PH 107: Quantum Physics and applications

Free Particle

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Recap

$$i\hbar\frac{1}{\chi}\frac{d\chi}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\phi}\frac{d^2\phi}{dx^2} + V\phi$$

The complete solution by separation of variable , $\Psi(x,t) = \phi(x)e^{-i\frac{E}{\hbar}t}$

To solve for $\phi(x)$, we need to solve TISE

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} + V\phi = E\phi}$$

Note:

- We cannot go any further with solving the TISE, unless we are given the form of $V = V(x)$. We will spend a lot of time in solving TISE for different types of $V(x)$.
- Solution is subjected to boundary conditions
- Acceptable solution $\phi(x)$ must be continuous, single valued and its derivative must be continuous.

Recap: Stationary States (does not mean static)

The complete solution by separation of variable , $\Psi(x,t) = \phi(x)e^{-i\frac{E}{\hbar}t}$

Probability $|\Psi(x,t)|^2 = \phi*(x)e^{i\frac{E}{\hbar}t}\phi(x)e^{-i\frac{E}{\hbar}t}$ **=** $\phi*(x)\phi(x)$ **=** $|\phi(x)|^2$

Normalisation, $$\int_{-\infty}^{\infty}|\boldsymbol{\Psi}(\boldsymbol{x},\boldsymbol{t})|^2\boldsymbol{dx} = \int_{-\infty}^{\infty}|\phi(x)|^2\boldsymbol{dx} = \mathbf{1}$$

This is independent of $\chi(t)$.

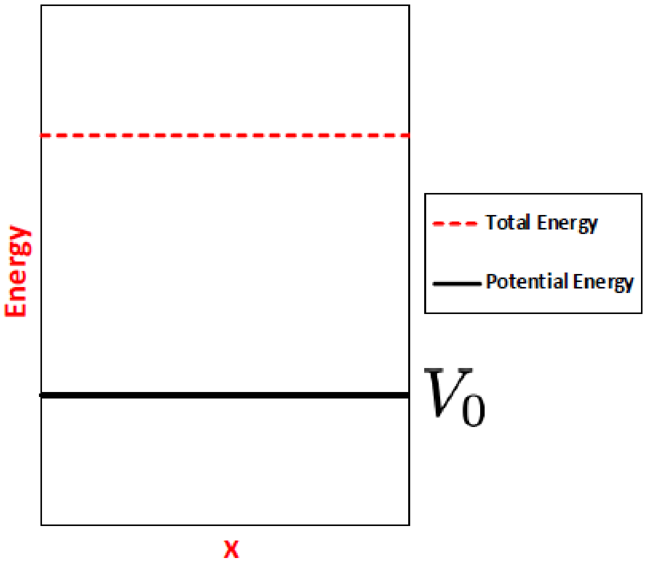
For this reason, solutions in separable form are called stationary states. Thus, for stationary states all probabilities are static.

$All\ calculation\ can\ be\ done\ using\ time\ \ independent\ wavefunction\ \phi(x).$

Free particle: *Classical*

Classically, a particle in following situation is referred to as a free particle

- No force is acting on particle. Motion is simple.
- Particle travels from left to right (right to left) with a constant speed (momentum)
- Speed is related to the difference between the total and potential energies



Free particle: *Quantum*

To study the "motion " of this system we will solve the TISE with a constant a constant potential energy

$$V(x) = V_0$$ Particle moving in a constant potential

$$V_0 = 0$$ **is a special case**

Aim :

- To get the eigen function(s) and write down the corresponding wave function(s)

- From these wave functions we write down the probability density function and calculate various expectation values

Free particle: ***No force is acting on the particle***

Let us write TISE as

$$-\frac{\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2}+V_0\phi(x)=E\phi(x)$$

$$k^2$$

$$-\frac{\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2}=(E-V_0)\phi(x)\implies\frac{d^2\phi(x)}{dx^2}=-\frac{2m(E-V_0)}{\hbar^2}\phi(x)$$

$$V_0=0$$

$$\implies\frac{d^2\phi(x)}{dx^2}=-k^2\phi(x)\quad\text{where } k=\frac{\sqrt{2m(E-Vo)}}{\hbar}=\frac{\sqrt{2mE}}{\hbar}$$

