

# **Free Particle Schrodinger Equation and Solutions**

## ***Recapitulate***

***Under separation of variables***

$$\Psi(x, t) = \psi(x)\phi(t) \qquad \phi(t) = e^{-iEt/\hbar} = e^{-i\omega t}$$

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

**Find E from time independent Schrödinger Equation**

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

***Given  $V(x)$ , solve time independent Schrodinger equation to obtain E and  $\psi(x)$***

***$\psi(x)$  must be continuous, single valued, differentiable, and subject to boundary conditions***

$$\underbrace{\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right]}_{\text{Hamiltonian } H = KE + PE} \psi(x) = E \psi(x) \quad \equiv \quad H \psi(x) = E \psi(x)$$

**Expectation value of operator  $\hat{A}$**

$$\hat{A} \psi(x) = \alpha \psi(x)$$

Multiplying both sides on left by  $\psi^*(x)$

$$\psi^*(x) \hat{A} \psi(x) = \psi^*(x) \alpha \psi(x) = \alpha \psi^*(x) \psi(x)$$

*Since  $\alpha$  is a number*

$$\int_{-\infty}^{\infty} \psi^*(x) \hat{A} \psi(x) dx = \int_{-\infty}^{\infty} \alpha \psi^*(x) \psi(x) dx = \alpha \int_{-\infty}^{\infty} \psi^*(x) \psi(x) dx$$

$$= \alpha$$

# Time dependent behaviour of a Gaussian Wave packet

*(Example 6.3 and 6.4 of Serway/Moses/Moyer)*

**Please follow the discussion in the book.**

*In the book the expressions are give without proof. These are built in these notes under 'supporting material'. Purpose of this material is to help you understand the examples 6.3 and 6.4 in your text book. **You are not required to memorize the derivations in the supporting material.** You may have difficulties in understanding some of the steps in the derivation, although enough details are provided. If you follow, it is well and good; if you do not follow, just leave it. The only information you need is (a) expression for the time dependent width, (b) behaviour of the peak amplitude (suppression of amplitude and shifting of the peak) of the wave packet.*

## ***Gaussian Wave packet***

**Let us create a Gaussian wave packet at  $t=0$  such that**

$$a(k) = \exp\left(-\frac{(k - k_0)^2}{2(\Delta k)^2}\right)$$

Mean:  $k_0$   
Variance:  $(\Delta k)^2$

$$\psi(x,0) = \int_{-\infty}^{\infty} \exp\left(-\frac{(k - k_0)^2}{2(\Delta k)^2}\right) \exp(ikx) dk$$

*From our discussions on Gaussian wave packet, we know that the width of  $\psi(x,0)$  is given by*

$$\Delta x(0) = \frac{1}{\Delta k}$$

This is the width of at  **$t=0$**

***We want to know how this width changes with time***

We construct

$$\Psi(x, t) = \psi(x)\phi(t) \qquad \phi = e^{-iEt/\hbar} = e^{-i\omega t}$$

$$\Psi(x, t) = \psi(x)e^{-i\omega t}$$

However, in this problem,  $\omega = \omega(k)$  **(Dispersion relation)**

Therefore,

$$\Psi(x, t) \neq e^{-i\omega t} \int_{-\infty}^{\infty} \exp\left(-\frac{(k - k_0)^2}{2(\Delta k)^2}\right) \exp(ikx) dk$$

But,

$$\Psi(x, t) = \int_{-\infty}^{\infty} \exp\left(-\frac{(k - k_0)^2}{2(\Delta k)^2}\right) \exp(ikx) \exp[-i\omega(k)t] dk$$

$$\Psi(x, t) = \int_{-\infty}^{\infty} \exp\left(-\frac{(k - k_0)^2}{2(\Delta k)^2}\right) \exp(ikx) \exp[-i\omega(k)t] dk$$

What we want to find is the **width** of this wave packet at a function of time  **$[\Delta x(t)]$**  given that the initial width (at time  $t=0$ ) is  **$\Delta x(0)=[\Delta k]^{-1}$**

