak{R} = \frac{\int_{-\infty}^{x_L} dx \psi^*(x,t)\psi(x,t)}{\langle \psi(t) \mid \psi(t) \rangle} \tag{3.400}$$

Before calculating $\mathfrak{R}$ and $\mathfrak{I}$, let us note the following useful relations:

(a) We have

$$\int_{-\infty}^{\infty} \frac{dx}{2\pi} e^{\pm i(k'-k)x} = \delta(k'-k) \tag{3.401}$$

(b) Let

$$g(x,t) = \frac{1}{\sqrt{\Delta}} \int_{E_0}^{E_0+\Delta} dE\, e^{\pm ikx} e^{-i\frac{Et}{\hbar}} C(E) \tag{3.402}$$

where Δ is small and

$$\frac{dk}{dE} = \frac{1}{\hbar v} \tag{3.403}$$

We will encounter integrals of the form

$$\int_{-\infty}^{\infty} dx\, g^*(x,t) g(x,t) \tag{3.404}$$

We have

$$\begin{aligned}
&\int_{-\infty}^{\infty} dx\, g^*(x,t) g(x,t) \\
&\quad = \int_{-\infty}^{\infty} dx \left[\frac{1}{\sqrt{\Delta}} \int_{E_0}^{E_0+\Delta} dE\, e^{\mp ikx} e^{i\frac{Et}{\hbar}} C^*(E) \right] \left[\frac{1}{\sqrt{\Delta}} \int_{E_0}^{E_0+\Delta} dE'\, e^{\pm ik'x} e^{-i\frac{E't}{\hbar}} C(E') \right] \\
&\quad = \frac{1}{\Delta} \int_{E_0}^{E_0+\Delta} dE \int_{E_0}^{E_0+\Delta} dE'\, C^*(E) C(E') e^{i\frac{Et}{\hbar}} e^{-i\frac{E't}{\hbar}} \int_{-\infty}^{\infty} dx\, e^{\pm i(k'-k)x} \\
&\quad = \frac{1}{\Delta} \int_{E_0}^{E_0+\Delta} dE \int_{E_0}^{E_0+\Delta} dE'\, C^*(E) C(E') e^{i\frac{Et}{\hbar}} e^{-i\frac{E't}{\hbar}} 2\pi\delta(k'-k)
\end{aligned}$$

Note that

$$\int dE' F(E,E')\delta(k'-k) = \int dk' \left(\frac{dE'}{dk'}\right) F(E,E')\delta(k'-k)$$
$$= \left[\left(\frac{dE'}{dk'}\right) F(E,E')\right]_{k'=k} = \left(\frac{dE}{dk'}\right) F(E,E)$$

so that

$$\int_{-\infty}^{\infty} dx\, g^*(x,t)g(x,t) = \frac{1}{\Delta}\int_{E_0}^{E_0+\Delta} dE \int_{E_0}^{E_0+\Delta} dE'\, C^*(E)C(E')e^{i\frac{Et}{\hbar}}e^{-i\frac{E't}{\hbar}}2\pi\delta(k'-k)$$
$$= \frac{2\pi}{\Delta}\int_{E_0}^{E_0+\Delta} dE \int_{E_0}^{E_0+\Delta} dk' \left(\frac{dE'}{dk'}\right) C^*(E)C(E')e^{i\frac{Et}{\hbar}}e^{-i\frac{E't}{\hbar}}\delta(k'-k)$$
$$= \frac{2\pi}{\Delta}\int_{E_0}^{E_0+\Delta} dE \left(\frac{dE}{dk}\right) C^*(E)C(E)e^{i\frac{Et}{\hbar}}e^{-i\frac{Et}{\hbar}}$$
$$= \frac{2\pi\hbar}{\Delta}\int_{E_0}^{E_0+\Delta} dE\, v\,|C(E)|^2 \approx \frac{2\pi\hbar}{\Delta}\left(v_0\,|C(E_0)|^2\,\Delta\right) = 2\pi\hbar v_0\,|C(E_0)|^2 \tag{3.405}$$

Now we can calculate $\mathfrak{R}$ and $\mathfrak{I}$ directly

$$1 = \langle\psi(t)\mid\psi(t)\rangle = \int_{-\infty}^{\infty} dx\psi^*(x,t)\psi(x,t) \tag{3.406}$$

$$\mathfrak{R} = \lim_{t\to+\infty}\int_{-\infty}^{x_L} dx\ \underbrace{\psi^*(x,t)\psi(x,t)}_{\psi^*_{refl}(x,t)\psi_{refl}(x,t)}$$
$$= \lim_{t\to+\infty}\int_{-\infty}^{x_L} dx\psi^*_{refl}(x,t)\psi_{refl}(x,t) = \lim_{t\to+\infty}\int_{-\infty}^{\infty} dx\psi^*_{refl}(x,t)\psi_{refl}(x,t)$$

where the last limit replacement $x_L \to +\infty$ is valid because $\psi_{refl} \neq 0$ only for $x \to -\infty (as\ t \to +\infty)$. Therefore

$$\mathfrak{R} = \lim_{t\to+\infty}\int_{-\infty}^{\infty} dx\,\psi^*_{refl}(x,t)\psi_{refl}(x,t) = 2\pi\hbar v_{L0}\left|B_L^{(1)}(E_0)\right|^2 \tag{3.407}$$

Similarly,

$$\mathfrak{I} = \lim_{t\to+\infty} \int_{x_R}^{\infty} dx \quad \underbrace{\psi^*(x,t)\psi(x,t)}_{\psi^*_{trans}(x,t)\psi_{trans}(x,t)}$$

$$= \lim_{t\to+\infty} \int_{x_R}^{\infty} dx \psi^*_{trans}(x,t)\psi_{trans}(x,t) = \lim_{t\to+\infty} \int_{-\infty}^{\infty} dx \psi^*_{trans}(x,t)\psi_{trans}(x,t)$$

where the last limit replacement $x_R \to -\infty$ is valid because $\psi_{trans} \neq 0$ only for $x \to +\infty (as\ t \to +\infty)$. Therefore

$$\mathfrak{I} = \lim_{t\to+\infty} \int_{-\infty}^{\infty} dx\, \psi^*_{trans}(x,t)\psi_{trans}(x,t) = 2\pi\hbar v_{R0} \left|A_R^{(1)}(E_0)\right|^2 \tag{3.408}$$

Note that (3.406) is valid for any t. We can evaluate this integral at $t = -\infty$ and at $t = +\infty$ to obtain relationships obeyed by $A_L^{(1)}, A_R^{(1)}, B_L^{(1)}$.

