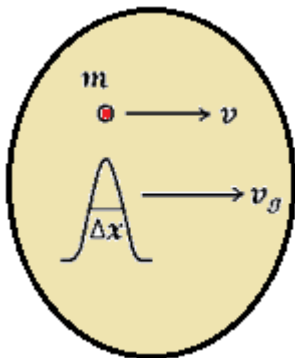


## Application to Spread of Gaussian Wave-Packet for a Free Particle in One Dimension: Concept of Wave Packet:

In the year 1901, the scientist **Max Planck** gave the concept of old quantum theory which is actually based on particle aspect of radiation. By this theory any monochromatic electromagnetic radiation can be considered as a stream of a number of discrete energy packet each containing finite amount of energy  $h\nu$  where  $h$  is **Planck's constant** ( $h = 6.626 \times 10^{-34}$  J.sec) and  $\nu$  is the frequency of that monochromatic radiation. This energy packet is called photon or quanta and thus if the given radiation contains  $n$  number of such discrete monochromatic photon then the total energy of that radiation will be  $E = nh\nu$

After that Planck established this quantum concept theoretically by explaining the characteristics of Black body radiation with the help of this concept. In the year 1905,



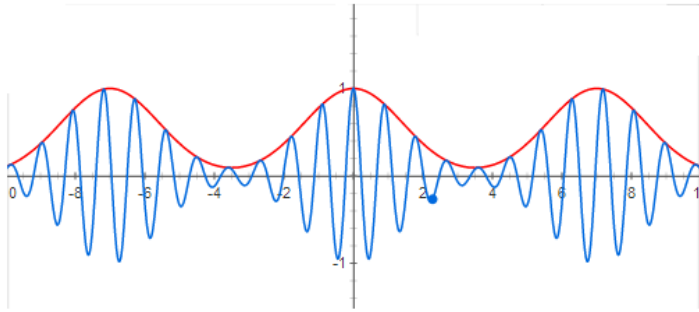
**Einstein** gave the quantum explanation of photo electric effect by the help of this theory given by Planck. Again in 1921 the scientist **Compton** gave the explanation of Compton scattering by this quantum theory. Also the scientist **Dirac** gave the explanation of Pair production with the help of this quantum theory. By this manner Planck's quantum theory was well established.

After a few years, in 1928 the great philosopher **de Broglie** gave the wave aspect of particle motion which is known as wave particle duality. By this aspect, any particle motion can be replaced the motion of matter wave which is basically the wave packet and according to **de Broglie** the wave length of that wave packet is inversely proportional to the momentum of the corresponding particle motion and it is given by  $\lambda = \frac{h}{p} = \frac{h}{mv}$

The basic characteristics of this matter wave are

- It is not a single continuous wave extending from  $-\infty$  to  $+\infty$ , it is actually a wave packet which can be obtained by the superposition of a number of single wave having slightly varying frequency and wavelength.
- The width of the wave packet is the estimation of the position uncertainty ( $\Delta x$ ) and thus this wave particle duality is supported by **Heisenberg's uncertainty principle**.
- The wave packet or the matter wave is a localized wave which can theoretically constructed by **Fourier analysis** and it moves with group velocity which must be equal to the particle velocity as required for perfect replacement.

d) The concept of wave packet motion as a representative of particle motion is also supported by Bohr's quantization of angular momentum which was the basis of Bohr's atomic structure. Thus this wave particle duality is supported by Bohr's atomic theory.



When at least two or more than two waves of slightly different frequency and wavelength superimposes with each other then the amplitude of the resultant wave obtained will propagate in wave manner. The phase velocity of that amplitude wave is called

group velocity in wave motion. Let us now consider the superposition of two waves having respective frequency  $\omega_1$  and  $\omega_2$  and propagation constant  $k_1$  and  $k_2$ . Thus by the principle of superposition the resultant wave will be

$$y = y_1 + y_2 = A\sin(\omega_1 t - k_1 x) + A\sin(\omega_2 t - k_2 x)$$

$$= 2A \sin\left(\frac{\omega_1 + \omega_2}{2} t - \frac{k_1 + k_2}{2} x\right) \cos\left(\frac{\omega_1 - \omega_2}{2} t - \frac{k_1 - k_2}{2} x\right) = A_0 \sin\left(\frac{\omega_1 + \omega_2}{2} t - \frac{k_1 + k_2}{2} x\right)$$

$$\Rightarrow y = A_0 \sin(\omega t - kx) \text{ for } \omega_1 \approx \omega_2 \approx \omega \text{ and } k_1 \approx k_2 \approx k$$