It can be shown that for  $\Psi(x,t)$  defined as above  
(see supporting material)

$$|\psi(x,t)|^2 = \frac{2\pi}{\Delta x(t)\Delta x(0)} \exp\left(-\frac{(x - v_g t)^2}{[\Delta x(t)]^2}\right) \quad \Rightarrow \quad \text{Time evolution of probability}$$

$$\Delta x(t) = \sqrt{[\Delta x(0)]^2 + \left[\frac{\hbar t}{2m\Delta x(0)}\right]^2} \quad \Rightarrow \quad \text{Time evolution of the width of the wave packet}$$

$m$  = mass of the particle (nonrelativistic)

$v_g$  = Group velocity of the wave packet



## Important observations

$$|\psi(x,t)|^2 = \frac{2\pi}{\Delta x(t)\Delta x(0)} \exp\left(-\frac{(x - v_g t)^2}{[\Delta x(t)]^2}\right) \quad \Delta x(t) = \sqrt{[\Delta x(0)]^2 + \left[\frac{\hbar t}{2m\Delta x(0)}\right]^2}$$

(1) The centre of the wave packet keeps shifting to  $v_g t$  (**see the factor  $(x - v_g t)$  in the exponent**)

(2) Width of the wave packet keeps increasing with time (**see the expression for  $\Delta x(t)$** )

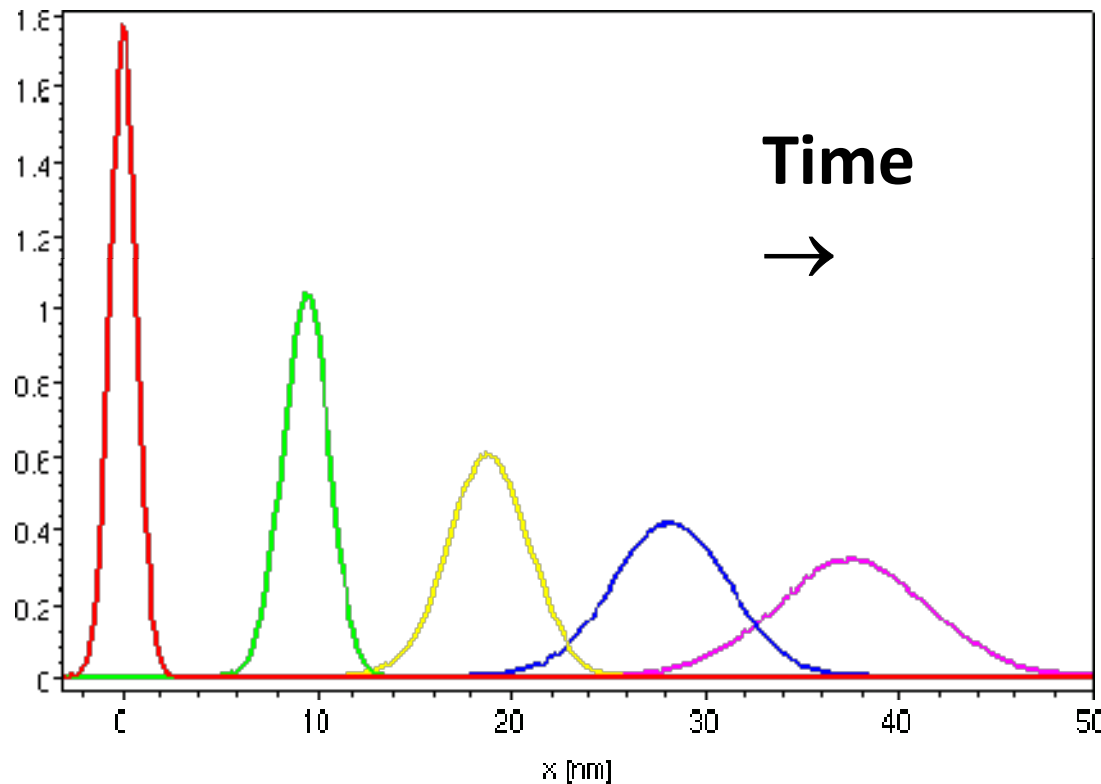
(3) Since,  $P(x,t) = \psi^*(x,t)\psi(x,t)$

$$\frac{P(0,t)}{P(0,0)} = \frac{\Delta x(0)}{\Delta x(t)} \quad \Rightarrow \quad \frac{\psi(0,t)}{\psi(0,0)} = \sqrt{\frac{\Delta x(0)}{\Delta x(t)}} \quad \psi(0,t) \text{ is the peak amplitude of } \psi(x,t)$$