$$1 = \int_{-\infty}^{\infty} dx \psi^*(x,t)\psi(x,t) \underset{t\to-\infty}{=} \int_{-\infty}^{x_L} dx \psi^*_{inc}(x,t)\psi_{inc}(x,t)$$

$$= \int_{-\infty}^{\infty} dx \psi^*_{inc}(x,t)\psi_{inc}(x,t) = 2\pi\hbar v_{L0} \left|A_L^{(1)}(E_0)\right|^2 \tag{3.409}$$

where the last limit replacement $x_R \to +\infty$ is valid because $\psi_{inc} \neq 0$ only for $x \to -\infty (as\ t \to -\infty)$.

$$1 = \int_{-\infty}^{\infty} dx \psi^*(x,t)\psi(x,t) \underset{t\to\infty}{=} \int_{-\infty}^{x_L} dx \psi^*_{refl}(x,t)\psi_{refl}(x,t) + \int_{x_R}^{\infty} dx \psi^*_{trans}(x,t)\psi_{trans}(x,t)$$

$$= \int_{-\infty}^{\infty} dx \psi^*_{refl}(x,t)\psi_{refl}(x,t) + \int_{-\infty}^{\infty} dx \psi^*_{trans}(x,t)\psi_{trans}(x,t)$$

$$= 2\pi\hbar v_{L0} \left|B_L^{(1)}(E_0)\right|^2 + 2\pi\hbar v_{R0} \left|A_R^{(1)}(E_0)\right|^2 \tag{3.410}$$

where the last limit replacement $x_R \to -\infty$ is valid because $\psi_{trans} \neq 0$ only for $x \to +\infty (as\ t \to +\infty)$ and the last limit replacement $x_L \to +\infty$ is valid because $\psi_{refl} \neq 0$ only for $x \to -\infty (as\ t \to +\infty)$.

Summarizing we have:

$$\mathfrak{R} = 2\pi\hbar v_{L0} \left|B_L^{(1)}(E_0)\right|^2 \tag{3.411}$$

$$\mathfrak{I} = 2\pi\hbar v_{R0} \left|A_R^{(1)}(E_0)\right|^2 \tag{3.412}$$

$$1 = 2\pi\hbar v_{L0} \left|A_L^{(1)}(E_0)\right|^2 \tag{3.413}$$

$$1 = 2\pi\hbar v_{L0} \left|B_L^{(1)}(E_0)\right|^2 + 2\pi\hbar v_{R0} \left|A_R^{(1)}(E_0)\right|^2 \tag{3.414}$$

When one invokes the time-independent Schrodinger equation for $u_{CE}^{(1)}$, one obtains $B_L^{(1)}$ and $A_R^{(1)}$ in terms of $A_L^{(1)}$. $A_L^{(1)}$ is usually chosen as the arbitrary constant one gets when solving the differential equation for $u_{CE}^{(1)}$.

We then impose

$$\left|A_L^{(1)}\right|^2 = \frac{1}{2\pi\hbar v_{L0}} \tag{3.415}$$

by requiring that $\langle\psi(t) \mid \psi(t)\rangle = 1$. Then we have

$$\mathfrak{R} = 2\pi\hbar v_{L0}\left|B_L^{(1)}(E_0)\right|^2 = \left|\frac{B_L^{(1)}(E_0)}{A_L^{(1)}(E_0)}\right|^2 \tag{3.416}$$

and

$$\mathfrak{I} = 2\pi\hbar v_{R0}\left|A_R^{(1)}(E_0)\right|^2 = \frac{v_{R0}}{v_{L0}}\left|\frac{A_R^{(1)}(E_0)}{A_L^{(1)}(E_0)}\right|^2 \tag{3.417}$$

where

$$\frac{v_{R0}}{v_{L0}} = \frac{k_{R0}}{k_{L0}} \text{ because } v = \frac{\hbar k}{m} \tag{3.418}$$

Thus,

$$\mathfrak{R} = \left|\frac{B_L^{(1)}(E_0)}{A_L^{(1)}(E_0)}\right|^2 \quad , \quad \mathfrak{I} = \frac{k_{R0}}{k_{L0}}\left|\frac{A_R^{(1)}(E_0)}{A_L^{(1)}(E_0)}\right|^2 \tag{3.419}$$

where

$$u_{CE}^{(1)} = \left\{ \begin{array}{ll} A_L^{(1)}e^{ik_L x} + B_L^{(1)}e^{-ik_L x} & for \quad x < x_L \\ A_R^{(1)}e^{ik_R x} & for \quad x > x_R \end{array} \right\} \tag{3.420}$$

We also have that

$$\begin{aligned} 1 &= 2\pi\hbar v_{L0}\left|B_L^{(1)}(E_0)\right|^2 + 2\pi\hbar v_{R0}\left|A_R^{(1)}(E_0)\right|^2 \\ &= \left|\frac{B_L^{(1)}(E_0)}{A_L^{(1)}(E_0)}\right|^2 + \frac{v_{R0}}{v_{L0}}\left|\frac{A_R^{(1)}(E_0)}{A_L^{(1)}(E_0)}\right|^2 \\ &= \mathfrak{R} + \mathfrak{I} \end{aligned} \tag{3.421}$$

which simply says that the probability of finding the particle somewhere when $t \to +\infty$ is unity.

One can show that $\mathfrak{R} + \mathfrak{I} = 1$ directly from the time-independent Schrodinger equation.

Proof: Let $u = u_{CE}^{(1)}$. Then

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} + V(x)u = Eu \tag{3.422}$$

Multiplying by u^* we have

$$-\frac{\hbar^2}{2m}u^*\frac{d^2u}{dx^2}+V(x)u^*u=Eu^*u \tag{3.423}$$

The complex conjugate of this equation (V and E are real) is

$$-\frac{\hbar^2}{2m}u\frac{d^2u^*}{dx^2}+V(x)u^*u=Eu^*u \tag{3.424}$$

Subtracting (3.424) from (3.423) we get:

$$-\frac{\hbar^2}{2m}\left[u^*\frac{d^2u}{dx^2}-u\frac{d^2u^*}{dx^2}\right]=0=-\frac{\hbar^2}{2m}\frac{d}{dx}\left[u^*\frac{du}{dx}-u\frac{du^*}{dx}\right]$$

so that

$$u^*\frac{du}{dx}-u\frac{du^*}{dx}=W=\text{ constant} \tag{3.425}$$

for all x.

For $x>x_R$, $u=A_R^{(1)}e^{ik_Rx}\Rightarrow W=2ik_R\left|A_R^{(1)}\right|^2$

For $x<x_L$, $u=A_L^{(1)}e^{ik_Lx}+B_L^{(1)}e^{-ik_Lx}\Rightarrow W=2ik_L\left|A_L^{(1)}\right|^2-2ik_L\left|B_L^{(1)}\right|^2$

Equating these two expressions for the constant W we get

$$2ik_R\left|A_R^{(1)}\right|^2=2ik_L\left|A_L^{(1)}\right|^2-2ik_L\left|B_L^{(1)}\right|^2$$

$$1=\frac{k_R}{k_L}\frac{\left|A_R^{(1)}\right|^2}{\left|A_L^{(1)}\right|^2}+\frac{\left|B_L^{(1)}\right|^2}{\left|A_L^{(1)}\right|^2}=\mathfrak{I}+\mathfrak{R}$$

as we found earlier.