Free particle:

$$\frac{d^2\phi(x)}{dx^2} = -k^2\phi(x)$$

This is the equation of a simple harmonic oscillator in Mechanics with the following substitution

$$\phi(x) \longrightarrow x(t)\,, \quad x \longrightarrow t$$

Let us guess a solution $\phi(x) = Ae^{\lambda x}$

After substituting the guessed solution

$$\frac{d^2\phi(x)}{dx^2} = -k^2\phi(x) \Longrightarrow \lambda^2 Ae^{\lambda x} = -k^2 Ae^{\lambda x} \Longrightarrow \lambda = \pm ik$$

Free Particle : Solution to SE

Case I: $E > V_0 \implies k^2 > 0 \implies \lambda = \pm ik$

$$\phi(x) = Ae^{ikx} \text{ and/or } Ae^{-ikx}$$

In general, $\phi(x) = Ae^{ikx} + Be^{-ikx}$ Check this !!

$$k = \sqrt{\frac{2m(E - V_0)}{\hbar^2}} \implies E = \frac{\hbar^2 k^2}{2m} + V_0$$

In the case of free particle, $V_0 = 0$, $E = \frac{\hbar^2 k^2}{2m}$

- **There is no restriction on the value of *k*.**
- **Thus a free particle, even in quantum mechanics, can have any non-negative value of the energy**

Free Particle :

1. Is free particle wavefunction is an eigen function of momentum operator ?

$$\phi(x) = Ae^{ikx}$$ momentum operator $$\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$$

$$\hat{p}_x\phi(x) = -i\hbar\frac{\partial}{\partial x}Ae^{ikx} = -i\hbar(ik)Ae^{ikx} = \underbrace{\hbar k}_{\text{momentum } p_x}\ \phi(x)$$

$$\hat{p}_x\phi(x) = p_x\phi(x)$$

Similarly $\phi(x) = Be^{-ikx}$

$$\hat{p}_x\phi(x) = -\hbar k\phi(x) = p_x\phi(x)$$

YES !!

Free Particle: Which are the valid solutions?

- Possible solutions are

$$\phi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} \\ C\sin kx + D\cos kx \end{cases}$$

Which of these 2 correspond to free particle?
Momentum operator comes to the rescue!

$$\hat{p}_x \phi(x) = -i\hbar \frac{\partial}{\partial x} \phi(x)$$

- Exponentials are eigen-functions of Momentum operator
- Sin or Cosine are NOT eigen-functions of Momentum operator

$$-i\hbar \frac{\partial}{\partial x} \sin(kx) = -i(\hbar k)\ \cos(kx) \Longrightarrow \hat{p}_x \sin(kx) \neq p_x \cos(kx)$$

Free Particle: Time-dependent Wavefunction

- Solution corresponding to free particle with fixed momentum and energy

$$\phi(x) = Ae^{ikx} + Be^{-ikx}$$

- Momentum p can take on any real value between $-\infty$ and $+\infty$

e^{ikx}	$k > 0$	particle moving from left to right
e^{-ikx}	$k < 0$	particle moving from right to left

- To understand this further, let us consider the time-dependent part :

$$\phi(x) = \left(Ae^{ikx} + Be^{-ikx}\right) e^{-iEt/\hbar} = Ae^{i(kx-\omega t)} + Be^{-i(kx+\omega t)}$$

- These are travelling waves

$e^{i(kx-\omega t)}$	$p > 0$	wave traveling in the direction of increasing x
$e^{-i(kx+\omega t)}$	$p < 0$	wave traveling in the direction of decreasing x

Free Particle : Expectation value

2. Let us evaluate the expectation value of momentum operator .

$$\langle p_x \rangle = \frac{\int_{-\infty}^{\infty} \phi^*(x) \left(-i\hbar \frac{\partial}{\partial x}\right) \phi(x) dx}{\int_{-\infty}^{\infty} \phi^*(x)\phi(x) dx}$$

For $\phi(x) = Ae^{ikx}$

Travelling right

$$\langle p_x \rangle = \hbar k \frac{\int_{-\infty}^{\infty} \phi^*(x)\phi(x) dx}{\int_{-\infty}^{\infty} \phi^*(x)\phi(x) dx} = \hbar k$$

For $\phi(x) = Be^{-ikx}$

Travelling left

$$\langle p_x \rangle = -\hbar k \frac{\int_{-\infty}^{\infty} \phi^*(x)\phi(x) dx}{\int_{-\infty}^{\infty} \phi^*(x)\phi(x) dx} = -\hbar k$$