*Thus the peak amplitude of  $\psi(0,t)$  keeps decreasing with increase in time.*

(Refer to Fig.6.4 of *Serway/Moses/Moyer*)

$$\Delta x(t) = \sqrt{[\Delta x(0)]^2 + \left[ \frac{\hbar t}{2m\Delta x(0)} \right]^2}$$



*Evolution of  
wave packet  
in time*

***Width increases*** and ***amplitude decreases*** as ***time is increased***. The centre keeps shifting to  $x=v_g t$ . ***Wave packet disperses in time as  $t \rightarrow \infty$***

**Example 6.4:** An atomic electron is initially localized to a region of space 0.1 nm wide. How much time elapses before this localization is destroyed by dispersion?

$$\Delta x(t) = \sqrt{[\Delta x(0)]^2 + \left[ \frac{\hbar t}{2m\Delta x(0)} \right]^2}$$

The wave packet will completely disperse when  $\Delta x(t) \gg \Delta x(0)$

Assume  $\Delta x(t) = 10\Delta x(0)$

$$100[\Delta x(0)]^2 = [\Delta x(0)]^2 + \frac{\hbar^2 t^2}{4m^2[\Delta x(0)]^2}$$

$$\therefore 99[\Delta x(0)]^4 = \left( \frac{\hbar t}{2m} \right)^2 \quad \rightarrow \quad t = \frac{2m}{\hbar} \sqrt{99} [\Delta x(0)]^2$$

$$m = \text{electron mass} = 9.11 \times 10^{-31} \text{ kg} \quad \Delta x(0) = 0.1 \text{ nm} = 10^{-10} \text{ m}$$

$$t = 1.7 \times 10^{-15} \text{ s}$$

Repeat the calculations for a 1.0 g of marble localized to 0.1 mm

$$t = \frac{2m}{\hbar} \sqrt{99} [\Delta x(0)]^2$$

$$m = \text{mass of marble} = 1 \times 10^{-3} \text{ kg}$$

$$\Delta x(0) = 0.1 \text{ mm} = 10^{-4} \text{ m}$$

$$t = 1.9 \times 10^{24} \text{ s}$$

*Localization of electron is destroyed in a very short time scale.*

*Marble remains localized on any measurable time scale.*

# **Solving Schrodinger Equation for a Free Particle**

# Free Particle

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

$$V(x) = V_0 \quad \text{Particle moving in a constant potential}$$

$V_0 = 0$  is a special case.

**Time independent Schrodinger equation:**

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V_0 \psi(x) = E \psi(x)$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} = (E - V_0) \psi(x) \quad \Rightarrow \quad \frac{\partial^2 \psi(x)}{\partial x^2} = -\frac{2m(E - V_0)}{\hbar^2} \psi(x)$$

$$\frac{\partial^2 \psi(x)}{\partial x^2} = -\frac{2m(E - V_0)}{\hbar^2} \psi(x) \quad \Rightarrow \quad \frac{\partial^2 \psi(x)}{\partial x^2} = -k^2 \psi(x)$$

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

**Let us try trial solution**  $\psi(x) = Ae^{\lambda x}$

$$\frac{\partial^2 \psi(x)}{\partial x^2} = -k^2 \psi(x) \quad \Rightarrow \quad \lambda^2 Ae^{\lambda x} = -k^2 Ae^{\lambda x} \quad \Rightarrow \quad \lambda = \pm ik$$