3.8.1.1. Summary of Important Results

$$u_{CE}^{(1)}(x)=\begin{cases}A_L^{(1)}e^{ik_Lx}+B_L^{(1)}e^{-ik_Lx} & \text{for } x<x_L\\ A_R^{(1)}e^{ik_Rx} & \text{for } x>x_R\\ \text{complicated} & \text{for } x_L<x<x_R\end{cases} \tag{3.426}$$

This solution is represented by Figure 3.30 below.

Now

$$\psi(x,t)=\frac{1}{\sqrt{\Delta}}\int_{E_0}^{E_0+\Delta}dE\,u_{CE}^{(1)}(x)e^{-i\frac{Et}{\hbar}} \tag{3.427}$$

represents a *particle* at $t=-\infty$ with the following properties:

1. It is *localized* at $x=-\infty$ at $t=-\infty$.

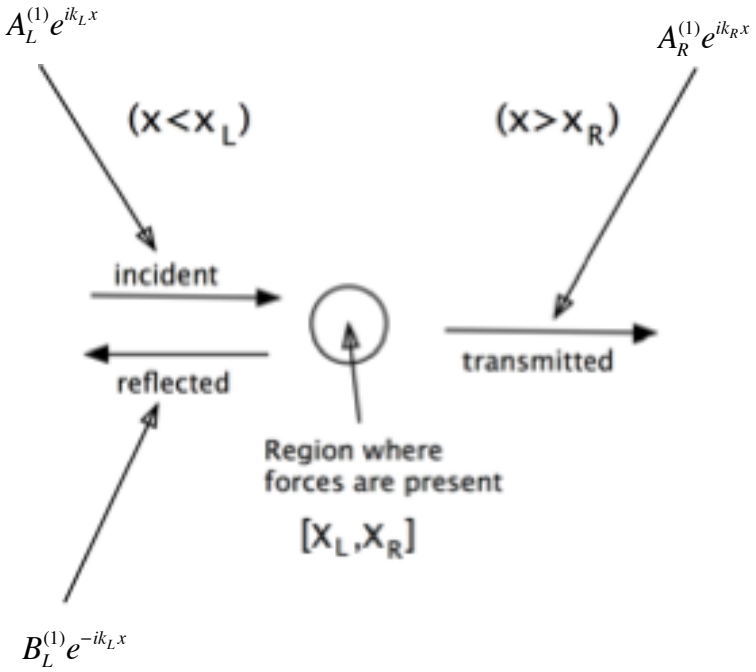


Figure 3.30: $u_{CE}^{(1)}(x)$

2. It has energy approximately equal to E (previously called E_0) with a small spread Δ in energy values.

3. It is traveling in the $+x$ direction with speed v_L at $t = -\infty$.

The transmission and reflection coefficients ($\mathfrak{I}$ and $\mathfrak{R}$) are functions of energy E and can be determined directly from $u_{CE}^{(1)}(x)$:

$$k_R = k \quad for\ transmitted\ wave = k_{trans} \tag{3.428}$$

$$k_L = k \quad for\ incident\ and\ reflected\ waves = k_{inc} = k_{refl} \tag{3.429}$$

$$\mathfrak{I} = \frac{k_{trans}}{k_{inc}} \frac{|transmitted\ wave\ coefficient|^2}{|incident\ wave\ coefficient|^2} = \frac{k_R}{k_L} \frac{\left|A_R^{(1)}\right|^2}{\left|A_L^{(1)}\right|^2} \tag{3.430}$$

$$\mathfrak{R} = \frac{|reflected\ wave\ coefficient|^2}{|incident\ wave\ coefficient|^2} = \frac{\left|B_L^{(1)}\right|^2}{\left|A_L^{(1)}\right|^2} \tag{3.431}$$

$$\mathfrak{R} + \mathfrak{I} = 1 \tag{3.432}$$

Given a potential energy $V(x)$, it is simple to find the transmission and reflection coefficients as a function of the energy E. For a particle incident from the left

with $E > V_R > V_L$, solve the time-independent Schrodinger equation for $u_{CE}^{(1)}(x)$. This will give $B_L^{(1)}$ and $A_R^{(1)}$ in terms of $A_L^{(1)}$ and E. $\mathfrak{I}^{(1)}$ and $\mathfrak{R}^{(1)}$ can then be calculated using the results just derived. For a particle incident from the right with $E > V_R > V_L$, solve the time-independent Schrodinger equation for $u_{CE}^{(2)}(x)$. This will give $B_L^{(2)}$ and $A_R^{(2)}$ in terms of $B_R^{(2)}$ and E. $\mathfrak{I}^{(2)}$ and $\mathfrak{R}^{(2)}$ can then be measured *experimentally* in the following way:

1. $\mathfrak{I}^{(1)}$ and $\mathfrak{R}^{(1)}$: Send a beam of N particles of approximate energy E toward the interaction region $[x_L, x_R]$ from the far left. If $N_{\mathfrak{R}}$ are reflected and $N_{\mathfrak{I}}$ particles are transmitted, then

$$\mathfrak{R}^{(1)} = \frac{N_{\mathfrak{R}}}{N} \text{ and } \mathfrak{I}^{(1)} = \frac{N_{\mathfrak{I}}}{N} \text{ for large } N \tag{3.433}$$

2. $\mathfrak{I}^{(2)}$ and $\mathfrak{R}^{(2)}$: Send a beam of N particles of approximate energy E toward the interaction region $[x_L, x_R]$ from the far right. If $N_{\mathfrak{R}}$ are reflected and $N_{\mathfrak{I}}$ particles are transmitted, then

$$\mathfrak{R}^{(2)} = \frac{N_{\mathfrak{R}}}{N} \text{ and } \mathfrak{I}^{(2)} = \frac{N_{\mathfrak{I}}}{N} \text{ for large } N \tag{3.434}$$

