

# Lecture Notes on Quantum Mechanics & Quantum Computing Part - I

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# 1. Lecture 1

## 1.1 Wave packet

A localized Wave Function is called a wave packet. A wave packet consists of different waves of differing amplitude, different phases and different wavelengths. An isolated wave doesn't make much physical sense in the quantum realm. A wave packet is what we associate with the physical world. As seen in the De Broglie wave-matter relation. Here the  $\lambda$  is associated with the wave packet's group velocity.

$$p = \frac{h}{\lambda} \quad (1.1)$$

One common Misconception, electron doesn't stay in the first orbit of a hydrogen atom. It has the highest probability of being found there. Even if we send all photons of same energy, the outcome will still be random.

When we measure a quantum phenomenon, the wave packet's superposition disappears and we are left with one particular value.

## 1.2 Interpretations of Quantum Mechanics

### 1.2.1 Copenhagen Interpretation

The idea is that quantum mechanics is intrinsically indeterministic, with probabilities calculated using the Born rule, and the principle of complementarity, which states that objects have certain pairs of complementary properties which cannot all be observed or measured simultaneously. Moreover, the act of "observing" or "measuring" an object is irreversible, no truth can be attributed to an object except according to the results of its measurement.

**The main one used in the lectures. Simply put unless you measure something it doesn't exist**

### 1.2.2 Pilot wave theory

Particles, which always have positions, are guided by the wavefunction. The wavefunction evolves according to the Schrödinger wave equation, and the wavefunction never collapses. The theory takes place in a single spacetime, is non-local, and is deterministic. The simultaneous determination of a particle's position and velocity is subject to the usual uncertainty principle constraint.

### 1.2.3 Many world theory

A universal wavefunction obeys the same deterministic, reversible laws at all times; in particular there is no (indeterministic and irreversible) wavefunction collapse associated with measurement. The phenomena associated with measurement are claimed to be explained by decoherence, which occurs when states interact with the environment. More precisely, the parts of the wavefunction describing observers become increasingly entangled with the parts of the wavefunction describing their experiments. Although all possible outcomes of experiments continue to lie in the wavefunction's support, the times at which they become correlated with observers effectively "split" the universe into mutually unobservable alternate histories.

## 1.3 Quantum Entanglement

### 1.3.1 Einstein's approach

Suppose one mother particle is broken such that two particles move to the opposite side of the universe. Now if we measure the spin of one of those particles, we may find up/down spin. But because of this measurement, the wavefunction collapses which in turn means that the other particle will surely be in the opposite spin.

$$v_p v_g > c^2$$

**group velocity cannot be greater than light velocity.**

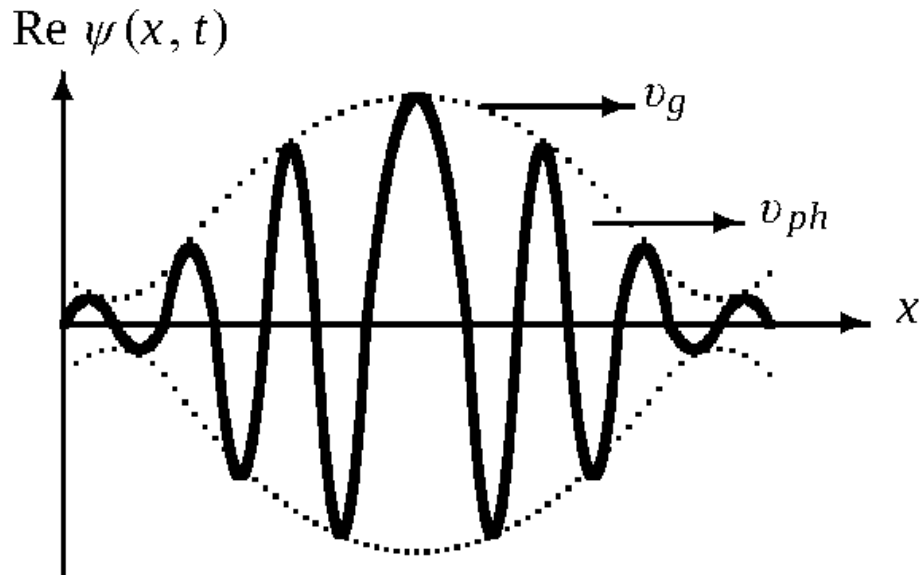


Figure 1.1: Phase velocity and group velocity

### 1.3.2 Bell's Inequality

Bell deduced that if measurements are performed independently on the two separated particles of an entangled pair, then the assumption that the outcomes depend upon hidden variables within each half implies a mathematical constraint on how the outcomes on the two measurements are correlated. This constraint would later be named the Bell inequality. Bell then showed that quantum physics predicts correlations that violate this inequality. Consequently, the only way that hidden variables could explain the predictions of quantum physics is if they are "nonlocal", which is to say that somehow the two particles were able to interact instantaneously no matter how widely the two particles are separated.

Everything in this world is predetermined and only the unconscious particles know the outcome in advance.

### 1.3.3 Locality vs Non Locality

Consider electric field, gravitational field effects as local and at infinity they become non local effects. Simply local means some sort of connection or bond, non local means completely separated, no means of communication in real sense. Quantum Mechanics suggests non local effects.

### 1.3.4 EPR Paradox

Einstein proposed a thought experiment that if two particles are entangled and we measure the position or momentum of one of the particles then the second particles corresponding position or state gets fixed. Which implies before the measurement both the position and momentum were in a superposition state. But this is not possible due to Heisenberg's uncertainty principle.