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

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

$$\text{In general, } \psi(x) = Ae^{ikx} + Be^{-ikx}$$

**Expectation value of momentum=  $\langle p_x \rangle$**

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

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

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

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

**$\psi(x)$  is an eigenfunction of momentum operator  $\hat{p} \psi(x) = p \psi(x)$**

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad \Rightarrow \quad \psi(x, t) = (Ae^{ikx} + Be^{-ikx}) e^{-iEt/\hbar}$$

$$\psi(x, t) = Ae^{i(kx - \omega t)} + Be^{-i(kx + \omega t)}$$

**Travelling right**

**Travelling left**



## Normalization

$$\psi(x) = Ae^{ikx} \quad \Rightarrow \quad \psi^*(x) = A^*e^{-ikx} \quad \Rightarrow \quad \psi^*(x)\psi(x) = |A|^2$$

Probability of finding a particle is constant everywhere!

Wave function  $\psi(x)$  cannot be normalized

*$\psi(x)$  is an eigen function of momentum operator, therefore position is delocalized.*

**Special case**  $V_0 = 0$

$$\text{In general,} \quad k = \sqrt{\frac{2m(E - V_0)}{\hbar^2}} \quad E = V_0 + \frac{\hbar^2 k^2}{2m}$$

$$\text{For } V_0 = 0 \quad \text{and } E > 0, \quad k = \sqrt{\frac{2mE}{\hbar^2}} \quad \text{and} \quad E = \frac{\hbar^2 k^2}{2m}$$

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

Travelling right    Travelling left

**What is the average value of momentum?**

$$\begin{aligned} \langle p \rangle &= \frac{\int_{-\infty}^{\infty} \psi^*(x) \left( -i\hbar \frac{\partial}{\partial x} \right) \psi(x) dx}{\int_{-\infty}^{\infty} \psi^*(x) \psi(x) dx} = \frac{(-i\hbar) \int_{-\infty}^{\infty} (A^* e^{-ikx} + B^* e^{ikx}) \left( \frac{\partial}{\partial x} \right) (Ae^{ikx} + Be^{-ikx}) dx}{\int_{-\infty}^{\infty} (A^* e^{-ikx} + B^* e^{ikx}) (Ae^{ikx} + Be^{-ikx}) dx} \\ &= (-i\hbar)(ik) \frac{\int_{-\infty}^{\infty} (A^* e^{-ikx} + B^* e^{ikx}) (Ae^{ikx} - Be^{-ikx}) dx}{\int_{-\infty}^{\infty} (A^* e^{-ikx} + B^* e^{ikx}) (Ae^{ikx} + Be^{-ikx}) dx} \\ &= \hbar k \frac{\int_{-\infty}^{\infty} (|A|^2 - |B|^2 + AB^* e^{2ikx} - A^* B e^{-2ikx}) dx}{\int_{-\infty}^{\infty} (|A|^2 + |B|^2 + AB^* e^{2ikx} + A^* B e^{-2ikx}) dx} \end{aligned}$$