3.8.2. General Comments

1. Consider the potential energy function in Figure 3.31 above. Let $E > V_R \geq V_L$ and let $E < V_{\max}$

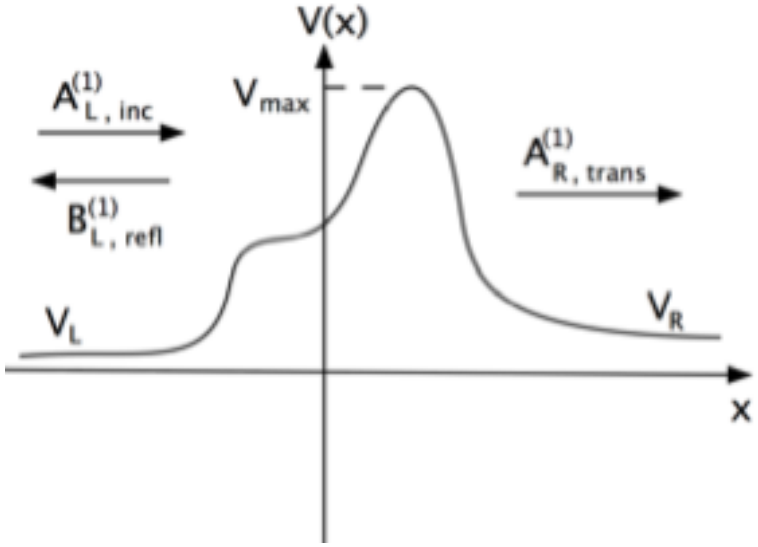


Figure 3.31: General Potential Energy Function

Classically, no particles can be transmitted because a transmitted particle

would have to pass through a region in which $E < V(x)$, that is, kinetic energy < 0. This is classically impossible!

Note: $A_R^{(1)} \neq 0$: The proof is simple: If $A_R^{(1)} = 0$, then $u_{CE}^{(1)} = 0$ for all $x > x_R$. Therefore, at a given point $x > x_R$, $u_{CE}^{(1)} = 0$ and $du_{CE}^{(1)}/dx = 0$. But these two values *uniquely* determine $u_{CE}^{(1)}(x)$ for all $x \in [-\infty, +\infty]$ because the Schrodinger equation is a second-order differential equation. Thus, $u_{CE}^{(1)} = 0$ for all $x \in [-\infty, +\infty]$. But an eigenfunction must not be identically zero.

Quantum mechanically, $\Im \neq 0$ because $A_R^{(1)} \neq 0$. Thus, there is a non-zero probability for a particle to be transmitted through the classically forbidden region. This phenomenon is called *tunneling*.

2. Suppose that $E > V_{\max}$ for the potential energy shown in Figure 3.31. Classically, all particles will be transmitted - there cannot be any reflection. Classically, a particle is reflected at a turning point, where $v = 0$ (v can change sign) or where $E = V(x)$. For $E > V_{\max}$, kinetic energy > 0 everywhere and there is no point where $v = 0$.

   Quantum mechanically, $B_L^{(1)}$ can be non-zero (although at certain energies $B_L^{(1)}$ can be zero) and there is a non-zero probability of reflection!

3. Consider the potential energy function shown in Figure 3.32 below.

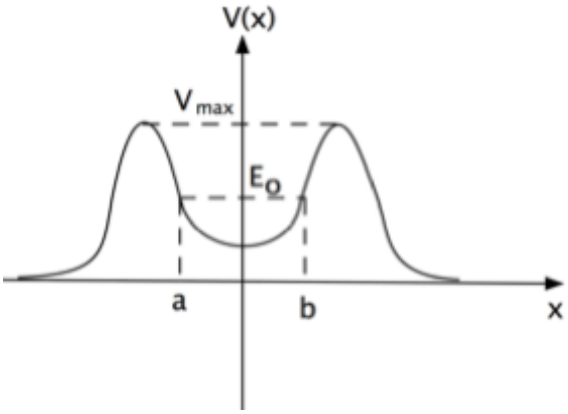


Figure 3.32: A potential energy function

Classically, a particle of energy E_0 and initially located between a and b will remain bound within this region for all t.

Quantum mechanically, we can form a wave function

$$\psi(x,t) = \frac{1}{\sqrt{\Delta}} \int_{E_0}^{E_0+\Delta} dE\, e^{-i\frac{Et}{\hbar}} \left\{ C^{(1)}(E) u_{CE}^{(1)}(x) + C^{(2)}(E) u_{CE}^{(2)}(x) \right\} \tag{3.435}$$

with Δ small and such that $\psi(x,t)$ is negligible outside the region $[a,b]$ at $t = 0$. However, $\lim_{t\to\infty} \psi(x,t) = 0$ for any fixed (finite) x (see earlier discussion). Thus, the particle (the probability actually) eventually *leaks* out (*tunnels* out) of the bound region $[a,b]$. At $t \to \infty$, the probability of finding the particle inside the bound region $[a,b]$ is zero!

One might refer to the state described by the wave function as an unstable bound state - at $t = 0$ the particle is bound within $[a,b]$; however, after a sufficiently long time, the particle will have completely tunneled out of the bound region. Contrast this situation with the case of a true bound state (well potential already discussed). This particular potential energy function has no bound states. A bound state $u_n(x)$ is normalizable.

Thus,

$$\psi(x,t) = u_n(x) e^{-i\frac{E_n t}{\hbar}} \tag{3.436}$$

is a possible wave function (with no integration over energies occurring). $|\psi(x,t)| = |u_n(x)|$ for all t. In particular,

$$\lim_{t\to+\infty} |\psi(x,t)| = |u_n(x)| \tag{3.437}$$

which approaches zero as $|x| \to \infty$ and which is non-negligible in some bounded region of the $x-$axis - the particle stays bound for all time!

3.9. The Symmetrical Finite Potential Well

We now consider the potential energy function shown in Figure 3.33 below.

We found the bound states for this potential earlier. In this case, we have added a constant potential energy $-V_0$ everywhere in space to the previous symmetrical well in order to obtain this symmetrical well.

We have

$$V_R = V_L = 0 \quad , \quad E > 0 \tag{3.438}$$

$$k_R = k_L = k = \sqrt{\frac{2mE}{\hbar^2}} \quad , \quad k_2 = \sqrt{\frac{2m(E+V_0)}{\hbar^2}} \tag{3.439}$$

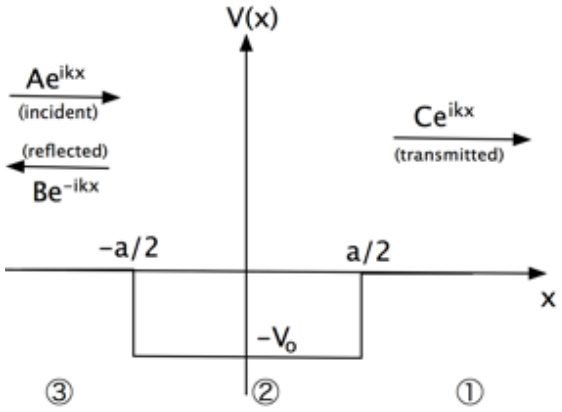


Figure 3.33: A potential energy function

Let a particle of energy $E > 0$ be incident from the left. We therefore look for the eigenfunction $u(x)$ of the form:

$$u(x) = \begin{cases} u_3(x) = Ae^{ikx} + Be^{-ikx} & \text{for } x < -a/2 \\ u_1(x) = Ce^{ikx} & \text{for } x > a/2 \\ u_2(x) = \alpha e^{ik_2 x} + \beta e^{-ik_2 x} & \text{for } -a/2 < x < a/2 \end{cases} \tag{3.440}$$

so that

$$\mathfrak{I} = \frac{k}{k}\frac{|C|^2}{|A|^2} = \frac{|C|^2}{|A|^2} \text{ and } \mathfrak{R} = \frac{|B|^2}{|A|^2} = 1 - \mathfrak{I} \tag{3.441}$$

To find $\mathfrak{I}$ we must find C in terms of A.

