PH 112: Quantum Physics and Applications

S. Shankaranarayanan
shanki@iitb.ac.in

Week 04 Lecture 2: Free particle

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Classical-Mechanical Observables and Their Corresponding Quantum-Mechanical Operators

Observable		Operator	
Name	Symbol	Symbol	Operation
Position	x	$\hat{X}$	Multiply by x
	$\mathbf{r}$	$\hat{\mathbf{R}}$	Multiply by $\mathbf{r}$
Momentum	p_x	$\hat{P}_x$	$-i\hbar\frac{\partial}{\partial x}$
	$\mathbf{p}$	$\hat{\mathbf{P}}$	$-i\hbar(\mathbf{i}\frac{\partial}{\partial x}+\mathbf{j}\frac{\partial}{\partial y}+\mathbf{k}\frac{\partial}{\partial z})$
Kinetic energy	T_x	$\hat{T}_x$	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
	T	$\hat{T}$	$-\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2})$ $=-\frac{\hbar^2}{2m}\nabla^2$

Schrodinger equation is an eigenvalue equation!

- Schrodinger equation is

$$E = T + V = \frac{p^2}{2m} + V$$

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

- Hamiltonian (Energy) operator is

$$\hat{H} = \hat{T} + \hat{V}$$

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \hat{V}$$

$$\hat{H}\psi(x) = E\psi(x)$$

- Hamiltonian operates on the eigenfunction $(\psi(x))$ giving a constant eigenvalue (E) times the eigenfunction $(\psi(x))$. Eigen means same in German.

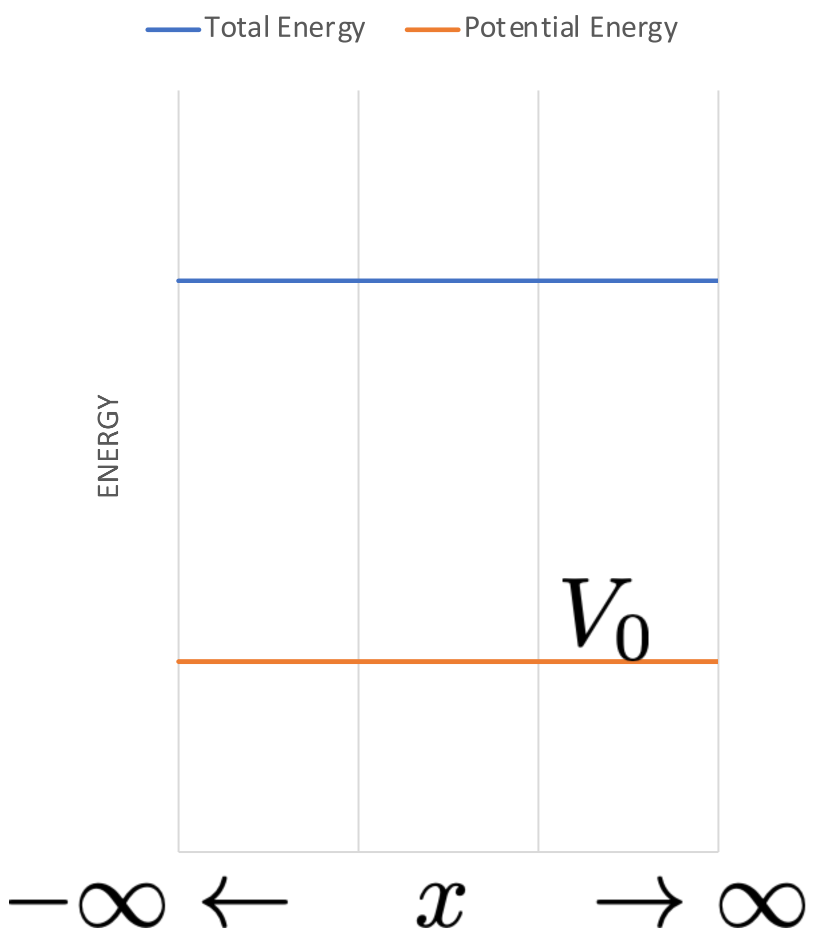
First Application of Schrödinger equation

Free Particle: Classical

- Consider the following setup:

1. No net force acting on particle. Motion is simple.
2. Particle travels from left to right (or right to left) with a constant speed (momentum).
3. Speed is related to the difference between the total and potential energies.
4. Particle's energy is constant $$E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$

Classically, a particle in this situation is referred to as a free particle.