### 1.3.5 Fourier basics

Consider the following for orthonormal basis.

$$\Psi(\vec{r}, t) = \sum_{-\infty}^{\infty} C_n \Phi(\vec{r}, t)$$

$$\int_{-\infty}^{\infty} |\Psi(\vec{r}, t)|^2 dV = 1 = \sum_{-\infty}^{\infty} |C_n|^2$$

**Food for thought:** Bound electrons have discrete energy but not free electrons. Consider this from Fourier perspective

Engineering notation and Physics notation

$$i = -j$$

## 2. Lecture 2

### 2.1 Fourier

#### 2.1.1 Orthonormal functions

Let  $\phi_i$  &  $\phi_j$  be two functions such that  $\phi_i, \phi_j \in C[a, b]$

$$\langle \phi_i | \phi_j \rangle = \int_a^b \phi_i^*(x) \phi_j(x) dx$$

if we get

$$\int_a^b \phi_i^*(x) \phi_j(x) dx = \delta_{ij} = \begin{cases} 0, & \text{if } i \neq j \\ 1, & \text{if } i=j \end{cases}$$

then we call the functions orthonormal

#### 2.1.2 Fourier Series

Let  $\{\phi_i(x)\}$  be such orthonormal basis for  $f(x)$  then

$$f(x) = \sum_i C_i \phi_i(x)$$

now to find any  $C_i$  we can do the following

$$\begin{aligned} \langle \phi_k(x) | f(x) \rangle &= \int_a^b \phi_k^*(x) \sum_i C_i \phi_i(x) dx \\ &= \sum_i C_i \delta_{ik} |\phi_i|^2 \\ &= C_k |\phi_k|^2 \end{aligned}$$

thus we get

$$C_k = \frac{\langle \phi_k | f(x) \rangle}{|\phi_k|^2}$$

Fourier coefficients.

then for a set of orthonormal basis consisting of sin and cosine functions we get the following

$$f(x) = \frac{a_0}{2} + \sum_n a_n \sin\left(\frac{nx\pi}{l}\right) + \sum_m b_m \cos\left(\frac{mx\pi}{l}\right)$$

for complex equations commonly seen in physics text books

$$\begin{aligned} f(x) &= \sum_{-\infty}^{\infty} C_n e^{i \frac{nx\pi}{L}} \\ C_m &= \frac{1}{2L} \int_{-L}^L f(x) e^{i \frac{mx\pi}{L}} dx \end{aligned}$$

Inner product notation problem

$$\begin{aligned} \text{Bra - Ket} &= \langle \phi_m | \phi_n \rangle \\ \text{Inner - product} &= \langle \phi_n, \phi_m \rangle \\ &= \int \phi_m^* \phi_n dx \end{aligned}$$

### 2.1.3 Why do we need fourier in quantum mechanics

$$\Psi_{Before} = \sum C_n \phi_n$$

$$\Psi_{After} = \phi_n$$

The function collapses to a definitive value after the experiment.

$$\langle \text{final state} | \text{all states} \rangle$$

**for hilbert space and quantum mechanics(covered in later lectures)** we consider  $\Psi$  to be a function of everything,if we want to get the Energy of that state we simply take the energy projection of  $\Psi$

### 2.1.4 Fourier Transform and wave particle duality

Starting from the complex representation of fourier Series.

$$f(x) = \sum_{-\infty}^{\infty} \frac{1}{2L} \int_{-L}^L f(x) e^{\left(\frac{-inx\pi}{L}\right)} e^{\left(\frac{inx\pi}{L}\right)} dx$$

Let

$$k_n = \frac{n\pi}{L}$$

$$\Delta k = k_{n+1} - k_n = \frac{\pi}{L}$$

Then,

$$\frac{1}{2L} = \frac{\Delta k}{2\pi}$$

$$f(x) = \sum_{-\infty}^{\infty} \frac{\Delta k}{2\pi} \int_{-L}^L f(x) e^{-ik_n x} e^{ik_n x} dx$$

letting

$$L \rightarrow \infty$$

$$\Delta k \rightarrow 0$$

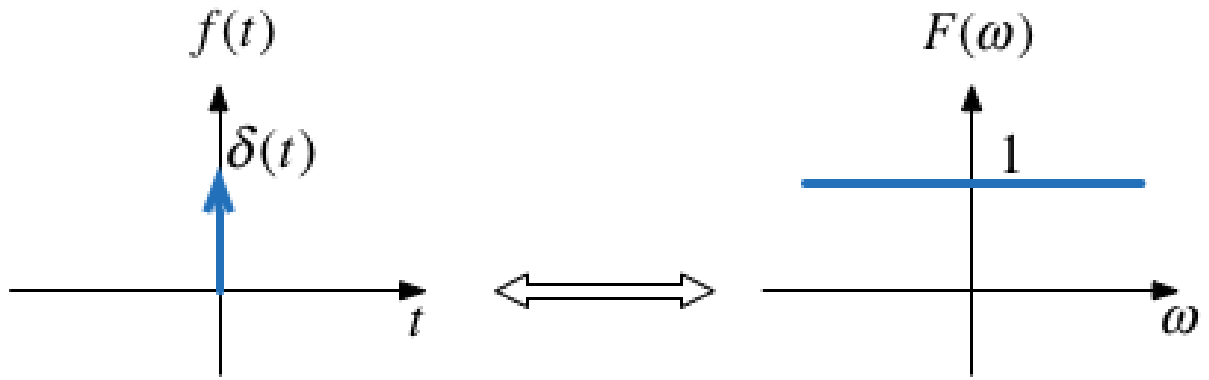
we get the followings transformations

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left\{ \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} f(x) e^{-ikx} dx \right\} e^{ikx} dk$$

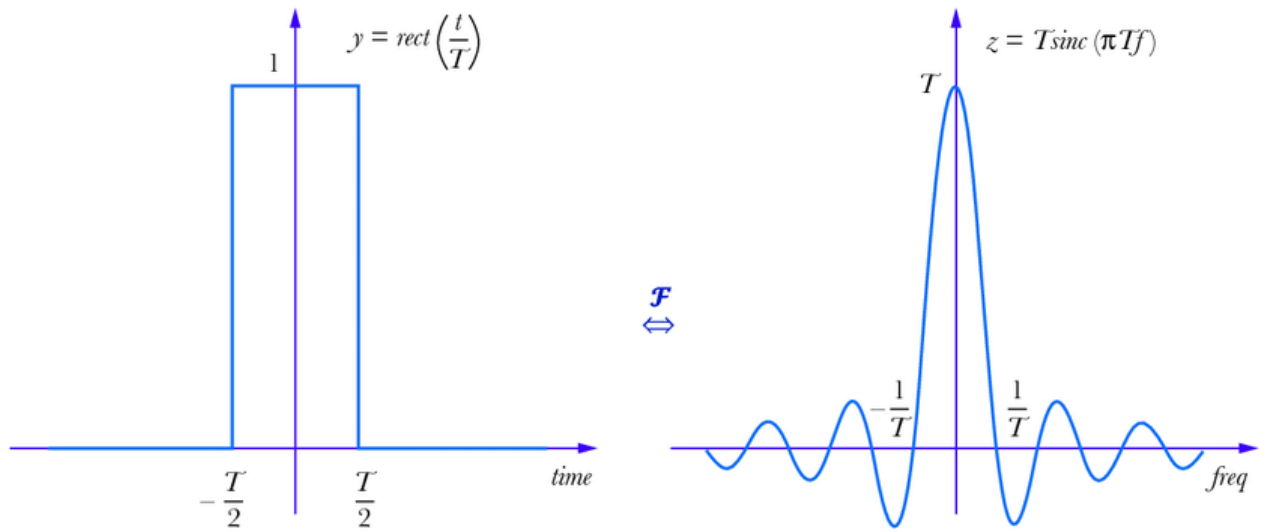
Thus we get the following

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k) e^{ikx} dk$$

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx$$



(a)