Terms  $\exp(\pm 2ik)$

integrate out to zero

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

**Average value of the momentum =**  $\langle p \rangle = \hbar k \frac{|A|^2 - |B|^2}{|A|^2 + |B|^2}$

$\frac{|A|^2}{|A|^2 + |B|^2}$  **is the fraction which has**  $\hbar k > 0$

$\frac{|B|^2}{|A|^2 + |B|^2}$  **is the fraction which has**  $\hbar k < 0$



## Summary of Results: Case I

### Schrodinger wave equation

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

**Assuming trial solution**  $\psi(x) = Ae^{\lambda x}$  **we obtain**  $\lambda = \pm ik$

**For**  $E > V_0$  ,  $k^2 > 0$  ,   $\psi(x) = Ae^{ikx} + Be^{-ikx}$

**Case II :**  $E < V_0$    $k^2 < 0$    $k = \sqrt{-\frac{2m|E - V_0|}{\hbar^2}} = i\kappa$

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

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

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

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

***This implies*** when  $E < V_0$

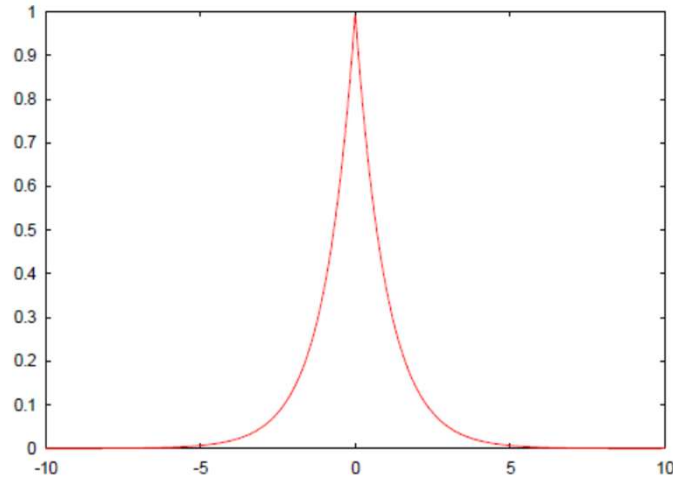
$$\psi(x) = Ce^{\kappa x} \text{ for } x < 0$$

$$\psi(x) = De^{-\kappa x} \text{ for } x > 0$$

***The wave function needs to be continuous and single valued***

$$\therefore C = D$$

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



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

The wave function is continuous at  $x=0$ ,  
*but the derivative of the function is not continuous at  $x=0$*

$$\psi(x) = Ce^{\kappa x}$$

$$\left. \frac{\partial \psi(x)}{\partial x} \right|_{x=0} = \kappa C e^{\kappa x} \Big|_{x=0} = \kappa C$$

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

$$\left. \frac{\partial \psi(x)}{\partial x} \right|_{x=0} = -\kappa C e^{-\kappa x} \Big|_{x=0} = -\kappa C$$

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

**➡ 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 !*

## Supporting material

**How to show**  $\Delta x(t) = \sqrt{[\Delta x(0)]^2 + \left[ \frac{\hbar t}{2m\Delta x(0)} \right]^2}$

$$\Psi(x, t) = \int_{-\infty}^{\infty} \exp\left(-\frac{(k - k_0)^2}{2(\Delta k)^2}\right) \exp(ikx) \exp[-i\omega(k)t] \quad (1)$$

Expand  $\omega(k)$  in Taylor's series and retain terms till second order. Why only up to the second order, you shall know a little later.

$$\begin{aligned} \omega(k) &= \omega(k_0) + (k - k_0) \left. \frac{\partial \omega}{\partial k} \right|_{k=k_0} + \frac{1}{2} (k - k_0)^2 \left. \frac{\partial^2 \omega}{\partial k^2} \right|_{k=k_0} + \dots \\ &= \omega(k_0) + (k - k_0) v_g + \frac{1}{2} (k - k_0)^2 \alpha + \dots \end{aligned}$$

Note,  $d\omega/dk = v_g$   
and  $d^2\omega/dk^2 = \alpha$

$$\Psi(x, t) = \int_{-\infty}^{\infty} \exp\left(-\frac{(k - k_0)^2}{2(\Delta k)^2}\right) \exp\left(i \left[ kx - \omega(k_0)t - (k - k_0)v_g t + \frac{1}{2} (k - k_0)^2 \alpha t \right]\right) dk$$

$$\begin{aligned}
\Psi(x, t) &= \int_{-\infty}^{\infty} \exp\left(-\frac{(k-k_0)^2}{2(\Delta k)^2}\right) \exp\left(i\left[kx - \omega(k_0)t - (k-k_0)v_g t + \frac{1}{2}(k-k_0)^2 \alpha t\right]\right) dk \\
&\quad \text{write } kx = (k-k_0)x + k_0 x \\
&= \exp(i[k_0 x - \omega(k_0)t]) \int_{-\infty}^{\infty} \exp\left(-\frac{(k-k_0)^2}{2}\right) \left(\frac{1}{(\Delta k)^2} + i\alpha t\right) \exp(i(k-k_0)(x - v_g t)) dk \\
&= \exp(i[k_0 x - \omega(k_0)t]) \int_{-\infty}^{\infty} \exp(-\xi(k)) dk \tag{2}
\end{aligned}$$