Note: $V(x) = V(-x)$ which implies that $[\Pi, H] = 0$. However, the particular $u(x)$ we are looking for (a particle incident from the left) is *not* a parity eigenfunction. This does not contradict the compatibility of H and parity because the eigenfunctions of H for $E > 0$ are 2–fold degenerate and a given eigenfunction of H for $E > 0$ need not be a simultaneous eigenfunction of parity. Compatibility only implies that there exists 2 linearly independent simultaneous eigenfunctions of H and parity for $E > 0$. For a bound state, $E_n < 0$, there is non-degeneracy and the corresponding eigenfunction of H must be an eigenfunction of parity also.

Matching $u(x)$ at the boundaries $a/2$ and $-a/2$ we have:

$$u_1(a/2) = u_2(a/2) \Rightarrow Ce^{i\frac{ka}{2}} = \alpha e^{i\frac{k_2 a}{2}} + \beta e^{-i\frac{k_2 a}{2}} \tag{3.442}$$

$$\frac{du_1(a/2)}{dx} = \frac{du_2(a/2)}{dx} \Rightarrow ikCe^{i\frac{ka}{2}} = ik_2\alpha e^{i\frac{k_2 a}{2}} - ik_2\beta e^{-i\frac{k_2 a}{2}} \tag{3.443}$$

$$u_2(-a/2) = u_3(-a/2) \Rightarrow \alpha e^{-i\frac{k_2 a}{2}} + \beta e^{i\frac{k_2 a}{2}} = Ae^{-i\frac{ka}{2}} + Be^{i\frac{ka}{2}} \tag{3.444}$$

$$\frac{du_2(-a/2)}{dx} = \frac{du_3(-a/2)}{dx} \Rightarrow ik_2\alpha e^{-i\frac{k_2 a}{2}} - ik_2\beta e^{i\frac{k_2 a}{2}} = ikAe^{-i\frac{ka}{2}} - ikBe^{i\frac{ka}{2}} \tag{3.445}$$

We have 4 linear equation in the 5 unknowns A, B, C, α, β. We can solve for B, C, α, β in terms of A. A straightforward calculation gives:

$$\frac{C}{A} = \frac{4e^{-ika}}{4\cos(k_2 a) - 2i\left(\frac{k_2}{k} + \frac{k}{k_2}\right)\sin(k_2 a)} \tag{3.446}$$

Thus,

$$\begin{aligned}
\mathfrak{I} = \frac{|C|^2}{|A|^2} &= \frac{16}{16\cos^2(k_2 a) + 4\left(\frac{k_2}{k} + \frac{k}{k_2}\right)^2 \sin^2(k_2 a)} \\
&= \frac{16}{16(1 - \sin^2(k_2 a)) + 4\left(\frac{k_2}{k} + \frac{k}{k_2}\right)^2 \sin^2(k_2 a)} \\
&= \frac{16}{16 + 4\left(\left(\frac{k_2}{k} + \frac{k}{k_2}\right)^2 - 4\right)\sin^2(k_2 a)} = \frac{16}{16 + 4\left(\frac{k_2}{k} - \frac{k}{k_2}\right)^2 \sin^2(k_2 a)} \\
&= \frac{1}{1 + \frac{1}{4}\left(\frac{k_2}{k} - \frac{k}{k_2}\right)^2 \sin^2(k_2 a)}
\end{aligned} \tag{3.447}$$

with

$$k = \sqrt{\frac{2mE}{\hbar^2}} \quad , \quad k_2 = \sqrt{\frac{2m(E + V_0)}{\hbar^2}} \tag{3.448}$$

Notes:

1. $E = 0 \Rightarrow k = 0,\ k_2 \neq 0 \Rightarrow \mathfrak{I} = 0$
2. $E \to \infty \Rightarrow k \to k_2 \neq 0 \Rightarrow \mathfrak{I} \to 1$
3. $\mathfrak{I} = 1$ for $k_2 a = N\pi$, $N = 0, 1, 2, ...$, where we must accept only energies $E \geq 0$, which further restricts N.

$$k_2 = \frac{2\pi}{\lambda_2} \Rightarrow N = \frac{a}{(\lambda_2/2)} \text{ for } \mathfrak{I} = 1 \tag{3.449}$$

$N = a/(\lambda_2/2)$ corresponds to the number of half-wavelengths in the well and implies that this must be an integer for $\mathfrak{I} = 1$. The energies at which $\mathfrak{I} = 1$ are called *resonances*.

$$\mathfrak{I} = 1 \text{for} N^2\pi^2 = k_2^2 a^2 = \frac{2m(E+V_0)a^2}{\hbar^2} \tag{3.450}$$

Therefore,

$$E_{resonance} = -V_0 + \frac{\hbar^2\pi^2 N^2}{2ma^2} \text{for} N = 1, 2, 3, ... \tag{3.451}$$

with the restriction that only N values occur for which $E_{res} \geq 0$ ($N = 0$ is clearly not allowed). It is interesting to note that the resonance energies occur at the bound-state energies of the well

$$V(x) = \begin{cases} -V_0 & \text{for } -a/2 < x < -a/2 \\ \infty & \text{for } |x| > a/2 \end{cases} \tag{3.452}$$

A plot of of $\mathfrak{I}(E)$ is shown in Figure 3.34 below.

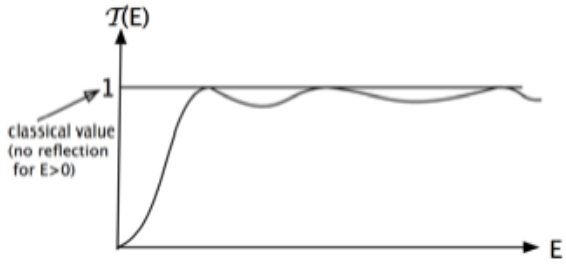


Figure 3.34: Transmission coefficient showing resonances

3.10. The Complex Energy Plane

Let

$$V(x) = \begin{cases} 0 & \text{for } x < x_L \\ 0 & \text{for } x > x_R \\ arbitrary\, V(x) & \text{for } x_L < x < x_R \end{cases} \tag{3.453}$$

where $V_L = V_R = 0$ and $V(x)$ is a *real* function of x.