(b)

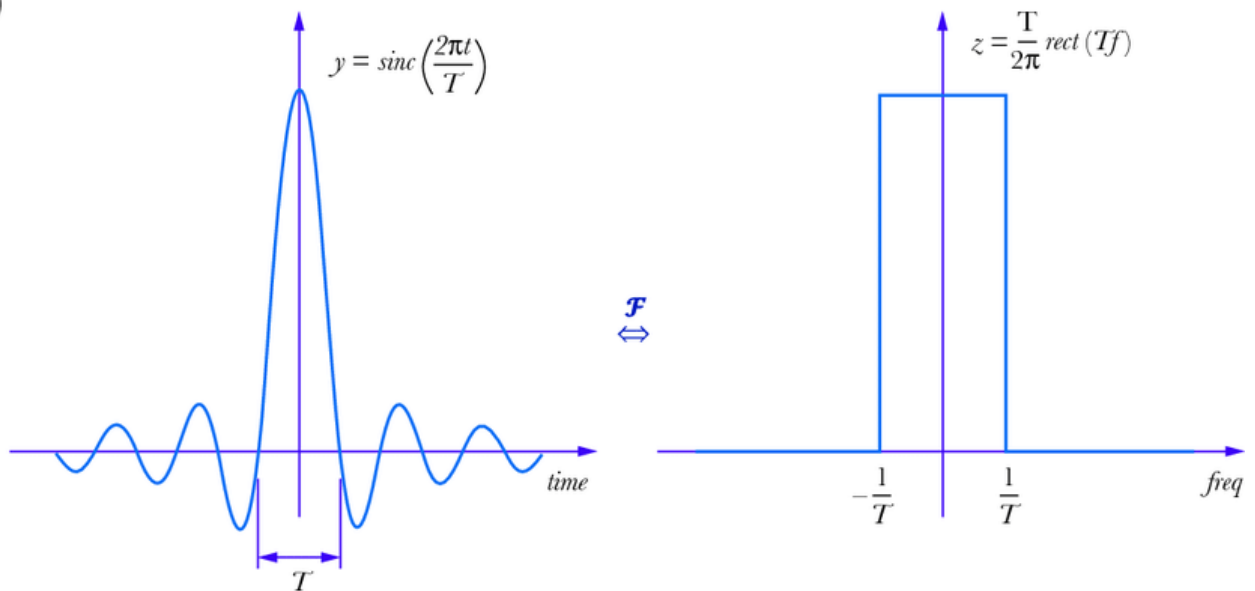


Figure 2.1: Some common fourier Transform. The first one is of dirac delta function denoting a single position or a single energy in position or energy space. The second and third are of localized wave packets and their corresponding fourier transform which is a sinc function

## 2.2 Single slit and double slit using quantum mechanics

### 2.2.1 Single Slit

Consider a Single slit experiment. The intensity in this case is a sinc function.

$$I = I_0 \left( \frac{\sin(az)}{z} \right)^2$$

Even if we send a single photon we will still see an interference pattern. If we change the slit's length, The interference pattern will further spread out. Here the intensity is dependent on  $z$ , but  $z$  is inversely proportional to wavelength. Also from De broglie's relation we know that momentum and wave length of a quantum particle is inversely proportional. Which means the intensity is proportional to momentum. As we are causing the position to be fixed, the momentum is getting more spread out, Which is causing the interference intensity to also spread out.

Another way to look at it, take the fourier of position function, which turns out to be a dirac delta function the more we narrow the slit. The fourier of dirac delta function is a spread out sinc function.

### 2.2.2 Double Slit

For double slit experiment consider the first slit and second slit wave function to be in a superposition state

$$|\Psi\rangle = C_1 |\Psi_1\rangle + C_2 |\Psi_2\rangle$$

so if we dont make any measurements, the final state vector's probability or intensity will be the

$$I = I(\text{first wave state}) + I(\text{second wave state}) + \text{interference terms}$$



## 3. Lecture 3

### 3.1 Motion created in quantum entity

Motion is created in quantum entity due to interference and dispersion. Consider the solution of the schrodinger equation.

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

The solution of the schrodinger equation can be written as below using the separation of variables.

$$\Psi(x, t) = \Psi(x, 0)e^{\frac{-iEt}{\hbar}}$$

and the probability density can thus be calculated without the time varying part.

$$|\Psi(x, t)|^2 = |\Psi(x, 0)|^2$$

So for a particular calculation or measurement we get a particular  $E_n$ . but after that measurement when we are not looking the state will once again change, we call this time varying phenomena as dispersion of wave packets.

When light wave travels through space, it gives a non-dispersive behaviour, but matter wave gives a dispersive behaviour.

**If a system has a well defined energy, then time evolution for that system doesn't occur, it remains in a stationary state. It remains frozen in time. That's why electrons in an orbit cannot have a fixed energy at every observation**

In order for motion to appear the wave function must be in a linear superposition of stationary states in interference.

$$\Psi = A\Psi(x, 0)e^{\frac{-iE_1t}{\hbar}} + B\Psi(x, 0)e^{\frac{-iE_2t}{\hbar}}$$

The time evolution in more general term.

$$\Psi(\vec{r}, t) = \sum_n C_n \Phi(\vec{r}, 0) e^{\frac{-iE_n t}{\hbar}}$$

if we confine our discussion to a two energy state of hydrogen atom with energies  $E_1$  and  $E_2$  then the probability becomes

$$\begin{aligned} P(x, t) &= |\Psi(x, t)|^2 \\ &= \frac{1}{a} |C_1\psi(x, t) + C_2\psi(x, t)|^2, [a = \sqrt{C_1^2 + C_2^2}] \\ &= \frac{1}{a} \{C_1^2\psi^2(x, 0) + C_2^2\psi^2(x, 0) + 2C_1C_2\cos(\frac{(E_2 - E_1)t}{\hbar})\} \end{aligned}$$

The interference term here consists of time varying variable. Thus its probability changes with time.