Here the amplitude wave of resultant motion will be

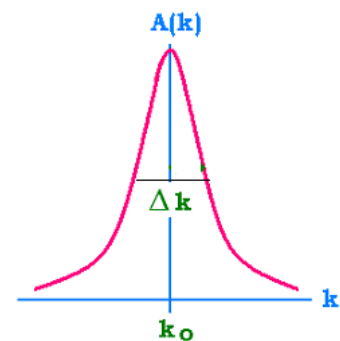
$$A_0 = 2A \cos\left(\frac{\omega_1 - \omega_2}{2} t - \frac{k_1 - k_2}{2} x\right) = 2A \cos\left(\frac{\Delta\omega}{2} t - \frac{\Delta k}{2} x\right)$$

And the phase velocity of this amplitude wave will be  $v_g = \frac{\frac{\Delta\omega}{2}}{\frac{\Delta k}{2}} = \frac{\Delta\omega}{\Delta k} = \frac{d\omega}{dk}$ .

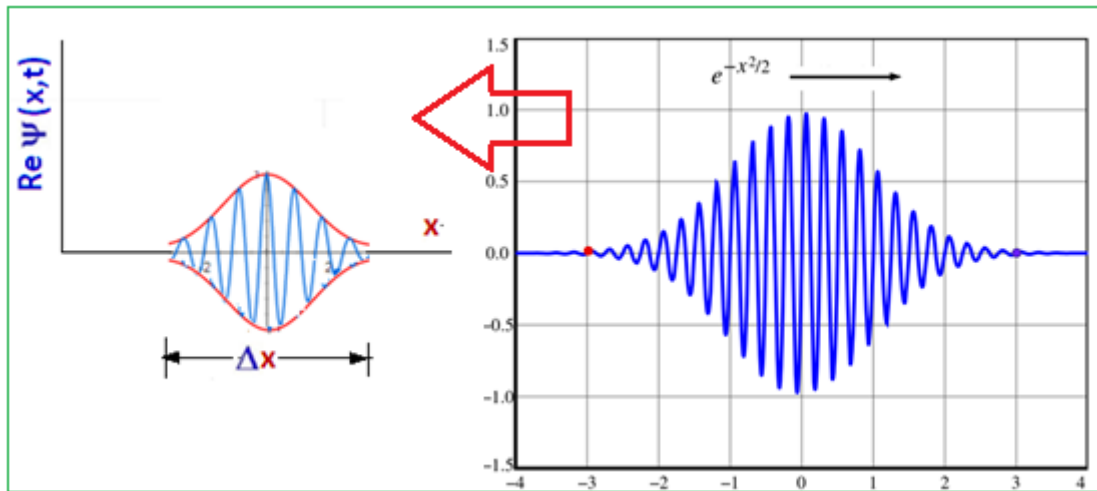
This is the group velocity of wave motion. The velocity of that so called wave packet is equal to this group velocity as predicted in wave particle duality.

Thus we have here the conclusion which is that the wave packet by which we can replace the particle motion has a very small extension which is basically localized wave propagation. It has small extension  $\Delta x$  as limited by uncertainty relation.

As shown in figure the wave packet presentation in position space (in one dim) is shown and this propagates with group velocity as discussed earlier. The presentation as it is described by the superposition of two plane waves with close frequencies or wavelengths but the same presentation can be made by the superposition of infinite number of plane waves with continuously varying frequencies and wave lengths and can be done by taking Fourier integral transform. But it is a fact that if the presentation of this wave packet be



taken in **k – space** i.e. in momentum space then it will be purely Gaussian wave function ( $\sim e^{-\alpha k^2}$ ) as shown in figure.



As we have mentioned earlier that for simple presentation of wave packet through the superposition of two **plane waves (harmonic waves)** the amplitude wave of the resultant wave will be taken as the wave packet propagation with group velocity and the **width** of that packet must be **consistent** with **uncertainty relation**, but for the superposition of infinite number of such plane wave or harmonic wave (one of which can simple be presented by  $Ae^{i(kx-\omega t)}$  in one dimension) with **continuously varying** frequencies or wave lengths, by Fourier's theorem, this wave packet can be expressed by the wave function in position space as

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

And by **inverse Fourier transformation**, the presentation in **momentum space** or **k – space** of the **wave packet** can usually be written as

$$A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x, t) e^{-i(kx-\omega t)} dx$$

This integral will give **Gaussian wave packet** in **k – space** and here we see that basically **A(k)** is not the function of time, thus  $\frac{dA(k)}{dt} = 0$  and that is why it is advantageous to study **Gaussian wave packet** in **k – space**.