We want to define a transmission coefficient $\mathfrak{I}(E)$ for all complex values of E. Such an object has physical significance only for E real and positive (where the physical continuum states are); however, it has interesting properties for

complex E.

The equation

$$\frac{d^2\phi}{dx^2} = \frac{2m}{\hbar^2}\left[V(x) - E\right]\phi \tag{3.454}$$

has 2 linearly independent solutions for any complex E. The additional requirement that $|\phi|$ does not become infinite as $|x| \to \infty$ restricts the allowed values of E to the real energies in the spectrum of the hermitian H.

To define $\mathfrak{I}(E)$ for complex E, we simply drop this additional requirement and look at solutions to the differential equation for complex E.

We have

$$for \quad x < x_L \quad \frac{d^2\phi}{dx^2} = -\frac{2mE}{\hbar^2}\phi \tag{3.455}$$

$$for \quad x > x_R \quad \frac{d^2\phi}{dx^2} = -\frac{2mE}{\hbar^2}\phi \tag{3.456}$$

Let

$$k = \sqrt{\frac{2mE}{\hbar^2}} \tag{3.457}$$

Because E is complex, we must define $\sqrt{E}$ carefully. Let $E = |E|\, e^{i\varepsilon}$. Therefore, $\sqrt{E} = |E|^{1/2}\, e^{i\varepsilon/2}$.

Now, if $\varepsilon \to \varepsilon + 2\pi N$, then $E \to E$, that is, E does not change when we change its phase by a multiple of 2π, but $\sqrt{E} \to \sqrt{E}e^{i\pi N} = (-1)^N\sqrt{E}$. Thus, $\sqrt{E}$ is not well-defined unless we specify the range in which ε lies. Let ε be in $[0, 2\pi]$. Then $\sqrt{E}$ is well-defined except when E is positive real, that is,

$$\varepsilon = 0 \Rightarrow \sqrt{E} = |E|^{1/2} \tag{3.458}$$

but

$$\varepsilon = 2\pi \Rightarrow \sqrt{E} = |E|^{1/2}\, e^{i\pi} = -\,|E|^{1/2} \tag{3.459}$$

Thus, there is a line of discontinuity in $\sqrt{E}$ along the positive real axis (called a *cut*). This situation is shown in Figure 3.35 below in a plot of complex energy plane

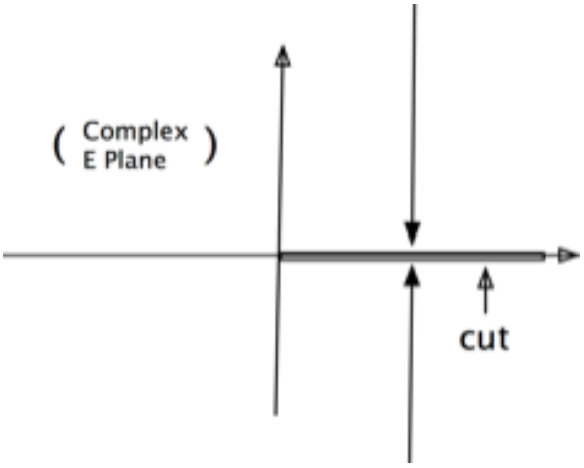
For E not on the cut,

$$\sqrt{E} = |E|^{1/2}\left[\cos\frac{\varepsilon}{2} + i\sin\frac{\varepsilon}{2}\right] \tag{3.460}$$

with ε in $[0, 2\pi]$ implying that $\mathrm{Im}(\sqrt{E}) > 0$. Now if

$$k = \sqrt{\frac{2mE}{\hbar^2}} = \alpha + i\beta \tag{3.461}$$

$$\varepsilon \to 0$$
$$\sqrt{E} \to |E|^{1/2}$$



$$\varepsilon \to 2\pi$$
$$\sqrt{E} \to -|E|^{1/2}$$

Figure 3.35: Cut in Complex E Plane

then $\beta > 0$ for E not positive real. We note that $k \to$ *positive real* if we approach the cut from above ($\varepsilon \to 0$).

Now,

$$for \quad x < x_L \quad \phi = Ae^{ikx} + Be^{-ikx} \tag{3.462}$$
$$for \quad x > x_R \quad \phi = Ce^{ikx} + De^{-ikx} \tag{3.463}$$

with E and k complex.

C and D may be chosen as the 2 arbitrary constants in the solution of the 2^{nd}–order differential equation. A and B will then depend on C and D as well as E. Consider the solution for $D = 0$ and $C = 1$.

$$for \quad x < x_L \quad \phi = A(E)e^{ikx} + B(E)e^{-ikx} \tag{3.464}$$
$$for \quad x > x_R \quad \phi = e^{ikx} \tag{3.465}$$

Define

$$\mathfrak{I}(E) = \frac{1}{|A(E)|^2} \tag{3.466}$$

for complex E.

For E positive real, this is the physical transmission coefficient if $k > 0$, that is,

$$A(E)e^{ikx} \quad \textit{is the incident wave in the } +x \textit{ direction} \tag{3.467}$$

$$B(E)e^{-ikx} \quad \textit{is the wave reflected toward the } -x \textit{ direction} \tag{3.468}$$

$$e^{ikx} \quad \textit{is the transmitted wave in the } +x \textit{ direction} \tag{3.469}$$

Thus, the physical $\mathfrak{I}(E)$ is obtained as we approach the cut from above ($\varepsilon \to 0$).

For positive, real E and $k > 0$, we have $\mathfrak{I} + \mathfrak{R} = 1$ with $\mathfrak{I}$ and $\mathfrak{R}$ non-negative (this is not true for complex E). Thus, $\mathfrak{I} \neq \infty$ as we approach the cut from above.

Does $\mathfrak{I} = \infty$ at any complex value of E? Equivalently, does $A(E) = 0$ at any complex value of E? We have

$$\phi(x) = \begin{cases} A(E)e^{i\alpha x}e^{-\beta x} + B(E)e^{-i\alpha x}e^{+\beta x} & \text{for } x < x_L \\ e^{i\alpha x}e^{-\beta x} & \text{for } x > x_R \end{cases} \tag{3.470}$$

with $\beta > 0$ except on the cut (E positive real).

For $\beta > 0$, $A(E) = 0$ if and only if ϕ is normalizable because

$$e^{-\beta x} \to \infty \text{ for } x \to -\infty$$
$$e^{+\beta x} \to 0 \text{ for } x \to -\infty$$
$$e^{-\beta x} \to 0 \text{ for } x \to +\infty$$

But ϕ is normalizable if and only if E is a bound state energy eigenvalue. Furthermore, the hermiticity of H implies that these energy eigenvalues occur only for real E. For $V_R = V_L = 0$, the bound states (if they exist) have energy E real and negative. Thus, in the cut complex energy plane ($\beta > 0$).