When no measurement is being done on the electrons in the figure 1 they obey the schrodinger's equation. But after being measured they behave like a particle.

**When no measurement is being done, the quantum entity follows schrodinger's equation and follows time evolution. But when a measurement is done the other states get destroyed and we see only one state. schrodinger's equation doesn't handle this.**

[measurement] $\psi = (\text{energy value})\psi_{\text{particular value}}$
--

### 3.2 Dirac delta

The Dirac delta can be loosely thought of as a function on the real line which is zero everywhere except at the origin, where it is infinite,

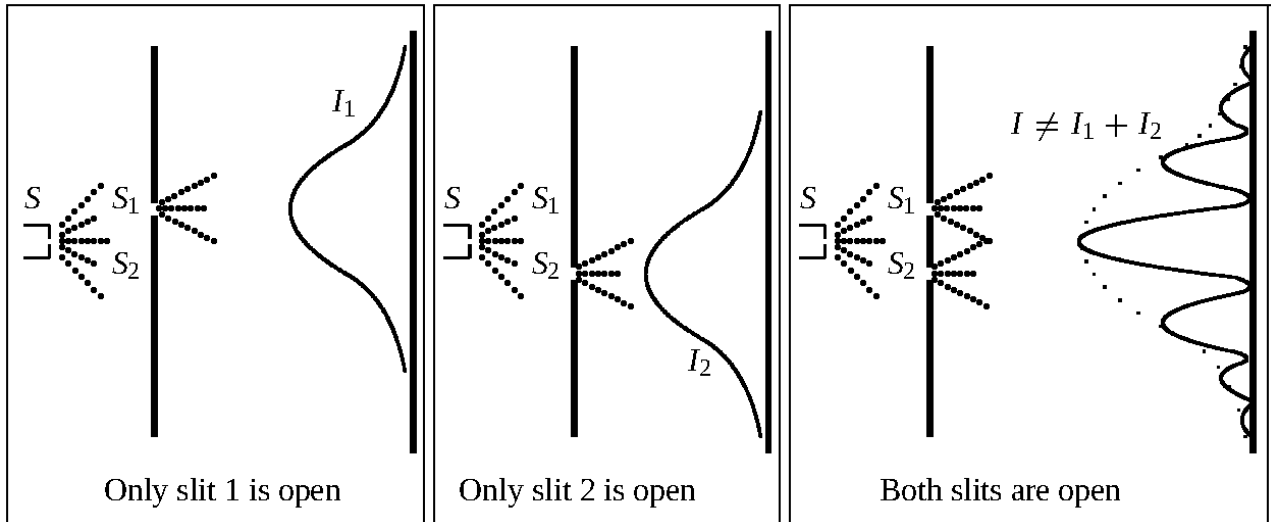


Figure 3.1: Sources are electrons. When both slits are open the total intensity is equal to sum of  $I_1$  and  $I_2$  plus some oscillating term

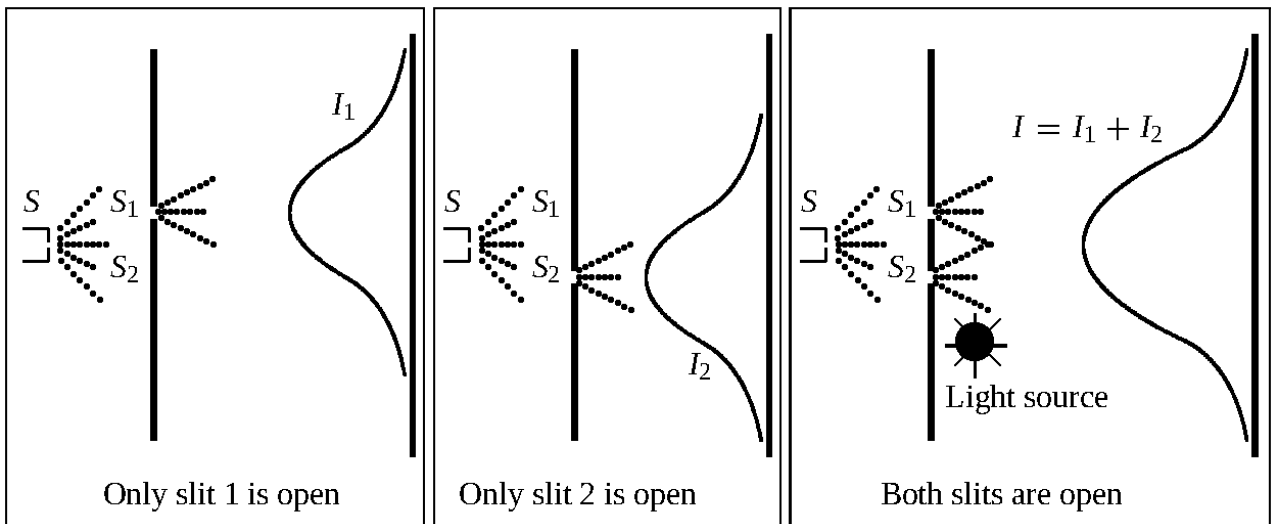


Figure 3.2: Sources are electrons. When both slits are open the total intensity is equal to the sum of  $I_1$  and  $I_2$  in the presense of an observer

$$\delta(x - x_n) \simeq \begin{cases} +\infty, & \text{if } x = x_n \\ 0, & \text{if } x \neq x_n \end{cases}$$

and

$$\int_{-\infty}^{\infty} \delta(x - x_n) = 1$$

so we get

$$\int_{-\infty}^{\infty} f(x) \delta(x - a) = f(a)$$

### 3.3 Operators in quantum mechanics

using

$$\Psi(x) = \sum_n C_n \psi(x)$$

and

$$\Psi_{bm}(x) = \sum_n \Psi(x_n)$$

we can write

$$\begin{aligned} \Psi_{bm}(x) &= \sum_n \delta(x - x_n) \Psi(x) \\ &= \sum_n \delta(x - x_n) C_n \psi(x) \end{aligned}$$

the same thing can also be written by changing the x variable to momentum variable or time or energy.  
the below Operators are written while the measurement domain in position

### 3.4 Fourier transformation Properties

The Operators used in quantum mechanics can be directly derived from fourier transformation Properties.