$$\text{where } \xi(k) = -\frac{1}{2}(k-k_0)^2 \left(\frac{1}{(\Delta k)^2} + i\alpha t\right) + i(k-k_0)(x - v_g t)$$

$$\begin{aligned}
\text{Let } k - k_0 &= \kappa \\
&= -\frac{1}{2}\kappa^2 \left(\frac{1}{(\Delta k)^2} + i\alpha t\right) + i\kappa(x - v_g t) \\
&= -\frac{1}{2} \left(\frac{1}{(\Delta k)^2} + i\alpha t\right) \left(\kappa^2 - \frac{2i\kappa(x - v_g t)}{[(1/\Delta k)^2 + i\alpha t]}\right)
\end{aligned}$$



$$\begin{aligned}
\xi(k) &= -\frac{1}{2} \left( \frac{1}{(\Delta k)^2} + i\alpha t \right) \left( \kappa^2 - \frac{2i\kappa(x - v_g t)}{[(1/\Delta k)^2 + i\alpha t]} \right) \\
&= -\frac{1}{2} \left( \frac{1}{(\Delta k)^2} + i\alpha t \right) \left( \kappa^2 - \frac{2i\kappa(x - v_g t)}{[(1/\Delta k)^2 + i\alpha t]} - \frac{(x - v_g t)^2}{[(1/\Delta k)^2 + i\alpha t]^2} + \frac{(x - v_g t)^2}{[(1/\Delta k)^2 + i\alpha t]^2} \right) \\
&= -\frac{1}{2} \left( \frac{1}{(\Delta k)^2} + i\alpha t \right) \left( \kappa - \frac{i(x - v_g t)}{[(1/\Delta k)^2 + i\alpha t]} \right)^2 - \frac{1}{2} \frac{(x - v_g t)^2}{[(1/\Delta k)^2 + i\alpha t]} \tag{3}
\end{aligned}$$

$$\begin{aligned}
\int_{-\infty}^{\infty} \exp(-\xi(k)) dk &= \exp \left( -\frac{1}{2} \frac{(x - v_g t)^2}{[(1/\Delta k)^2 + i\alpha t]} \right) \times \\
&\quad \int_{-\infty}^{\infty} \exp \left[ -\frac{1}{2} \left( (1/\Delta k)^2 + i\alpha t \right) \left( \kappa - \frac{i(x - v_g t)}{[(1/\Delta k)^2 + i\alpha t]} \right)^2 \right] d\kappa \tag{4}
\end{aligned}$$

$$\text{Let } \kappa - \frac{i(x - v_g t)}{(1/\Delta k)^2 + i\alpha t} = \beta$$

$$\begin{aligned} \int_{-\infty}^{\infty} \exp(-\xi(k)) dk &= \exp\left(-\frac{1}{2} \frac{(x - v_g t)^2}{[(1/\Delta k)^2 + i\alpha t]}\right) \int_{-\infty}^{\infty} \exp\left[-\frac{1}{2} ((1/\Delta k)^2 + i\alpha t) \beta^2\right] d\beta \\ &= \exp\left(-\frac{1}{2} \frac{(x - v_g t)^2}{[(1/\Delta k)^2 + i\alpha t]}\right) \times \left(\sqrt{\frac{2\pi}{[(1/\Delta k)^2 + i\alpha t]}}\right) \quad (5) \end{aligned}$$

*The second bracket is the value of the Gaussian integral*

*Inserting (5) into (2)*

$$\begin{aligned} \psi(x, t) &= \exp(i[k_0 x - \omega(k_0)t]) \int_{-\infty}^{\infty} \exp(-\xi(k)) dk \\ &= \sqrt{\frac{2\pi}{[(1/\Delta k)^2 + i\alpha t]}} \times \exp\left(-\frac{1}{2} \frac{(x - v_g t)^2}{[(1/\Delta k)^2 + i\alpha t]}\right) \times \exp(i[k_0 x - \omega(k_0)t]) \quad (6) \end{aligned}$$