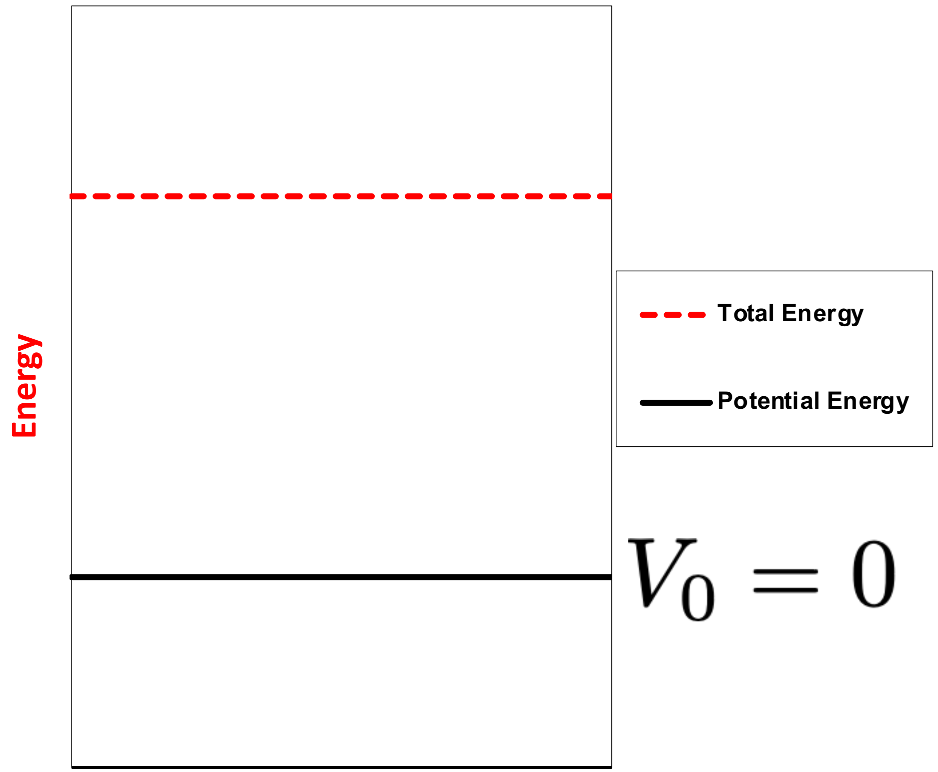
Free Particle: Quantum

- To study the "motion" of this system, we will solve the time independent Schrödinger equation with a constant potential energy.

- We will set $V(x) = V_0 = 0$

- Aim:

1. To get the eigenfunction(s) and then write down the corresponding wave function(s).
2. From these wave functions we write down the probability density function and calculate expectation values.



$-\infty \leftarrow \quad x \quad \rightarrow \infty$

Energy and Momentum of the particle are constants at all times!

Free Particle: Solutions to Schrödinger equation

- Time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x) \quad \Longrightarrow \frac{d^2}{dx^2}\psi(x) + \frac{2m}{\hbar^2}E\psi(x) = 0$$

- We define $k^2 = \dfrac{2mE}{\hbar^2}$ or $E = \dfrac{\hbar^2 k^2}{2m} = \dfrac{p^2}{2m}$

- Thus the Schrödinger equation becomes: $\dfrac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0$

- This is the equation of a simple harmonic oscillator in Mechanics with the following substitution $\psi(x) \to x(t)\,, \quad x \to t$

Free Particle: Solutions to Schrodinger equation

- Possible solutions are

$$\psi(x) = \ \text{const} \begin{cases} \sin kx \\ \cos kx \\ e^{\pm ikx} \end{cases}$$

- There is no restriction on the value of *k or momentum (p)*.

- Thus a free particle, even in quantum mechanics, can have any non-negative value of the energy

$$E = \frac{\hbar^2 k^2}{2m} \geq 0$$

- Energy levels correspond to the same continuum of kinetic energy shown by a classical particle.

Physical understanding of the solutions

Free Particle: Which are valid solutions?

- Possible solutions are

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

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

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

- Substituting exponentials in the above expression, we have

$$\hat{p}_x e^{\pm ikx} = -i\hbar \frac{\partial}{\partial x} e^{\pm ikx} = (\pm \hbar k)\, e^{\pm ikx} \Longrightarrow \hat{p}_x e^{\pm ikx} = p_x e^{\pm ikx}$$

Free Particle: Which are the valid solutions?

- Possible solutions are

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

- Sin or Cosine leads to

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

Free Particle solutions: What do they correspond to?

- Solution corresponding to free particle with fixed momentum and energy

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

- 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

Free Particle solutions: What do they correspond to?

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

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

- Rewriting: $$\Psi(x,t) = Ae^{ik(x-vt)} + Be^{-ik(x+vt)} \qquad v \equiv v_{\text{quantum}} = \frac{\hbar k}{2m}$$

- These are travelling waves

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

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

Free Particle solutions: What do they correspond to?

