International Journal of Physics and Mathematical Sciences ISSN: 2277-2111 (Online)
An Online, International Journal, Available at http://www.cibtech.org/jpms.htm
2022 Vol. 12, pp. 21-34/Sudin
Research Article (Open Access)

A THEORETICAL RETRACING ON THE STUDY OF WAVE PACKET DYNAMICS

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ABSTRACT
In this article, a localized wave packet of a free particle initially at time '$t = 0$' is considered. The wave functions [$\psi(x,0)$ and $\psi(x,t)$] describing the motion of the wave packet at different intervals of time in position space are obtained mathematically. At later instant of time 't', the wave packet moving with group velocity starts spreading or being dispersed. The time-dependence of the spreading indicates that there is a characteristic time-scale known as 'dispersion-time-scale' over which the spreading takes place. The widths of the wave packet for the wave functions $\psi(x,0)$ and $\psi(x,t)$ are found to be 'Gaussian' in nature. Further, the change of minimum wave packet with time and its dynamical spread have been discussed. It has been observed that the amplitude factor of the wave function of the initial wave packet depends upon the standard deviation but at later instant of time 't' when the wave packet starts spreading, the amplitude factor no longer depends upon the standard deviation. Moreover, 'the measure of the rate at which the wave packet spreads' has been discussed in terms of the sizes of the uncertainties in position and momentum space in this article. The dynamics of the wave packet in light of its spreading has also been discussed graphically.

Keywords: *Dispersion-time-scale, Fourier transforms, Gaussian function, Localized wave packet, Standard deviation, Width of wave packet.*

INTRODUCTION
The construction of wave packets was not an easy task over a long period of time and for this reason; the real practical use of wave packets was not possible to observe in the fields of science. The concept of wave packets introduced by Erwin Schrödinger had endowed the classical trajectory in reducing the gap between the classical and quantum descriptions of nature (Schrödinger, 1926). This approach was proved to be useful in describing Ehrenfest's theorem which states that in the classical limit the quantum mechanical expectation values behave classically (Ehrenfest, 1927). The recent advancements in the field of physics and chemistry of laser interactions with atoms and molecules paved the way of wave packet and its dynamics into the limelight. Wave packets are used in other areas of physics also. Such as, the low temperatures achieved in laser cooling lead to cold collisions of atoms that require a wave packet dynamics (Julienne *et al.*, 1992). Wave packet finds its useful application in the field of atom optics and in semiconductor physics too. A wave function which is localized in small region of space can be regarded as a wave packet. A wave packet therefore comprises of a group of waves of slightly different wavelengths, with phases and amplitudes so chosen such that they interfere constructively over a small region of space, outside of which they produce amplitude that reduces to zero rapidly as a result of destructive interference. Not only are the wave packets useful in the description of 'isolated' particles that are confined to certain spatial region, they also play a key role in understanding the connection between quantum mechanics and classical mechanics. The concept of wave packets is therefore regarded as a useful mathematical tool which can describe not only the particle-like behaviour but the wave-like behaviour also.

In this article, a localized wave packet of a free particle at its initial time '$t = 0$' is considered. A wave packet localized in a very small region can be regarded as a point and its motion may be described by the motion of a single particle. The wave functions [$\psi(x,0)$ and $\psi(x,t)$] describing the motion of the wave packet at different intervals of time in position space are obtained mathematically. At later instant of time 't' the wave packet starts moving with group velocity and simultaneously the spreading or dispersion occurs. The spreading or the dispersion is independent of its velocity. The widths of the wave packet for the wave functions $\psi(x,0)$ and $\psi(x,t)$ are found to be 'Gaussian' in nature. The momentum of the packet also has a width associated with it. However, in the absence of a potential this remains constant. The time-dependence of the spreading indicates that there is a characteristic time-scale known as 'dispersion-time-scale' over which the spreading takes place. Subsequently the change of minimum wave packet with time and the dynamical changes of the spread of the wave packet have been discussed theoretically. It has been observed that the amplitude factor of the wave function of the initial wave packet depends on the standard deviation (σ) but at later instant of time 't' when the wave packet starts spreading, the amplitude factor no longer remains dependent on the standard deviation (σ). Later, 'the measure of the rate at which the wave packet spreads' has been discussed in detailed in terms of the sizes of the uncertainties in position and momentum space. The spreading is quadratic in time, for small time t, becoming linear in time for large t. It is clear that there is characteristic time-scale over which the spreading takes place which is known as dispersion-time-scale (Garraway and Suominen, 1995; Zettili, 2009/2018).
The article is organized as follows: Section-2 i.e. Materials and Methods, has been focused on obtaining the expression that shows the minimum wave packet has the shape of a Gaussian wave and a measure of the spread which is given by the uncertainty Δx expressed in terms of Standard deviation (σ).