Table 3.1: Operators in quantum mechanics in space domain

$f(x)$	Any function of position, such as $x$ , or potential $V(x)$	$f(x)$
$p_x$	$x$ component of momentum ( $y$ and $z$ same form)	$\frac{\hbar}{i} \frac{\partial}{\partial x}$
$E$	Hamiltonian (time independent)	$\frac{p_{op}^2}{2m} + V(x)$
$E$	Hamiltonian (time dependent)	$i\hbar \frac{\partial}{\partial t}$
$KE$	Kinetic energy	$\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$
$L_z$	$z$ component of angular momentum	$-i\hbar \frac{\partial}{\partial \phi}$

Table 3.2: Fourier transformation Properties

Function, $f(t)$	Fourier Transform, $F(\omega)$
<i>Definition of Inverse Fourier Transform</i>	<i>Definition of Fourier Transform</i>
$f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(\omega) e^{j\omega t} d\omega$	$F(\omega) = \int_{-\infty}^{\infty} f(t) e^{-j\omega t} dt$
$f(t - t_0)$	$F(\omega) e^{-j\omega t_0}$
$f(t) e^{j\omega_0 t}$	$F(\omega - \omega_0)$
$f(\alpha t)$	$\frac{1}{ \alpha } F\left(\frac{\omega}{\alpha}\right)$
$F(t)$	$2\pi f(-\omega)$
$\frac{d^n f(t)}{dt^n}$	$(j\omega)^n F(\omega)$
$(-jt)^n f(t)$	$\frac{d^n F(\omega)}{d\omega^n}$
$\int_{-\infty}^t f(\tau) d\tau$	$\frac{F(\omega)}{j\omega} + \pi F(0) \delta(\omega)$
$\delta(t)$	1
$e^{j\omega_0 t}$	$2\pi \delta(\omega - \omega_0)$
$\text{sgn}(t)$	$\frac{2}{j\omega}$

Table 3.3: Some important fourier transformation

**Table of Common Functions and their Fourier Transforms**

Function name	Function in the time domain	Fourier Transform (in the frequency domain)
	$w(t)$	$\hat{W}(f)$
<b>Dirac delta</b>	$\delta(t)$	1
<b>Constant</b>	1	$\delta(f)$
<b>Cosine</b>	$\cos(2\pi f_0 t)$	$\frac{\delta(f - f_0) + \delta(f + f_0)}{2}$
<b>Sine</b>	$\sin(2\pi f_0 t)$	$\frac{\delta(f - f_0) - \delta(f + f_0)}{2j}$
<b>Unit step function</b>	$u(t) = \begin{cases} 0, & \text{if } t < 0 \\ 1, & \text{if } t \geq 0 \end{cases}$	$\frac{1}{j\omega}$ (for $\omega = 2\pi f$ )
<b>Decaying exponential (for <math>t &gt; 0</math>)</b>	$e^{-\alpha t}u(t),$	$\frac{1}{\alpha + j2\pi f}, \alpha > 0$
<b>Box or rectangle function</b>	$\text{rect}(at) = \begin{cases} 0, & \text{if }  at  > \frac{1}{2} \\ 1, & \text{if }  at  \leq \frac{1}{2} \end{cases}$	$\frac{1}{ a } \text{sinc}\left(\frac{f}{a}\right) = \frac{\sin(\pi f/a)}{\pi f/a}$
<b>Sinc function</b>	$\text{sinc}(at) = \frac{\sin(\pi at)}{\pi at}$	$\frac{1}{ a } \text{rect}\left(\frac{f}{a}\right)$
<b>Comb function</b>	$\sum_{n=-\infty}^{\infty} \delta(t - nT)$	$\frac{1}{T} \sum_{k=-\infty}^{\infty} \delta\left(f - \frac{k}{T}\right)$
<b>Gaussian</b>	$e^{-\alpha t^2}$	$\sqrt{\frac{\pi}{\alpha}} e^{-\frac{(\pi f)^2}{\alpha}}$

### 3.5 Dispersion of electron

Considering a free electron we get the following

$$\begin{aligned}E &= \frac{p^2}{2m} \\ \hbar\omega &= \frac{1}{2m}(\hbar^2 k^2) \\ \omega &= \frac{\hbar}{2m}k^2\end{aligned}$$

which is a non linear relation which is why **electron shows dispersive nature.**  
For photon ,we can write

$$\begin{aligned}E &= pc \\ \hbar\omega &= \hbar kc \\ \omega &= kc\end{aligned}$$

**photon doesnt show any dispersion**

for photon we can also use the Operators to get the electro-magnetic wave equation.

$$\begin{aligned}E^2 &= p^2 c^2 \\ \hat{E}\hat{E}y &= \hat{p}\hat{p}c^2 y \\ (i\hbar\frac{\partial}{\partial t})^2 y &= c^2[(-i\hbar\nabla)^2]y \\ \frac{1}{c^2}\frac{\partial^2 y}{\partial t^2} &= \nabla^2 y\end{aligned}$$

we can use y as it follows a non-dispersive nature but its not a general case

## 4. Lecture 4

### 4.1 Postulates of quantum mechanics from wave mechanics

1. **Description of the system** For every object ,there is an associated complex,single valued,continuous wave function  $\Psi(x, y, z, t)$  where x,y,z space coordinates, and t is the time.
2. **Description of Physical Quantities** Physical observables connected with quantum objects are represented by hermitian operators that operate on the wave function.
3. **Expansion Postulate** The eigenfunctions of the operators are orthonormal and form a basis.
4. **Measurement Postulate** If a Measurement of Physical observable represented by operators is carried out then the associated coefficient of the state is the probability of finding that state.

$$A|\Psi\rangle = A \sum_n C_n \psi_n$$

The probability of finding  $\psi_n$  is given by  $C_n^2$

5. **Reduction Postulate** After Measurement , the state found will remain static. Before the Measurement, the state is in a superposition. But after the Measurement has been made the state will remain in a definite state.
6. **Time evolution of a system** Between measurements, the time evolution of the system is given by the time dependent Schrodinger equation.