- To understand further, let us consider the expectation of momentum operator:

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

- These are travelling waves

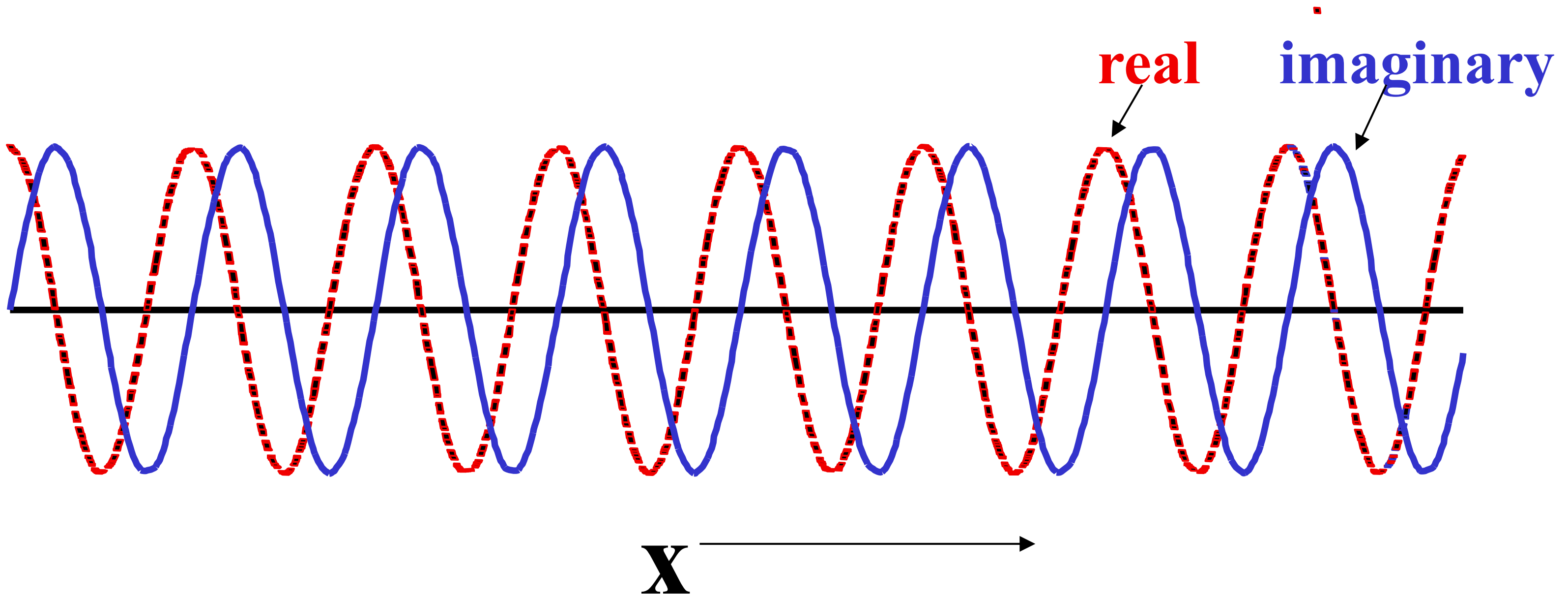
$$\phi(x) = Ae^{ikx} \qquad \langle p_x \rangle = \hbar k\frac{\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx}{\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx} = \hbar k$$

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

Properties of the free particle solutions

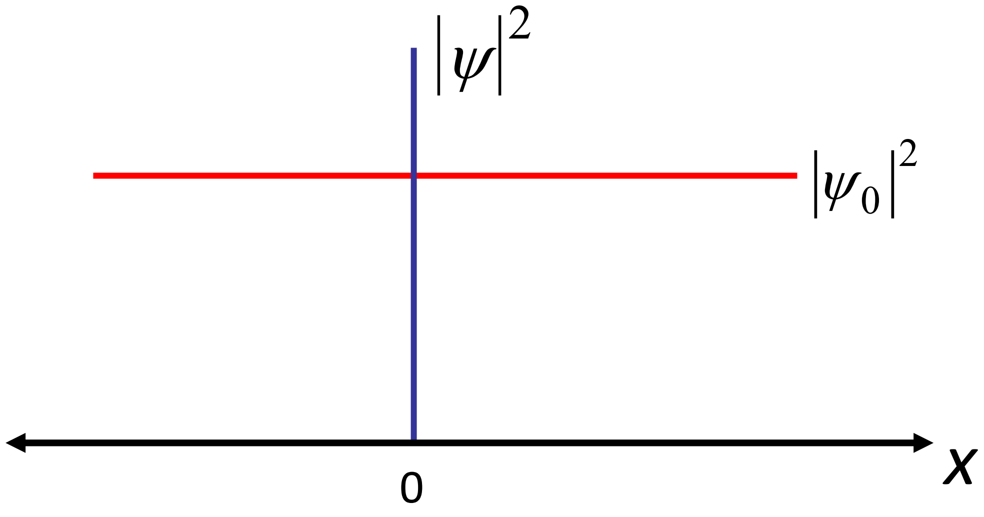
Probability density

- Assume that the free particle travels only in the positive *x-direction*
- Relabel A as $\psi_0 \Longrightarrow$ $$\psi(x) = \psi_0 e^{ikx} = \psi_0[\cos(kx) + i\sin(kx)]$$



Probability density

- The probability density is: $$|\psi(x)|^2 = |\psi_0 e^{ikx}|^2 = \psi_0^2 = \text{constant}$$



Key feature:

Probability density is the same for all values of *x*.