Now rationalizing the second exponent of Eq.(6)

$$\begin{aligned}
-\frac{1}{2} \frac{(x - v_g t)^2}{[(1/\Delta k)^2 + i\alpha t]} &= -\frac{1}{2} \frac{(x - v_g t)^2}{[(1/\Delta k)^2 + i\alpha t]} \frac{[(1/\Delta k)^2 - i\alpha t]}{[(1/\Delta k)^2 - i\alpha t]} \\
&= -\frac{1}{2} \frac{(x - v_g t)^2}{[(1/\Delta k)^4 + \alpha^2 t^2]} [(1/\Delta k)^2 - i\alpha t] \\
&= -\frac{1}{2} \frac{(x - v_g t)^2}{[(1/\Delta k)^4 + \alpha^2 t^2]} (1/\Delta k)^2 + \frac{1}{2} \frac{(x - v_g t)^2 (i\alpha t)}{[(1/\Delta k)^4 + \alpha^2 t^2]} \\
&= -\frac{1}{2} \frac{(x - v_g t)^2}{[(1/\Delta k)^2 + \alpha^2 t^2 (\Delta k)^2]} + \frac{1}{2} i\alpha t \frac{(x - v_g t)^2}{[(1/\Delta k)^4 + \alpha^2 t^2]}
\end{aligned} \tag{7}$$

Now using (7) in (6)

$$\begin{aligned}
 \psi(x, t) &= \sqrt{\frac{2\pi}{[(1/\Delta k)^2 + i\alpha t]}} \times \exp\left(-\frac{1}{2} \frac{(x - v_g t)^2}{[(1/\Delta k)^2 + i\alpha t]}\right) \times \exp(i[k_0 x - \omega(k_0)t]) \\
 &= \sqrt{\frac{2\pi}{[(1/\Delta k)^2 + i\alpha t]}} \times \exp(i[k_0 x - \omega(k_0)t]) \exp\left(\frac{i\alpha t}{2} \frac{(x - v_g t)^2}{[(1/\Delta k)^4 + \alpha^2 t^2]}\right) \\
 &\quad \times \exp\left(-\frac{1}{2} \frac{(x - v_g t)^2}{[(1/\Delta k)^2 + \alpha^2 t^2 (\Delta k)^2]}\right) \quad (8)
 \end{aligned}$$

Use (8) to obtain  $|\psi(x, t)|^2$  (this is done to get rid of imaginary quantities)

$$\begin{aligned}
 |\psi(x, t)|^2 &= \frac{2\pi}{\sqrt{(1/\Delta k)^4 + \alpha^2 t^2}} \exp\left(-\frac{(x - v_g t)^2}{[(1/\Delta k)^2 + \alpha^2 t^2 (\Delta k)^2]}\right) \\
 &\quad (9)
 \end{aligned}$$

Let us closely inspect Eq.(6) and Eq.(9)

$$\psi(x,t) = \sqrt{\frac{2\pi}{[(1/\Delta k)^2 + i\alpha t]}} \times \exp\left(-\frac{1}{2} \frac{(x - v_g t)^2}{[(1/\Delta k)^2 + i\alpha t]}\right) \times \exp(i[k_0 x - \omega(k_0)t]) \quad (6)$$

$$|\psi(x,t)|^2 = \frac{2\pi}{\sqrt{(1/\Delta k)^4 + \alpha^2 t^2}} \exp\left(-\frac{(x - v_g t)^2}{[(1/\Delta k)^2 + \alpha^2 t^2 (\Delta k)^2]}\right) \quad (9)$$

Since  $|\psi(x,t)|^2 = \psi^*(x,t)\psi(x,t)$ ,

Widths of  $|\psi(x,t)|^2$  and  $\psi(x,t)$  are related by the factor  $1/\sqrt{2}$

as we expect. We can therefore continue further analysis based on

$|\psi(x,t)|^2$  which is real.