### 4.2 Homogeneity of free space

Changing the coordinates of the system doesnt change the quantum behaviour of the system

$$\begin{aligned}\psi(x) &\longrightarrow C(p) \\ \psi(x - x_0) &\longrightarrow C(p)e^{ikx_0} \\ |\psi(x - x_0)|^2 &\longrightarrow |C(p)|^2\end{aligned}$$

so we will get the same behaviour in all coordinates.

### 4.3 Shifting property and conservation of probability

From the previous section we know that a confined position of a particle gives a spread out sinc form in the momentum domain. The reason behind this is the conservation of probability in both domain.

$$\int_{-\infty}^{\infty} |\Psi(\vec{r})|^2 d^3r = \int_{-\infty}^{\infty} |\Psi(\vec{p})|^2 d^3p \quad (4.1)$$

### 4.4 Separation of variables

$$\begin{aligned}i\hbar \frac{\partial \Psi(x, t)}{\partial t} &= -\frac{\hbar^2}{2m} \nabla^2 \Psi(x, t) + V(x) \Psi(x, t) \\ i\hbar \frac{\partial \phi(t)}{\partial t} \psi(x) &= -\frac{\hbar^2}{2m} \phi(t) \nabla^2 \psi(x) + V(x) \psi(x) \phi(t) \\ \frac{i\hbar}{\phi(t)} \frac{\partial \phi(t)}{\partial t} &= E = \frac{-\hbar^2}{2m\psi(x)} \nabla^2 \psi(x) + V(x)\end{aligned} \quad (4.2)$$



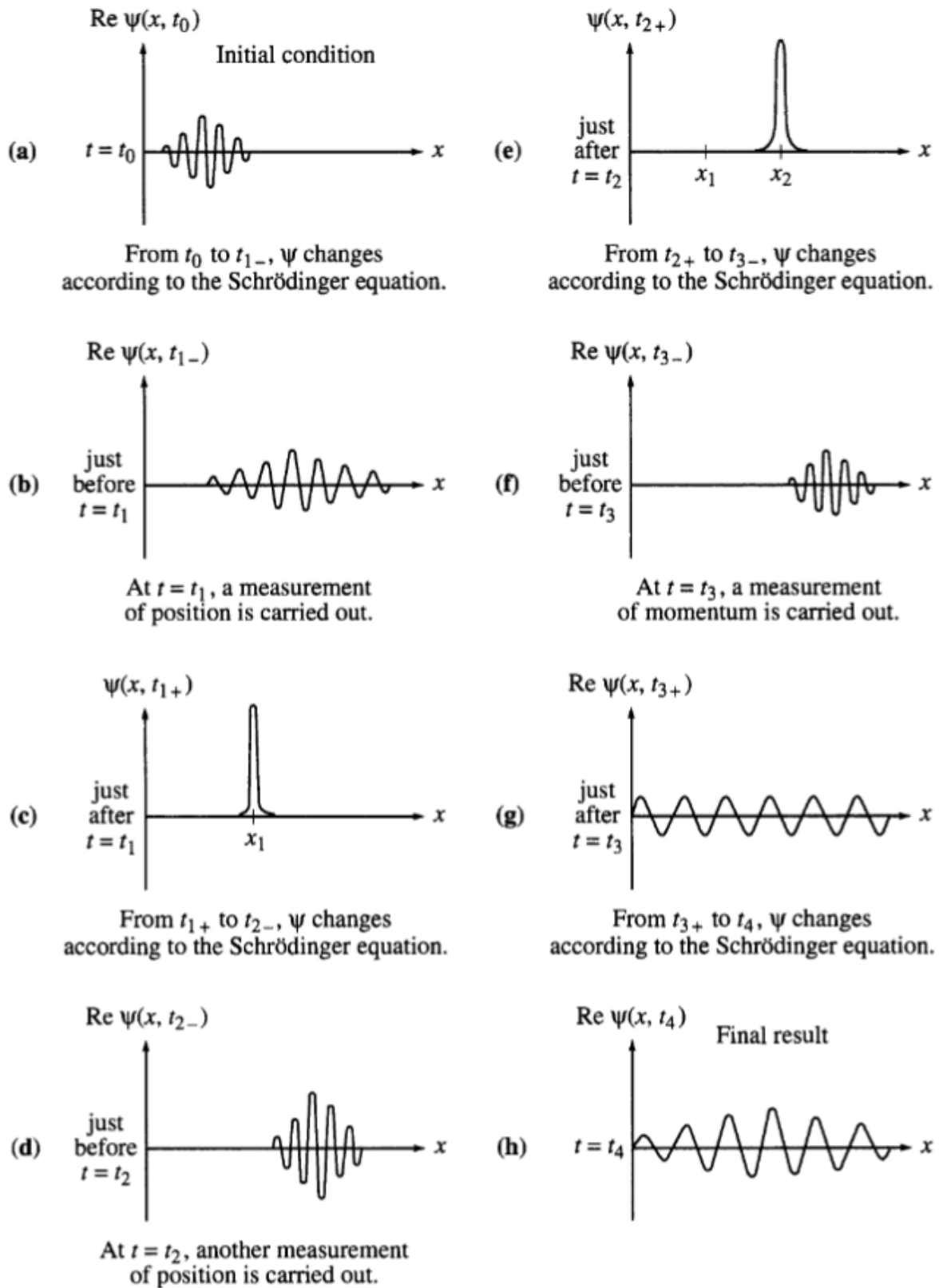


Figure 4.1: Time evolution of a wave packet due to dispersion

Then we get the following solutions

$$\begin{aligned}\frac{\partial \phi}{\partial t} - \frac{\phi E}{i\hbar} &= 0 \\ \phi(t) &= Ce^{\frac{-iEt}{\hbar}}\end{aligned}\tag{4.3}$$

incorporating the constant into the main solution we get

$$\Psi(x, t) = \psi(x)e^{\frac{-iEt}{\hbar}}$$

as its a linear equation the actual solution

$$\Psi(x, t) = \sum_n C_n \psi_n(x, 0) e^{\frac{-iE_n t}{\hbar}}\tag{4.4}$$

## 4.5 Expectation value and Standard Deviation

$$\bar{x} = \frac{1}{N} \sum_n x n(x)$$

$$\bar{x} = \sum_n x P(x)$$

For continuous variable

$$\bar{x} = \int x P(x) dx$$

for quantum mechanics from borns interpretation we can write

$$\bar{x} = \int_{-\infty}^{\infty} x |\Psi(x, t)|^2 dx$$

for momentum space

$$\bar{p} = \int_{-\infty}^{\infty} p |\Phi(p, t)|^2 dp$$

but we can use the operators to extract information from the  $\Psi(x, t)$

$$\bar{p} = \int_{-\infty}^{\infty} \Psi^*(x, t) \hat{p} \Psi(x, t) dx$$

$$\bar{p} = \langle \Psi | \hat{p} | \Psi \rangle$$

and the Standard Deviation

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

## 5. Lecture 5

### 5.1 Localized wave function in potential wells

For a particle trapped in a potential well, The wave function is localized due to the boundary condition. On the other hand for a particle found in a space, it is localized due to the superposition of many wave functions causing constructive interference in a particular region and destructive interference in other regions.