In Section-3 i.e. Results and Discussion, the mathematical expression(s) of the change of minimum wave packet with time and the dynamical changes of the spread of the wave packet have been discussed; indicating that there is characteristic time-scale over which the spreading takes place which is known as dispersion-time-scale. In general, such time-scale has been found from wave-packet spreading in the absence of a potential, whereas in case of a harmonic oscillator (Tsuru, 1991), it can be shown that there is no spreading of this kind. The dynamics of the wave packet in light of its spreading has also been discussed graphically.

Finally, Section-4 has been devoted for summarizing the present work with some concluding remarks.

MATERIALS AND METHODS

According to Heisenberg's uncertainty principle (Schiff, 1968/2011; Merzbacher 1970), the relation $\Delta x \Delta p \geq \frac{\hbar}{2}$ holds good for any wave packet. Let us now find shape of the wave packet for which the uncertainty principle attains its theoretical minimum value, so that $\Delta x \Delta p \geq \frac{\hbar}{2}$. The inequality sign can hold only if the functions entering the Schwartz inequality are proportional i.e. if

$$-i\hbar\frac{d\psi}{dx} = Bx\psi \qquad (1)$$

where, 'B' is a suitable multiplier.

$$\therefore (-i\hbar\frac{d\psi}{dx})^* = (B\,x\,\psi\,)^*$$

Or, $$i\hbar\frac{d\psi^*}{dx} = B^*\,x\,\psi^*. \qquad (2)$$

Again the relation,

$$\hbar^2 |\int \psi(x)\,dx|^2 = 4|Im\int (i\,\hbar)\frac{d\psi^*}{dx}\,x\,\psi\,dx|^2$$

$$\leq 4 \, | \int (i\,\hbar) \frac{d\psi^*}{dx} x\, \psi \, dx|^2 \qquad (3)$$

The equation (3) will not admit the inequality unless the integral $4 \, | \int (i\,\hbar) \frac{d\psi^*}{dx} x\, \psi \, dx|^2 = B^* \int x\, \psi^* \, x\, \psi dx$ is purely imaginary. Hence, 'B' must be a purely imaginary number.

Let us, for convenience write,

$$B = \frac{i\,\hbar}{d} \qquad (4)$$

$$\therefore \; -i\hbar \frac{d\psi}{dx} = Bx\psi$$

Or, $-i\hbar \frac{d\psi}{dx} = \frac{i\,\hbar}{d} x\, \psi$

Or, $\frac{d\psi}{dx} = -\, \frac{x}{d}\, \psi \qquad (5)$

The equation (5) can be written in integral form as,

$$\int \frac{d\psi}{\psi} = -\int \frac{x}{d} dx$$

$\ln \psi = -\,\frac{x^2}{d} + \ln N$, $\ln N$ is integration constant.

Or, $\psi = N\, e^{-\frac{x^2}{2d}}. \qquad (6)$

The above expression shows that the minimum wave packet has the shape of a Gaussian wave. It follows from that a Gaussian wave packet represents a particle whose position and momentum are simultaneously determined as closely as is allowed by the uncertainty principle.

The necessity of the integral $\int |\, \psi(x)|^2 \, dx$ for being convergent demands the value of 'd' to be positive.

If we set, $d = \sigma^2$, then equation (6) becomes

$$\psi = N\, e^{-\frac{x^2}{2\sigma^2}} . \qquad (7)$$

After the normalization of the wave function $\psi(x)$ we get,

$$N = \frac{1}{(\pi\sigma^2)^{\frac{1}{4}}}. \qquad (8)$$

Then the wave function representing the wave packet becomes

$$\psi(x) = \frac{1}{(\pi\sigma^2)^{\frac{1}{4}}}\, e^{-\frac{x^2}{2\sigma^2}}. \qquad (9)$$

The width of the wave packet is described in terms of the following relation:

$$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2 \qquad (10)$$

If the origin is chosen at the centre of the packet at time $t = 0$, then $\langle x \rangle = 0$ whence

$$(\Delta x)^2|_{t=0} = \langle x^2 \rangle - \langle x \rangle^2$$

$$= \langle x^2 \rangle = \int_{-\infty}^{\infty} \psi^* \, x^2 \, \psi dx$$

$$= \frac{1}{\sigma\sqrt{\pi}} \int_{-\infty}^{\infty} x^2 \, e^{-\frac{x^2}{\sigma^2}} dx \qquad (11)$$

To evaluate the above integration, one needs to use the following general formula:

$$\int_0^{\infty} x^{2n} \, e^{-\alpha x^2} dx = \frac{1 \cdot 3 \cdot 5 \cdots (2n-1)}{2^{n+1}\alpha^n} \sqrt{\frac{\pi}{\alpha}} \, ; \qquad (12)$$

Therefore, $\langle x^2 \rangle = \int_{-\infty}^{\infty} \psi^* \, x^2 \, \psi \, dx = \frac{\sigma^2}{2} \cdot \frac{1}{4(\frac{1}{\sigma^2})} \cdot \sqrt{\frac{\pi}{\frac{1}{\sigma^2}}} = \frac{\sigma^2}{2}$

The width of the wave packet at time $t = 0$ is therefore calculated as:

$$\Delta x|_{t=0} = \frac{\sigma}{\sqrt{2}} \qquad (13)$$

Since, $\Delta x \Delta p = \frac{\hbar}{2}$, the minimum width in momentum space is $\frac{\sigma}{\sqrt{2}} \, \Delta p = \frac{\hbar}{2}$

Or, $\Delta p = \frac{\hbar}{\sigma\sqrt{2}}$. $\qquad$ (14)

Thus, Δp remains constant as the wave packet moves.