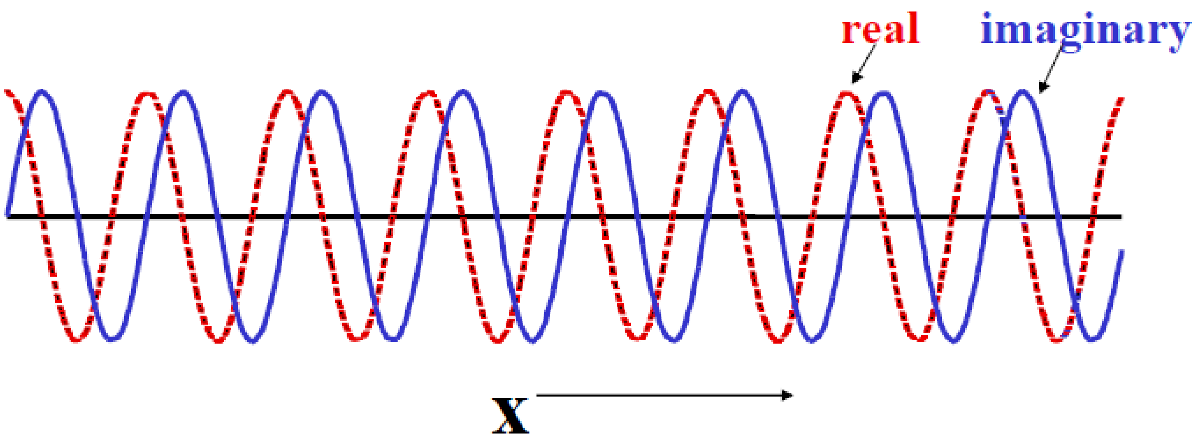
$$\langle p_x \rangle = -\hbar k$$

Free Particle : Probability Density

3. Probability Density.

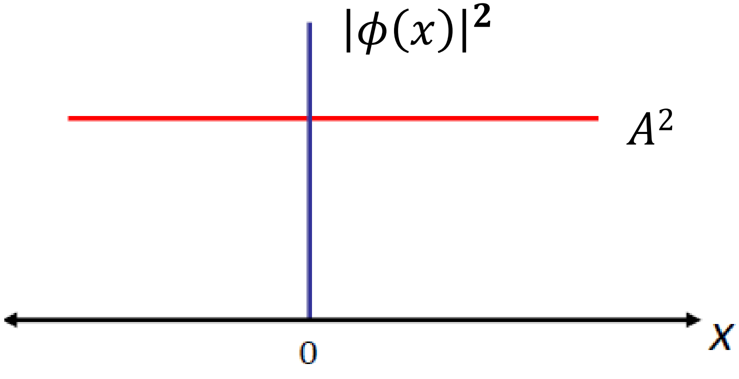
Assume that the particle travels only in the positive x-direction

$$\phi(x) = Ae^{ikx} = A\,[Cos(kx) + iSin\,(kx)]$$



3. Probability Density.

The probability density $|\phi(x)|^2 = A^2 = Constant$



Key feature:

Probability density is the same for all values of x.

all positions are equally likely expected

Momentum Uncertainty

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

For $\phi(x) = Ae^{ikx}$ we know $\langle p_x \rangle = \hbar k$

Now, $\langle p_x^2 \rangle == \dfrac{\int_{-\infty}^{\infty} \phi^*(x) \left(-i\hbar \frac{\partial}{\partial x}\right)^2 \phi(x) dx}{\int_{-\infty}^{\infty} \phi^*(x)\phi(x) dx} = (\hbar k)^2$

$$\Delta p_x = \sqrt{\langle p_x^2 \rangle - \langle p_x \rangle^2} = 0 \qquad \Longrightarrow \Delta x = \frac{\hbar}{2\Delta p_x} \to \infty$$

The Heisenberg's uncertainty principle

- In the example of a free particle, we see that if its momentum is completely specified, then its position is completely unspecified.

- When the momentum p is completely specified we write: $\Delta p = 0$ $\Delta p = p_1 - p_2 = 0$

- When the position x is completely unspecified we write $\Delta x \to \infty$

- As we showed earlier, it is impossible to simultaneously determine the position and momentum of a particle with complete precision.

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

Normalization

$$\phi(x) = Ae^{ikx} \implies \phi^*(x) = A^*e^{-ikx} \implies \phi^*(x)\phi(x) = |A|^2$$

Probability of finding a particle is constant everywhere!

$$\int_{-\infty}^{\infty} \phi^*(x)\phi(x)dx = |A|^2 \int_{-\infty}^{\infty} dx$$

Wavefunction can't be normalised.