Consider a particle of mass  $m$  trapped in a one dimensional box with the potential defined as below

$$V(x) = \begin{cases} 0, & \text{if } 0 \leq x \leq a \\ \infty & \text{if otherwise} \end{cases}$$

The schrodinger equation is

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + 0 = E\Psi$$

which can be written as

$$\frac{\partial^2 \Psi}{\partial x^2} + k^2 \Psi = 0$$

where

$$k^2 = \frac{2mE}{\hbar^2}$$

The solution to such equation is given by

$$\Psi(x) = A \sin(kx) + B \cos(kx)$$

using boundary conditions at  $x = 0$ ,

$$\Psi(0) = A \sin(0) + B \cos(0)$$

To satisfy this  $B$  has to be 0. also for  $x = a$

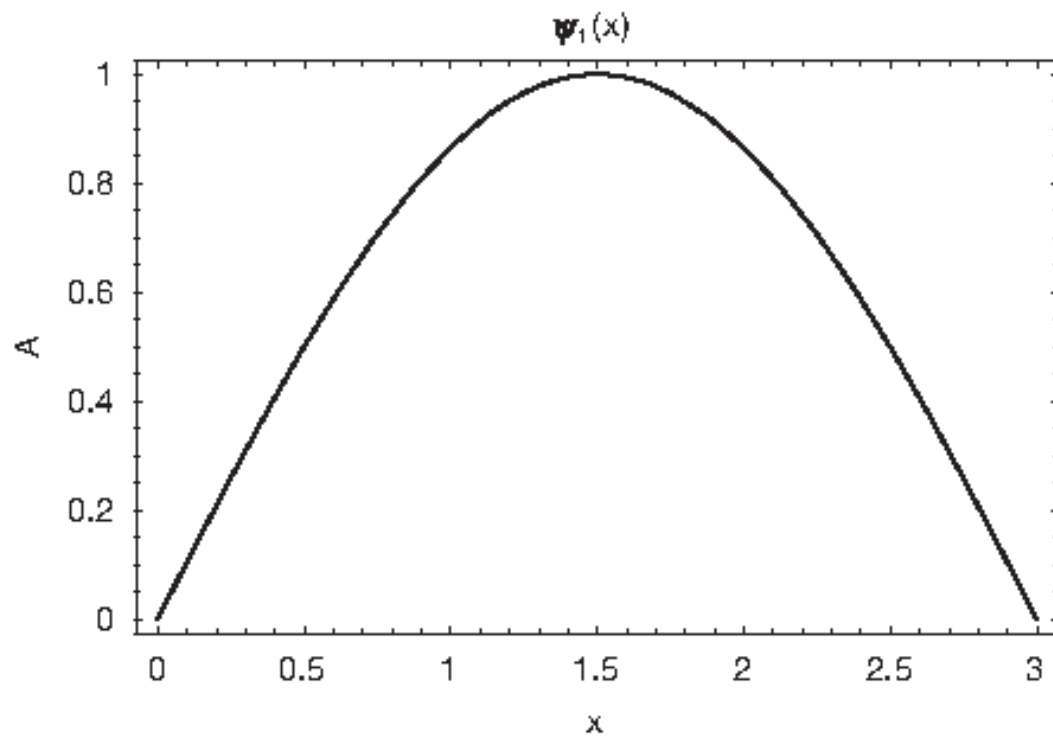
$$ka = n\pi$$

which turns out to be

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}, n \in \mathbb{N}$$

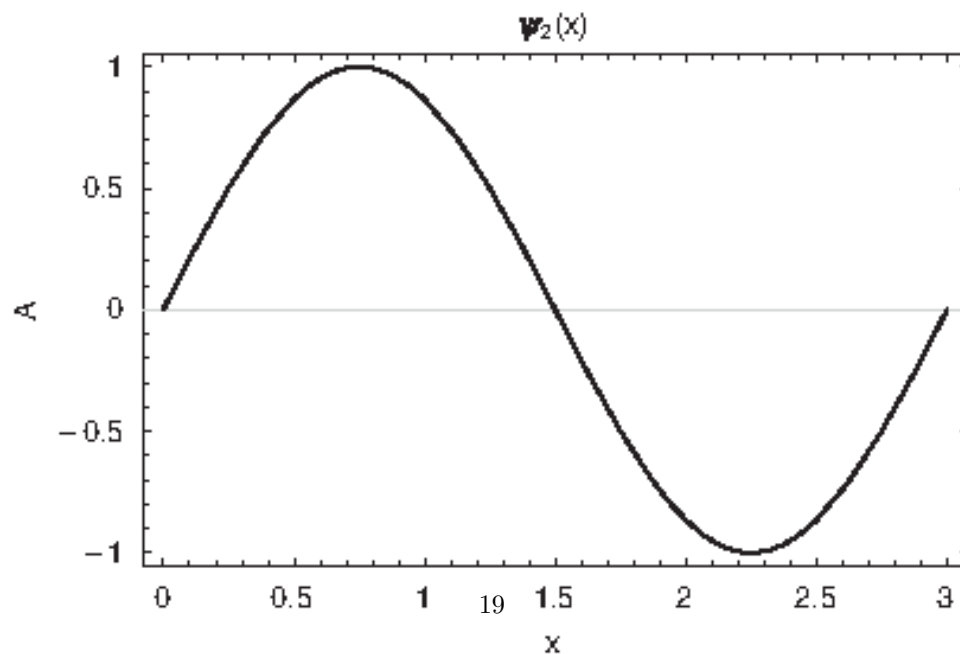
These are the energy eigen values of the bound state in a potential well.