In spite of this, (since wave packet is composed of the superposition of the **number of plane waves**, where a free particle wave function is a plane wave function, this **Gaussian wave function** is also the presentation of **Gaussian wave packet** for **free particle**) by

solving the 1<sup>st</sup> integral of Fourier transform as mentioned above, we also get **Gaussian wave packet** in position space multiplied by **harmonic function** and the result we have is

$$\psi(x) = \left(\frac{1}{\sigma\sqrt{\pi}}\right)^{\frac{1}{2}} e^{-x^2/2\sigma^2} \cdot e^{ikx} \quad (\text{As taken at } t = 0)$$

Where  $\sigma$  is the width of the shape and obviously the **probability** of finding particle within the spreading of such wave packet vanishes very rapidly for  $|x| > \sigma$  and more precisely and quantitatively, the **probability density** will be

$$\rho = \psi^* \psi = \frac{1}{\sigma\sqrt{\pi}} e^{-x^2/\sigma^2} \rightarrow \text{This is purely Gaussian function in nature.}$$

As we have mentioned repeatedly that such Gaussian wave packet for free particle motion is **consistent** and is also **limited** by **uncertainty principle** we now have

Since  $\psi(x)$  is **normalized**, we have  $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = \frac{1}{\sigma\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-x^2/\sigma^2} dx = 1$  and we get  $\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx = \frac{1}{\sigma\sqrt{\pi}} \int_{-\infty}^{\infty} x e^{-x^2/\sigma^2} dx = 0$ ,

Also we have  $\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi(x)|^2 dx = \frac{2}{\sigma\sqrt{\pi}} \int_{-\infty}^{\infty} x^2 e^{-x^2/\sigma^2} dx$

But we have a standard integral  $\int_0^{\infty} x^{2n} e^{-ax^2} dx = \frac{1.3.5 \dots (2n-1)}{2^{n+1} a^n} \sqrt{\frac{\pi}{a}}$

Thus we get  $\langle x^2 \rangle = \frac{2}{\sigma\sqrt{\pi}} \cdot \frac{1}{4(1/\sigma^2)} \cdot \sqrt{\frac{\pi}{1/\sigma^2}} = \frac{2}{1/\sigma^2} = \frac{2}{\sigma\sqrt{\pi}} \cdot \frac{\sigma^2}{4} \sigma\sqrt{\pi} = \frac{\sigma^2}{2}$

Similarly we should have  $\langle p \rangle = \langle p_x \rangle = \int \psi^* \left(-i\hbar \frac{\partial}{\partial x}\right) \psi dx$  we get

$\langle p \rangle = \langle p_x \rangle = \int_{-\infty}^{+\infty} \left(\frac{1}{\sigma\sqrt{\pi}}\right)^{\frac{1}{2}} e^{-\frac{x^2}{2\sigma^2}} \cdot e^{-ikx} (-i\hbar) \left(\frac{1}{\sigma\sqrt{\pi}}\right)^{\frac{1}{2}} e^{-\frac{x^2}{2\sigma^2}} \cdot e^{ikx} \left[-\frac{x}{\sigma^2} + ik\right] dx$  and we finally

get  $\langle p \rangle = \langle p_x \rangle = \frac{1}{\sigma\sqrt{\pi}} (-i\hbar)(ik) 2 \int_0^{\infty} e^{-\frac{x^2}{\sigma^2}} dx = \frac{1}{\sigma\sqrt{\pi}} 2\hbar k \cdot \frac{1}{2} \sqrt{\frac{\pi}{1/\sigma^2}} = \hbar k$

Also similarly we get  $\langle p_x^2 \rangle = \int \psi^* \left(-i\hbar \frac{\partial}{\partial x}\right)^2 \psi dx = -\hbar^2 \int \psi^* \frac{\partial^2 \psi}{\partial x^2} dx$

And by some mathematical approach we get  $\langle p_x^2 \rangle = \frac{\hbar^2}{2\sigma^2} + \hbar^2 k^2$

Finally we get  $(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2 = \frac{\sigma^2}{2}$  and  $(\Delta p_x)^2 = \langle p_x^2 \rangle - \langle p_x \rangle^2 = \frac{\hbar^2}{2\sigma^2}$

And then  $(\Delta x)^2 (\Delta p_x)^2 = \frac{\hbar^2}{4}$  or,  $\Delta x \cdot \Delta p_x = \frac{\hbar}{2} \rightarrow$  this is **Uncertainty relation**.