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THEORY :-

(a)

Since, TISE is :-

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

Here, in case of free particle :-

$V(x) = 0$, everywhere

$$\therefore \frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}E\psi(x)$$

$$\left[\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi(x) = 0\right]$$

Let, ~~x~~ $\xi = x/L$

$$\frac{d^2\psi}{dx^2} = \frac{1}{L^2}\frac{d^2\psi}{d\xi^2}$$

$$\therefore \frac{1}{L^2}\frac{d^2\psi}{d\xi^2} + \frac{2m}{\hbar^2}E\psi(x) = 0$$

$$\therefore \left[\frac{d^2\psi}{d\xi^2} + \frac{2mL^2}{\hbar^2}E\psi(x) = 0\right]$$

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Now making Energy term dimensionless :-

Let $e = \frac{\hbar^2}{2mL^2}$

$$\therefore \left[\frac{d^2\psi}{d\xi^2} + e\psi = 0 \right]$$

[$\xi \rightarrow$ dimensionless length & $e \rightarrow$ dimensionless energy]

(b)

The stationary state can't represent physically relizable states because the wave function is not normalizable in this state. ~~the~~
That means a free particle can't exist in stationary state or there is no such things as free particle with a definite energy.

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(1)

A wave packet is a group of superposed waves which together form a travelling disturbance.

Since, we know that the solution obtain by solving time independent solution though it is mathematically right but not acceptable physically. Therefore the general solution is the linear combination of separable solutions.

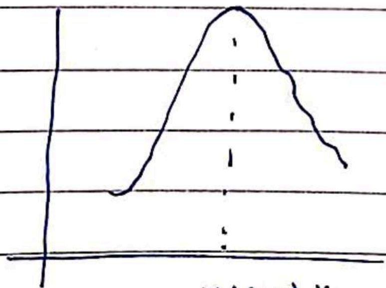
Given by:-

$$\left[\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) \cdot e^{i\left(kx - \frac{\hbar k^2}{2m} t\right)} dk \right]$$

This wave function can be normalized for appropriate $\phi(k)$. But it necessarily comes in a range of k's and hence range of energy and speeds.

It is called wave packet.

$\Psi(x,t)$



$$\left[v_g = \frac{dx(t)}{dt} \right]$$

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assume ,

$$C(k) = \begin{cases} 0 & \text{for } |k-k_0| > \Delta k/2 \\ \text{non-zero} & \text{for } k-\frac{\Delta k}{2} < k < k_0 + \frac{\Delta k}{2} \end{cases}$$

OR

$$C(p) = \begin{cases} 0 & \text{for } |p-p_0| > \Delta p/2 \\ & \end{cases}$$

$$p_0 = \hbar k_0 \qquad \Delta p = \hbar \Delta k$$

Harmonic wave = $e^{i(kx - \omega(k)t)}$

omega is non-zero only around $\omega(k_0)$. ω_0

$$\therefore \psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} C(k) \cdot e^{i(kx-\omega t)} dk$$

$$\left.\frac{d\phi(x,t)}{dx}\right|_{x = X(t)} = 0$$

$$\Rightarrow \int_{-\infty}^{+\infty} C(k) \cdot (ik) \cdot e^{i(kX(t) - \omega(t))} \cdot dk = 0$$

differentiating w.r.t t

$$\therefore \; kX' - \omega$$

$$= kX' - \left(\omega_0 + (k-k_0) \left.\frac{d\omega}{dk}\right|_{k=k_0}\right)$$

$$\therefore \left[\frac{dx}{dt} = \left.\frac{d\omega}{dk}\right|_{k=k_0} \right]$$

$\downarrow$ particle velocity

$\downarrow$ Group velocity.