Eq.(9) can be written in the standard format

$$|\psi(x,t)|^2 = \frac{2\pi}{\sqrt{(1/\Delta k)^4 + \alpha^2 t^2}} \exp\left(-\frac{(x - v_g t)^2}{[\Delta x(t)]^2}\right) \quad (9a)$$

where

$$[\Delta x(t)]^2 = \frac{1}{(\Delta k)^2} + \alpha^2 t^2 (\Delta k)^2$$

Initial width of the wave packet is  $\Delta x(0) = \frac{1}{\Delta k}$

$$[\Delta x(t)]^2 = [\Delta x(0)]^2 + \frac{\alpha^2 t^2}{[\Delta x(0)]^2} \quad (10)$$

*We need value of  $\alpha$ , which can be obtained from the dispersion relation*

## Dispersion relation:

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \hbar \omega \quad \Rightarrow \quad \omega = \frac{\hbar k^2}{2m}$$

$$v_g = \frac{\partial \omega}{\partial k} = \frac{\hbar k}{m} \quad \alpha = \frac{\partial^2 \omega}{\partial k^2} = \frac{\hbar}{m}$$

Substituting value of  $\alpha$  in Eq.(10)

$$[\Delta x(t)]^2 = [\Delta x(0)]^2 + \left[ \frac{\hbar t}{2m \Delta x(0)} \right]^2$$

$$\Delta x(t) = \sqrt{[\Delta x(0)]^2 + \left[ \frac{\hbar t}{2m \Delta x(0)} \right]^2} \quad (11)$$

*This is here you understand why we expanded  $\omega(k)$  up to second order. The dispersion relation is quadratic in  $k$ , therefore  $d^n \omega / dk^n = 0$  for  $n \geq 3$*

*This is the desired result.*

**We thus have**

$$|\psi(x, t)|^2 = \frac{2\pi}{\sqrt{(1/\Delta k)^4 + \alpha^2 t^2}} \exp\left(-\frac{(x - v_g t)^2}{[\Delta x(t)]^2}\right)$$

$$\begin{aligned} \Delta x(t) &= \sqrt{[\Delta x(0)]^2 + \left[\frac{\hbar t}{2m\Delta x(0)}\right]^2} = \sqrt{\frac{[\Delta x(0)]^4 + (\hbar t / 2m)^2}{[\Delta x(0)]^2}} \\ &= \frac{1}{[\Delta x(0)]} \sqrt{[\Delta x(0)]^4 + (\hbar t / 2m)^2} \end{aligned}$$

$$\therefore \Delta x(t)\Delta x(0) = \sqrt{[\Delta x(0)]^4 + (\hbar t / 2m)^2}$$

Now simplify the constant factor using  $\alpha = \frac{\hbar}{2m}$  and  $\Delta x(0) = \frac{1}{\Delta k}$

$$\sqrt{(1/\Delta k)^4 + \alpha^2 t^2} = \sqrt{[\Delta x(0)]^4 + \left(\frac{\hbar t}{2m}\right)^2} = \Delta x(t)\Delta x(0)$$



**Our final expression is**

$$|\psi(x,t)|^2 = \frac{2\pi}{\Delta x(t)\Delta x(0)} \exp\left(-\frac{(x - v_g t)^2}{[\Delta x(t)]^2}\right)$$

$$\Delta x(t) = \sqrt{[\Delta x(0)]^2 + \left[\frac{\hbar t}{2m\Delta x(0)}\right]^2}$$

***Important observations***

**(1) Width of the wave packet keeps increasing with time**

**(2) The centre of the wave packet keeps shifting to  $v_g t$**

**(3) Since,  $P(x,t) = \psi^*(x,t)\psi(x,t)$**

$$\frac{P(0,t)}{P(0,0)} = \frac{\Delta x(0)}{\Delta x(t)}$$

$$\frac{\psi(0,t)}{\psi(0,0)} = \sqrt{\frac{\Delta x(0)}{\Delta x(t)}}$$