Thus, $\mathfrak{I}(E) = \infty$ (called *poles* in complex E plane) if and only if E = a bound-state energy as shown in Figure 3.36 above.

We have also shown that $\mathfrak{I}(E)$ is finite as we approach the cut from above ($\varepsilon \to 0$).

As a check, consider the symmetrical potential well above. We have

$$\mathfrak{I}(E) = \left|\frac{C}{A}\right|^2 = \left|\frac{4e^{-ika}}{4\cos(k_2 a) - 2i\left(\frac{k_2}{k} + \frac{k}{k_2}\right)\sin(k_2 a)}\right|^2 = \infty \tag{3.471}$$

if

$$4\cos(k_2 a) = 2i\left(\frac{k_2}{k} + \frac{k}{k_2}\right)\sin(k_2 a) \tag{3.472}$$

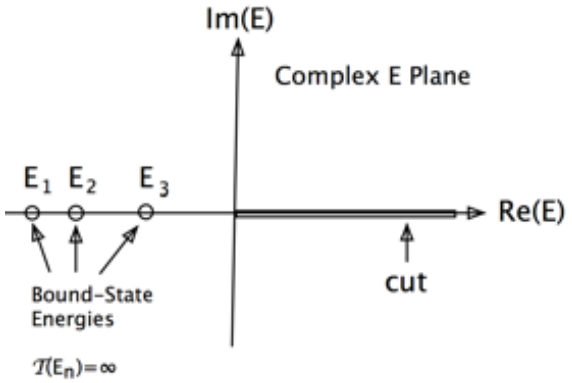


Figure 3.36: Cut and Poles in Complex E Plane

or

$$\begin{aligned} 4 &= 2i\left(\frac{k_2}{k}+\frac{k}{k_2}\right)\frac{\sin(k_2a)}{\cos(k_2a)} \\ &= 2i\left(\frac{k_2}{k}+\frac{k}{k_2}\right)\frac{2\sin(k_2a/2)\cos(k_2a/2)}{\cos^2(k_2a/2)-\sin^2(k_2a/2)} \\ &= 2i\left(\frac{k_2}{k}+\frac{k}{k_2}\right)\frac{2}{\cot(k_2a/2)-\tan(k_2a/2)} \end{aligned}$$

Therefore, $\mathfrak{I}(E) = \infty$ if

$$\cot(k_2a/2)-\tan(k_2a/2) = i\left(\frac{k_2}{k}+\frac{k}{k_2}\right) \tag{3.473}$$

or

$$\cot(k_2a/2) = -\frac{k_2}{ik} \text{ and } \tan(k_2a/2) = -\frac{ik}{k_2} \tag{3.474}$$

Now let $k = i\tilde{k}$. We then have

$$\cot(k_2a/2) = -\frac{k_2a/2}{\tilde{k}a/2} \text{ and } \tan(k_2a/2) = -\frac{\tilde{k}a/2}{k_2a/2} \tag{3.475}$$

for $\mathfrak{I}(E) = \infty$. These are just the transcendental equations which determine the bound states (look at our earlier solution and recall that $-V_0$ must be added to $V(x)$.

3.11. Problems

3.11.1. Free Particle in One-Dimension - Wave Functions

Consider a free particle in one-dimension. Let

$$\psi(x,0) = Ne^{-\frac{(x-x_0)^2}{4\sigma^2}}e^{i\frac{p_0x}{\hbar}}$$

where x_0, p_0 and σ are real constants and N is a normalization constant.

(a) Find $\tilde{\psi}(p,0)$

(b) Find $\tilde{\psi}(p,t)$

(c) Find $\psi(x,t)$

(d) Show that the *spread* in the spatial probability distribution

$$\wp(x,t) = \frac{|\psi(x,t)|^2}{\langle \psi(t) \mid \psi(t) \rangle}$$

increases with time.

3.11.2. Free Particle in One-Dimension - Expectation Values

For a free particle in one-dimension

$$H = \frac{p^2}{2m}$$

(a) Show $\langle p_x \rangle = \langle p_x \rangle_{t=0}$

(b) Show $\langle x \rangle = \left[\frac{\langle p_x \rangle_{t=0}}{m} \right] t + \langle x \rangle_{t=0}$

(c) Show $(\Delta p_x)^2 = (\Delta p_x)^2_{t=0}$

(d) Find $(\Delta x)^2$ as a function of time and initial conditions. HINT: Find

$$\frac{d}{dt} \langle x^2 \rangle$$

To solve the resulting differential equation, one needs to know the time dependence of $\langle x p_x + p_x x \rangle$. Find this by considering

$$\frac{d}{dt} \langle x p_x + p_x x \rangle$$

3.11.3. Time Dependence

Given

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

with

$$H = \frac{\vec{p} \cdot \vec{p}}{2m} + V(\vec{x})$$

(a) Show that $\frac{d}{dt} \langle \psi(t) \mid \psi(t) \rangle = 0$

(b) Show that $\frac{d}{dt}\langle x\rangle = \left\langle \frac{p_x}{m} \right\rangle$

(c) Show that $\frac{d}{dt}\langle p_x\rangle = \left\langle -\frac{\partial V}{\partial x} \right\rangle$

(d) Find $\frac{d}{dt}\langle H\rangle$

(e) Find $\frac{d}{dt}\langle L_z\rangle$ and compare with the corresponding classical equation $\left(\vec{L} = \vec{x} \times \vec{p}\right)$

3.11.4. Continuous Probability

If $p(x) = xe^{-x/\lambda}$ is the probability density function over the interval $0 < x < \infty$, find the mean, standard deviation and most probable value(where probability density is maximum) of x.

3.11.5. Square Wave Packet

Consider a free particle, initially with a well-defined momentum p_0, whose wave function is well approximated by a plane wave. At $t = 0$, the particle is localized in a region $-a/2 \le x \le a/2$, so that its wave function is

$$\psi(x) = \begin{cases} Ae^{ip_0 x/\hbar} & -a/2 \le x \le a/2 \\ 0 & \text{otherwise} \end{cases}$$

(a) Find the normalization constant A and sketch $\mathrm{Re}(\psi(x))$, $\mathrm{Im}(\psi(x))$ and $|\psi(x)|^2$

(b) Find the momentum space wave function $\tilde{\psi}(p)$ and show that it too is normalized.

(c) Find the uncertainties Δx and Δp at this time. How close is this to the minimum uncertainty wave function.

3.11.6. Uncertain Dart

A dart of mass $1\,kg$ is dropped from a height of $1\,m$, with the intention to hit a certain point on the ground. Estimate the limitation set by the uncertainty principle of the accuracy that can be achieved.