(d)

wave packet evolution is given by :-

$$\left[\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) \cdot e^{i\left(kx - \frac{\hbar k^2}{2m} t\right)} \cdot dk \right]$$

$$\omega(k) \cong \omega_0 + \omega_0'(k-k_0)$$

$$\psi(x,t) \cong \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k_0+s)\, e^{i[(k_0+s)x - (\omega_0 + \omega_0' s)t]} \cdot ds$$

at $t=0$

$$\therefore \psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k_0+s) \cdot e^{i(k_0+s)x} \cdot ds$$

at later time:-

$$\psi(x,t) \simeq \frac{1}{\sqrt{2\pi}} e^{i(\omega_0 t + k_0\omega_0' t)} \int_{-\infty}^{+\infty} \phi(k_0+s)\, e^{i(k_0+s)(x-\omega_0' t)} \cdot ds$$

$$\therefore \left[\psi(x,t) \simeq e^{-i(\omega_0 - k_0\omega_0')t}\, \psi(x-\omega_0' t, 0) \right]$$

1 Discussion

1. This is the plot for the probability density for finding the particle in position space at *time=0* after applying conditions given in the question.

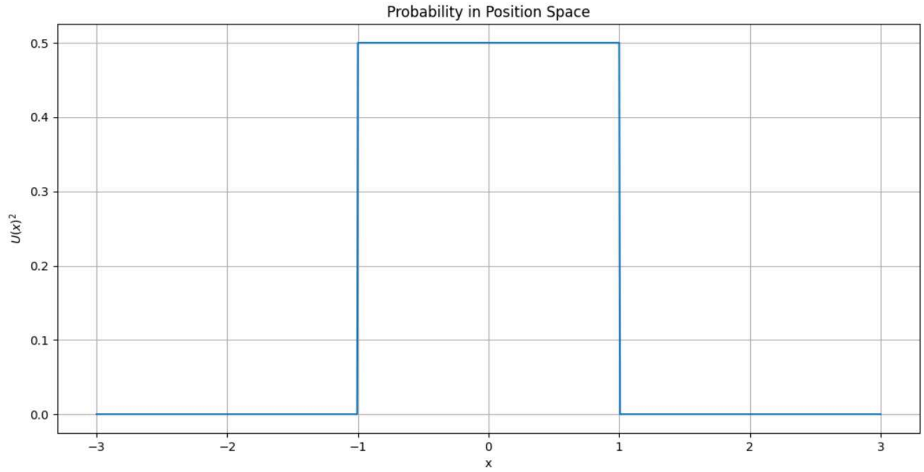

Figure 1:

2. This plot gives us the probability density for finding the particle in **Momentum space** at *time=0*.

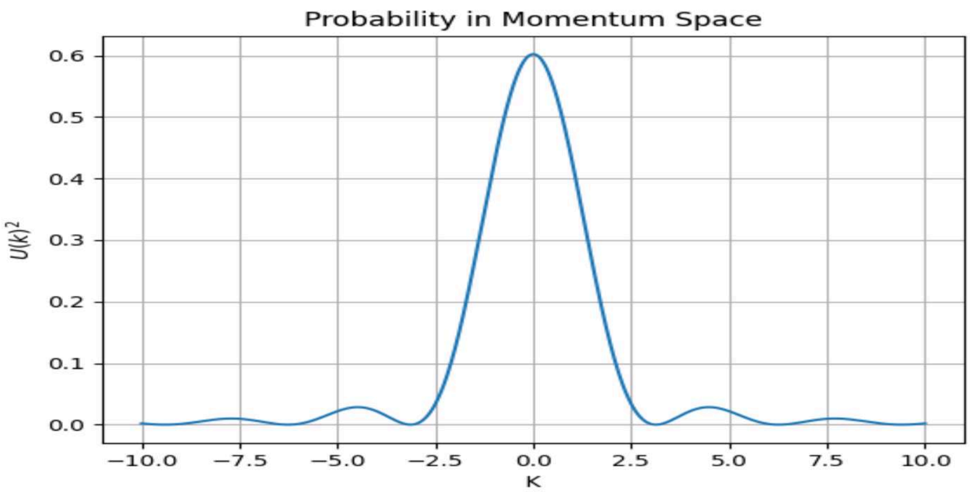

Figure 2:

3. This plot clearly shows the change on Probability Density with change in time in the position space.

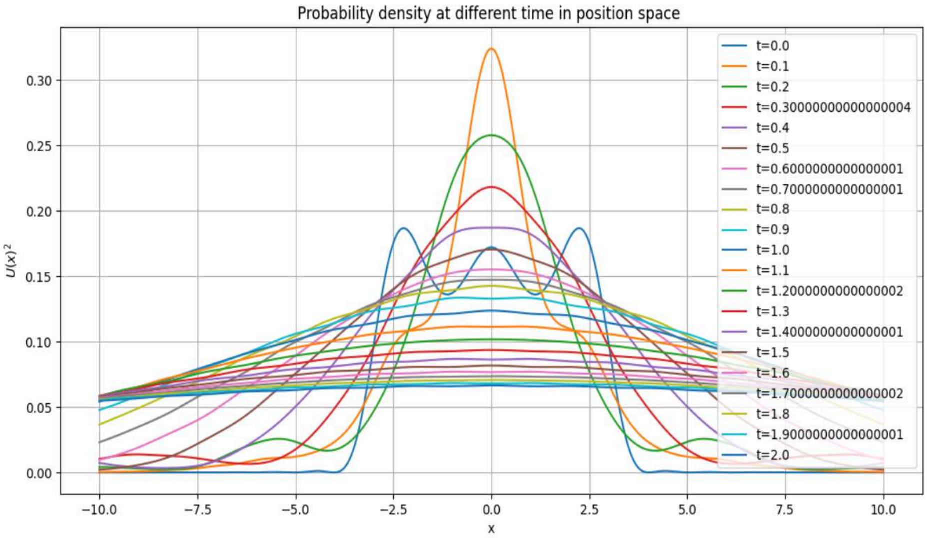

Figure 3:

4. Here I am plotting the probability density of a Gaussian wave packet at time equals to zero.

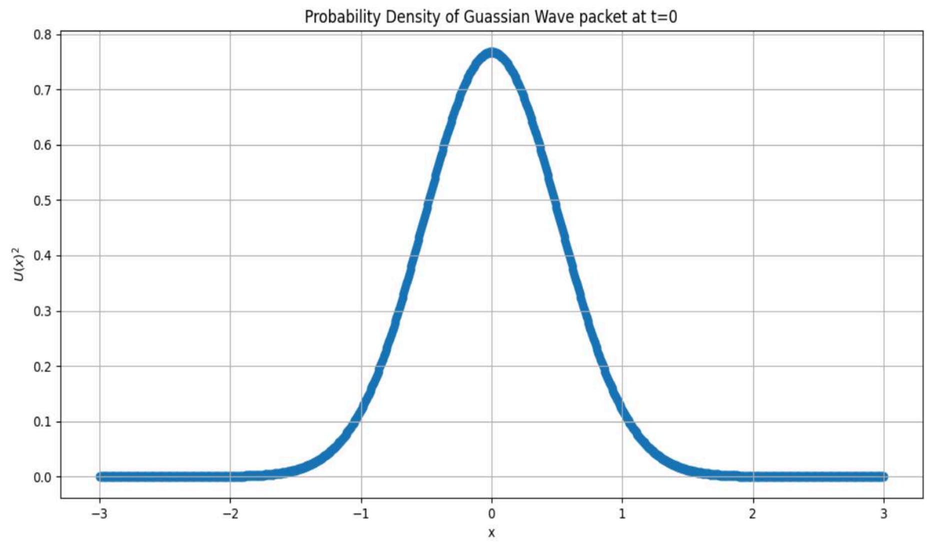

Figure 4:

5. This is the plot for Probability Density with change in time of a Gaussian wave packet.

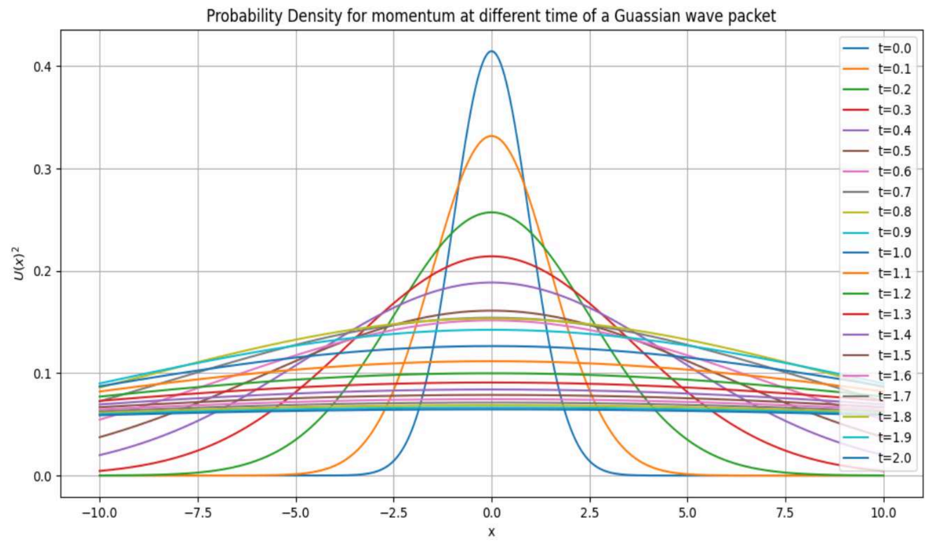

Figure 5:

B.Sc.(Hons.) Physics
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S.G.T.B. Khalsa College
Quantum Mechanics (2022-23)
Lab Assignment # 11
Time Evolution of Wave Packets

Due Date and Time :
25.09.2022, 11:59PM
Max. Marks : 20

The objective of this assignment is to

- understand that a wave packet can represent a free particle
- study the time evolution of a given wave packet numerically

1. (8 marks) **Theory**

   (a) Write down the Schrödinger Equation for a free particle in dimensionless form and determine the stationary states.

   (b) Discuss why the stationary states cannot represent a physical state.

   (c) What is a wave packet. Show that the group velocity of the wave packet corresponds to the speed of free particle.

   (d) How does the wave packet evolve with time?

   (e) Given that at $t = 0$, a quantum particle of mass m is described by the wave function

   $$\psi(x,\, 0) \quad = \quad \begin{cases} A & \text{for } |x| < b \\ 0 & \text{for } |x| > b \end{cases},$$

   normalise the wave function and determine the fourier components $a(k)$ given by

   $$\psi(x, 0) \quad = \quad \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} a(k) \exp\{ikx\}\, \mathrm{d}k \tag{1}$$

   (f) Use these $a(k)$ to write down the expression for wave function and the probability density at time t, $\psi(x,\, t)$ as an integral. Express these integrals in terms of dimensionless quantities.

2. (10 marks) **Programming**

   (a) Write a Python code to
      i. Plot the probability density for finding the particle in position space at $t = 0$.
      ii. Plot the probability density for the momentum of the particle at $t = 0$.

   (b) Extend the code to determine the probability density in position space at time t by evaluating the required integral numerically at $\tau = 0, 0.1, 0.2, \ldots 2.0$ where τ is the time in dimesnionless units.

   (c) Extend the code further to plot the probability density in position space at $\tau = 0, 0.1, 0.5,\, 1.0,\, \ldots 2.0$. Also plot the probability of finding the particle in the range $|x| < \frac{b}{2}$ as a function of τ.

   (d) Write another code to study the time evolution of a Gaussian wave packet and plot
      i. the wave packet at various times
      ii. the uncertainty in position and momentum as a function of time.

3. (2 marks) **Discussion**
   Discuss your results and compare with those of the Finite Difference Method.