Wavefunction is an eigen function of momentum operator, so position is delocalised.

- It means that the stationary states that we described do not represent physically realizable states, i.e. there can be no free particle with definite energy.
- We are still interested in these states: the general solution is a linear combination of stationary states.

Group velocity = Speed of particle

- If $\Psi(x,t) = Ae^{i(kx-\omega t)}$ is a solution to the Schrodinger equation, any superposition of such waves is also a solution: $\Psi(x,t) = \int_{-\infty}^{\infty} A(k)e^{i(kx-\omega t)}dk$ $\quad \omega = \frac{\hbar k^2}{2m}$

- For wave packet we can define two speeds: $v_{\text{phase}} = \frac{\omega}{k} \quad v_{\text{group}} = \frac{d\omega}{dk}$

- For this case, we get

$$v_{\text{phase}} = \frac{\hbar k}{2m}; \quad v_{\text{group}} = \frac{d\omega}{dk} = \frac{\hbar k}{m} = v_{\text{classical}}$$

- The speed of envelope (group velocity) corresponds to the particle velocity!

Free Particle Solutions

$$\frac{d^2\phi(x)}{dx^2} = -k^2\phi(x)$$

$$k = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

Assuming trial solution $\phi(x) = Ae^{\lambda x}$

Case I

For $E > V_0 \implies k^2 > 0 \implies \lambda = \pm ik$

We obtain $\phi(x) = Ae^{ikx} + Be^{-ikx}$

Case II

If $E < V_0 \Longrightarrow k^2 < 0 \qquad \Longrightarrow k = \sqrt{-\dfrac{2m|E-V_0|}{\hbar^2}} = i\kappa$

$$\kappa = \sqrt{\frac{2m|E-V_0|}{\hbar^2}}$$

In this case,

$$\boxed{\phi(x) = Ce^{\kappa x} + De^{-\kappa x}}$$

For $x > 0, x \to \infty, e^{\kappa x} \to \infty; x < 0, x \to -\infty, e^{-\kappa x} \to \infty$

Hence not a possible solution.

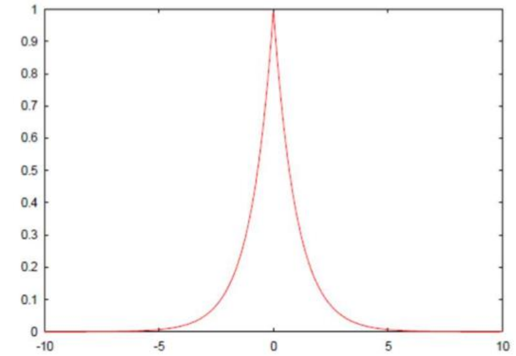
$When,\ E < V_0;$ $\qquad \phi(\mathrm{x}) = \mathrm{D}\ e^{-\kappa x}\ for\ x > 0$

and $\qquad \phi(\mathrm{x}) = \mathrm{C}\ e^{\kappa x}\ for\ x < 0$

The wave function must be continuous and single valued

Therefore, $\quad C = D \quad$ and $\quad \phi(x) = Ce^{-\kappa|x|}$

$$\phi(x) = Ce^{-\kappa|x|}$$



The wave function is continuous at x=0,

but the derivative of the function is not continuous at x = 0

$$\phi(x) = Ce^{\kappa x} \qquad \left.\frac{\partial \phi(x)}{\partial x}\right|_{x=0} = \kappa Ce^{\kappa x}|_{x=0} = \kappa C$$

$$\phi(x) = Ce^{-\kappa x} \qquad \left.\frac{\partial \phi(x)}{\partial x}\right|_{x=0} = -\kappa Ce^{-\kappa x}|_{x=0} = -\kappa C$$

For the derivative to be continuous, $\kappa C = -\kappa C \implies C = 0$

No physical solution exists for the case $E < V_0$ everywhere.

This does not mean that a solution does not exist if there are finite regions where E < V_0 and other regions where E > V_0. *We shall revisit this problem later !*

Summary

- **Free Particle**

Studied the simplest physical situation, an object that has no forces acting on it and thus has a constant potential energy everywhere!

- **Solutions**

1. Sin(kx) and Cos(kx) are solutions to Schrodinger equation. However, they are not eigenfunctions of momentum operator.
2. exp ($\pm i\ kx$) are solutions to Schrodinger equation and eigenfunctions of momentum operator.

- **Properties of solutions**

1. Probability density is the same for all values of x.
2. The free-particle wave functions are not normalizable.