3.11.7. Find the Potential and the Energy

Suppose that the wave function of a (spinless) particle of mass m is

$$\psi(r,\theta,\phi) = A\frac{e^{-\alpha r} - e^{-\beta r}}{r}$$

where A, α and β are constants such that $0 < \alpha < \beta$. Find the potential $V(r,\theta,\phi)$ and the energy E of the particle.

3.11.8. Harmonic Oscillator wave Function

In a harmonic oscillator a particle of mass m and frequency ω is subject to a parabolic potential $V(x) = m\omega^2 x^2/2$. One of the energy eigenstates is $u_n(x) = Axexp(-x^2/x_0^2)$, as sketched below.

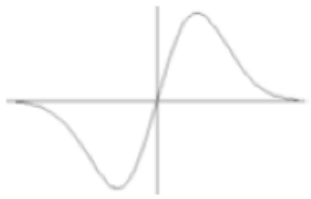


Figure 3.37: A Wave Function

(a) Is this the ground state, the first excited state, second excited state, or third?

(b) Is this an eigenstate of parity?

(c) Write an integral expression for the constant A that makes $u_n(x)$ a normalized state. Evaluate the integral.

3.11.9. Spreading of a Wave Packet

A localized wave packet in free space will spread due to its initial distribution of momenta. This wave phenomenon is known as *dispersion*, arising because the relation between frequency ω and wavenumber k is not linear. Let us look at this in detail.

Consider a general wave packet in free space at time $t = 0$, $\psi(x, 0)$.

(a) Show that the wave function at a later time is

$$\psi(x,t) = \int_{-\infty}^{\infty} dx'\, K(x,x';t)\psi(x')$$

where

$$K(x,x';t) = \sqrt{\frac{m}{2\pi i\hbar t}} exp\left[\frac{im(x-x')^2}{2\hbar t}\right]$$

is known as the *propagator*. [HINT: Solve the initial value problem in the usual way - Decompose $\psi(x, 0)$ into stationary states (here plane waves), add the time dependence and then re-superpose].

(b) Suppose the initial wave packet is a Gaussian

$$\psi(x,0) = \frac{1}{(2\pi a^2)^{1/4}} e^{ik_0 x} e^{-x^2/4a^2}$$

Show that it is normalized.

(c) Given the characteristic width a, find the characteristic momentum p_c, energy E_c and the time scale t_c associated with the packet. The time t_c sets the scale at which the packet will spread. Find this for a macroscopic object of mass $1\,g$ and width $a = 1\,cm$. Comment.

(d) Show that the wave packet probability density remains Gaussian with the solution

$$P(x,t) = |\psi(x,t)|^2 = \frac{1}{\sqrt{2\pi a(t)^2}} exp\left[-\frac{(x-\hbar k_0/m)^2}{2a(t)^2}\right]$$

with $a(t) = a\sqrt{1+t^2/t_c^2}$.

3.11.10. The Uncertainty Principle says ...

Show that, for the 1-dimensional wavefunction

$$\psi(x) = \begin{cases} (2a)^{-1/2} & |x| < a \\ 0 & |x| > a \end{cases}$$

the rms uncertainty in momentum is infinite (HINT: you need to Fourier transform ψ). Comment on the relation of this result to the uncertainty principle.

3.11.11. Free Particle Schrodinger Equation

The time-independent Schrodinger equation for a free particle is given by

$$\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial \vec{x}}\right)^2 \psi(\vec{x}) = E\psi(\vec{x})$$

It is customary to write $E = \hbar^2 k^2/2m$ to simplify the equation to

$$\left(\nabla^2 + k^2\right)\psi(\vec{x}) = 0$$

Show that

(a) a plane wave $\psi(\vec{x}) = e^{ikz}$

and

(b) a spherical wave $\psi(\vec{x}) = e^{ikr}/r$ $(r = \sqrt{x^2+y^2+z^2})$

satisfy the equation. Note that in either case, the wavelength of the solution is given by $\lambda = 2\pi/k$ and the momentum by the de Broglie relation $p = \hbar k$.

3.11.12. Double Pinhole Experiment

The double-slit experiment is often used to demonstrate how different quantum mechanics is from its classical counterpart. To avoid mathematical complications with Bessel functions, we will discuss two pinholes rather than two slits. Consider the setup shown below

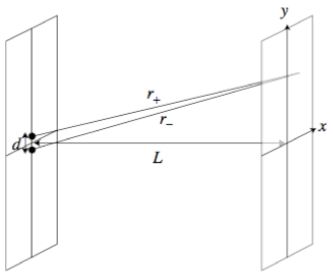


Figure 3.38: The Double Pinhole Setup

Suppose you send in an electron along the $z-$axis onto a screen at $z = 0$ with two pinholes at $x = 0$, $y = \pm d/2$. At a point (x, y) on another screen at $z = L \gg d$, λ the distance from each pinhole is given by $r_\pm = \sqrt{x^2 + (y \mp d/2)^2 + L^2}$.

The spherical waves from each pinhole are added at the point on the screen and hence the wave function is

$$\psi(x, y) = \frac{e^{ikr_+}}{r_+} + \frac{e^{ikr_-}}{r_-}$$

where $k = 2\pi/\lambda$. Answer the following questions.

(a) Considering just the exponential factors, show that constructive interference appears approximately at

$$\frac{y}{r} = n\frac{\lambda}{d} \qquad (n \in \mathbb{Z}) \tag{3.476}$$

where $r = \sqrt{c^2 + y^2 + L^2}$.

(b) Make a plot of the intensity $|\psi(0, y)|^2$ as a function of y, by choosing $k = 1$, $d = 20$ and $L = 1000$, Use the Mathematica Plot function. The intensity $|\psi(0, y)|^2$ is interpreted as the probability distribution for the electron to be detected on the screen, after repeating the same experiment many, many times.

(c) Make a contour plot of the intensity $|\psi(x, y)|^2$ as a function of x and y, for the same parameters, using the Mathematica ContourPlot function.

(d) If you place a counter at both pinholes to see if the electron has passed one of them, all of a sudden the wave function *collapses*. If the electron is observed to pass through the pinhole at $y = +d/2$, the wave function becomes

$$\psi_+(x, y) = \frac{e^{ikr_+}}{r_+}$$

If it is oberved to pass through the pinhole at $y = -d/2$, the wave function becomes

$$\psi_-(x, y) = \frac{e^{ikr_-}}{r_-}$$

After repeating this experiment many times with a 50:50 probability for each of the pinholes, the probability on the screen will be given by

$$|\psi_+(x, y)|^2 + |\psi_-(x, y)|^2$$

instead. Plot this function on the $y-$axis and also show the contour plot to compare its pattern to the case when you do not place a counter. What is the difference from the case without the counter?

3.11.13. A Falling Pencil

Using the uncertainty principle estimate how long a time a pencil can be balanced on its point.