$$\psi_1(x) = A \sin\left(\frac{\pi}{a}x\right), \text{ with energy } E_1 = \frac{\pi^2 \hbar^2}{2ma^2} :$$



**Fig. 2-2**

$$\psi_2(x) = A \sin\left(\frac{2\pi}{a}x\right), \text{ with energy } E_2 = \frac{4\pi^2 \hbar^2}{2ma_2} = 4E_1$$



## 5.2 Continuity equation

The probability density is

$$P(x, t) = \Psi^*(x, t)\Psi(x, t)$$

Then

$$\frac{\partial P}{\partial t} = \Psi^* \frac{\partial \Psi}{\partial t} + \frac{\partial \Psi^*}{\partial t} \Psi$$

Using the schrodinger equation we can write the following

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x} \left[ \frac{i\hbar}{2m} \left( \Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x} \Psi \right) \right]$$

This can be further written as

$$\frac{\partial P}{\partial t} + \frac{\partial J}{\partial x} = 0$$

or in a more general sense

$$\frac{\partial P}{\partial t} + \nabla \cdot \mathbf{J} = 0$$

This is known as the Continuity equation for probability in quantum mechanics. This implies that the probability of finding a particle in a region decreased as time goes on.

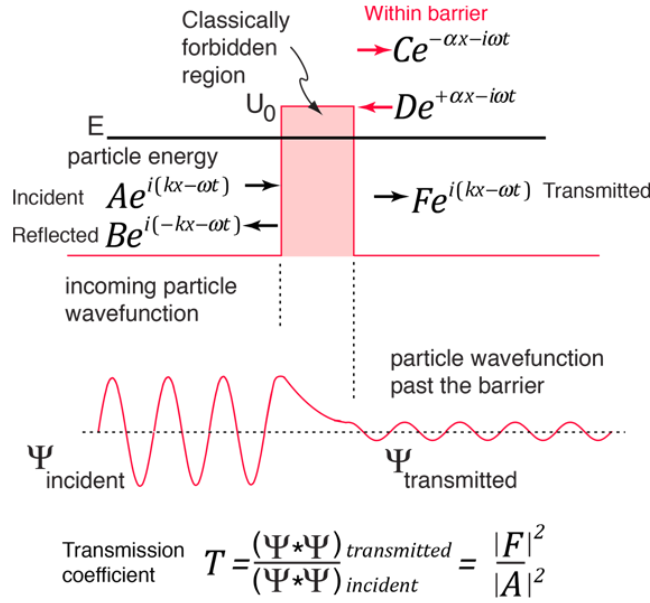


Figure 5.2: Schematic diagram of Tunneling effect

### 5.3 Tunneling effect

To evaluate a symmetric potential well, we consider the wave function

$$\Psi(x, 0) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & \text{Region 1} \\ Ce^{\alpha x} + De^{-\alpha x}, & \text{Region 2} \\ Fe^{ikx} & \text{Region 3} \end{cases}$$

Using the boundary conditions we get the following,

$$\begin{aligned} A + B &= C + D ; \Psi(x = 0) \\ ikA - ikB &= \alpha D - \alpha C ; \frac{\partial \Psi(x = 0)}{\partial x} \\ Ce^{\alpha L} + De^{-\alpha L} &= Fe^{ikL} ; \Psi(x = L) \\ (\alpha C)e^{\alpha L} - (\alpha D)e^{-\alpha L} &= ikFe^{ikL} ; \frac{\partial \Psi(x = L)}{\partial x} \end{aligned}$$

In this case the Transmission coefficient

$$T = \frac{\Psi_T^* \Psi_T}{\Psi_I^* \Psi_I} = \frac{|F|^2}{|A|^2} > 0$$

Which means unlike the classical case when ( $E < V$ ) The particle can not cross the high potential region, in the case of quantum particles there is a possibility of transmission to occur.

### 5.4 Ehrenfest Theorem

Expectation values of physical observable follow classical equations of motion if the potential is given in terms of a polynomial of degree 2 or less

This means for flat, linear or parabolic potentials follow both classical mechanics and quantum mechanics.

$$\begin{aligned} \langle P \rangle &= -i\hbar \int \Psi^* \frac{\partial \Psi}{\partial x} dx \\ \frac{d \langle P \rangle}{dt} &= -i\hbar \int \frac{\partial}{\partial t} \left( \Psi^* \frac{\partial \Psi}{\partial x} \right) dx \end{aligned}$$

But the term inside the paranthesis can be written as The V here is the potential.

$$\frac{\partial}{\partial t} \left( \Psi^* \frac{\partial \Psi}{\partial t} \right) = \frac{i\hbar}{2m} \left[ \Psi^* \frac{\partial^3 \Psi}{\partial x^3} - \frac{\partial^2 \Psi^*}{\partial x^2} \frac{\partial \Psi}{\partial x} \right] - \frac{i}{\hbar} \frac{\partial V}{\partial x} \Psi$$

Integrating we get the following

$$\begin{aligned}\frac{d\langle P \rangle}{dt} &= - \int_{-\infty}^{\infty} \Psi^* \frac{\partial V}{\partial x} \Psi dx \\ \frac{d\langle P \rangle}{dt} &= \langle -\frac{\partial V}{\partial x} \rangle \\ \frac{d\langle P \rangle}{dt} &= \langle F(x) \rangle\end{aligned}$$

but in general,

$$\langle F(x) \rangle \neq F(\langle x \rangle)$$

But if we expand the Expectation value of  $F(x)$  we get the following,

$$\begin{aligned}\langle F(x) \rangle &= \langle F(\langle x \rangle) + F'(\langle x \rangle)(x - \langle x \rangle) + \frac{1}{2}F''(\langle x \rangle)(x - \langle x \rangle)^2 + O(x^3) \rangle \\ \langle F(x) \rangle &= F(\langle x \rangle) + F' \langle x - \langle x \rangle \rangle + \langle \frac{1}{2}F''(\langle x \rangle)(x - \langle x \rangle)^2 \rangle + \langle O(x^3) \rangle\end{aligned}$$

The second term is zero, and if we consider the second and higher derivatives of  $F(x)$  to be 0 then we are left with the following

$$\langle F(x) \rangle = F(\langle x \rangle)$$

Which means for polynomial of power 2 or less The potential function follows classical mechanics as well as quantum mechanics.