All positions are equally likely

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: $\Delta p = p_1 - p_2 = 0$ $\Delta p = 0$

- When the position *x* is completely unspecified we write $\Delta x \to \infty$
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- As we showed earlier, it is impossible to simultaneously determine the position and momentum of a particle with complete precision.

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

Speed of wave

- We got the speed of wave as $$v_{\text{quantum}} = \frac{\hbar k}{2m} = \sqrt{\frac{E}{2m}}$$

- The classical speed of the particle is

$$E \equiv E_{\text{Kinetic}} = \frac{1}{2}mv^2 \implies v_{\text{classical}} = \frac{2E}{m} = 2v_{\text{quantum}}$$

- Therefore, it appears that the wave function travels at only half the speed of the particle that it is supposed to represent!

- Is there a problem?

Normalization of free particle wave function

- Another problem is the normalization of the wave function!

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx = |\psi_0|^2 \int_{-\infty}^{\infty} dx = |\psi_0|^2(\infty)$$

- What does it mean?

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: $\Psi(x,t) = \int_{-\infty}^{\infty} A(k)e^{i(kx-\omega t)}dk$ $\qquad \omega = \frac{\hbar k^2}{2m}$

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

- For this case, we get

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

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

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.

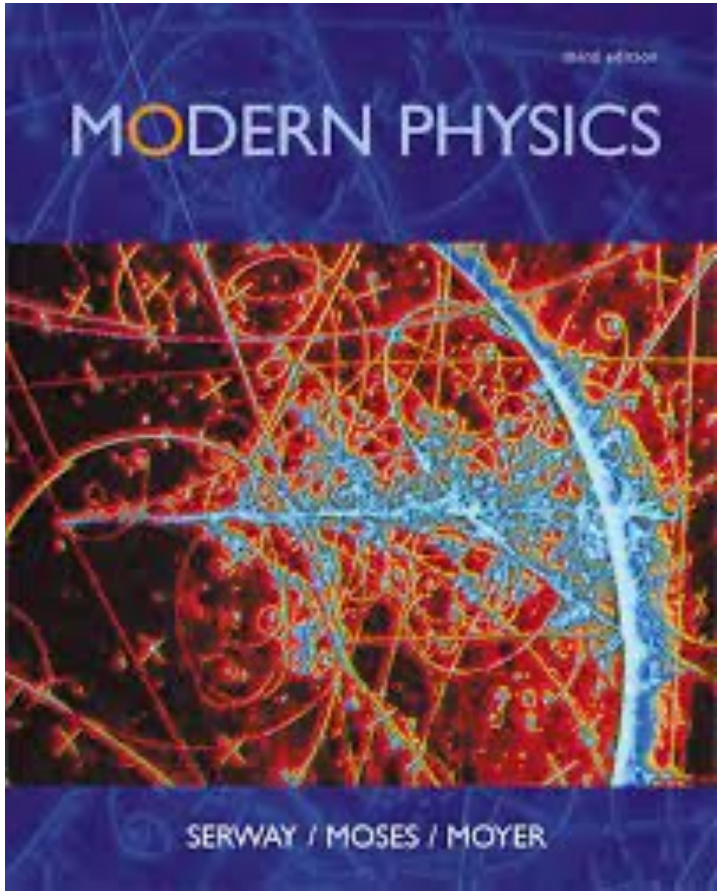
  2. $\exp(\pm i\ kx)$ are solutions to Schrodinger equation and eigenfunctions of momentum operator.

- Properties of solutions

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

Recommended Reading

Free particle section 6.2



Conservation of Probability: Proof

Normalizing the free particle wave function

- Since the integral of $|\psi|^2$ over all values of $x \in (-\infty, \infty)$ is infinite, it appears ψ is non-normalizable.
- We can imagine that the particle to be in a region $x \in (-L, L)$ and assume $L \to \infty$

$$\int_{-L}^{+L} \psi^*(x)\psi(x)dx = A^* \; A \int_{-L}^{L} e^{-ikx}e^{+ikx}dx = 1$$

$$|A|^2 \int_{-L}^{+L} dx \quad \Longrightarrow \quad A = [2\,L]^{-1/2}$$

- The same expression we get for the constant B.
- This is referred to as box normalization.