Let us now find the form of the wave packet:

The minimum uncertainty product can be obtained when the following term can be written as:

$$\int \psi^* \left(\hat{\alpha}\hat{\beta} + \hat{\beta}\hat{\alpha}\right) \psi dx = 0 \qquad (15)$$

and that the Schwartz inequality reduces to equality, which it does when $f = \hat{\alpha}\psi$ and $g = \hat{\beta}\psi$ are made proportional i.e. 'f' is proportional to 'g', then $f = \gamma g$.

i.e. $\hat{\alpha}\psi = \gamma\hat{\beta}\psi$; 'γ' is a constant. $\qquad$ (16)

We have chosen the followings:

$$\hat{\alpha} = \hat{x} - \langle x \rangle \qquad (17)$$

and

$$\hat{\beta} = \hat{p} - \langle p \rangle = -i\hbar \frac{d}{dx} - \langle p \rangle. \qquad (18)$$

Therefore, the equation (16) can be written in terms of the equations (17) and (18) as the following:

$$(\hat{x} - \langle x \rangle)\, \psi = \gamma[\left(-i\hbar \frac{d}{dx}\right) \psi - \langle p \rangle]\psi$$

Or, $\frac{d\psi}{dx} = [\frac{i}{\gamma\hbar}(x - \langle x \rangle) + \frac{i\,\langle p \rangle}{\hbar}]\psi$ $\qquad$ (19)

Integrating the equation (19) over 'x'; we get $\psi(x)$ as

$$\psi(x) = N\, e^{\left[\frac{i}{2\gamma\hbar}(x-\langle x\rangle)^2 + \frac{i\langle p\rangle x}{\hbar}\right]} \qquad (20)$$

where 'N' can be chosen to normalize the wave function.

To find out the value of 'γ', we make use of the equations (15) and (16) together and write them as the following:

$$\int \psi^* \left(\hat{\alpha}\hat{\beta} + \hat{\beta}\hat{\alpha}\right)\psi dx = \left(\frac{1}{\gamma} + \frac{1}{\gamma^*}\right)\int \psi^* \alpha^2\, \psi dx = 0 \qquad (21)$$

since, $\int \psi^* \left(\hat{\alpha}\hat{\beta}\right)\psi dx = \int \psi^*\, \hat{\alpha}\cdot\frac{1}{\gamma}\hat{\alpha}\psi = \frac{1}{\gamma}\int \psi^*\, \widehat{\alpha^2}\psi\, dx$ (22)

and $\int \psi^* \left(\hat{\beta}\hat{\alpha}\right)\psi dx = \int (\,\hat{\beta}\psi\,)^* \hat{\alpha}\, \psi\, dx,$ (23)

since $\hat{\beta}$ is hermitian operator, the equation (23) be written as

$$\int \psi^* \left(\hat{\beta}\hat{\alpha}\right)\psi dx = \frac{1}{\gamma^*}\int \psi^*\, \widehat{\alpha^2}\, \psi\, dx\,, \qquad (24)$$

since $\hat{\alpha}$ is real and hermitian.

Equation (21) then requires that 'γ' must be pure imaginary, as

$$\int \psi^*\, \widehat{\alpha^2}\, \psi\, dx = 0 \text{ and } \frac{1}{\gamma} + \frac{1}{\gamma^*} = 0. \qquad (25)$$

Also $\psi(x)$ must converge. In that case first term of exponent of the exponential term in equation (20) must be negative, so that 'γ' must be negative imaginary number, say $\gamma = -i\delta$; where δ is real.

To find the value of N, it is necessary to normalize the wave function $\psi(x) = N\, e^{\left[\frac{i}{2\gamma\hbar}(x-\langle x\rangle)^2 + \frac{i\langle p\rangle x}{\hbar}\right]}$ as below:

$$\int \psi^*\, \psi\, dx = N^* N \int e^{\,-(x-\langle x\rangle)^2/\delta\hbar}\, dx$$

Or, $N^* N = \dfrac{1}{\int e^{\,-(x-\langle x\rangle)^2/\delta\hbar} dx}$ (26)

The use of the standard integral $\int_{-\infty}^{\infty} e^{-\,\alpha x^2}\, dx = \sqrt{\frac{\pi}{\alpha}}$ leads the above equation (26) as,

$$|N| = \frac{1}{\sqrt{(\pi\delta\hbar)^{1/2}}} = (\pi\delta\hbar)^{-\frac{1}{4}} \qquad (27)$$

The integral, $\int \psi^*\, \widehat{\alpha^2}\psi\, dx = \int \psi^*\, (\hat{x} - \langle x\rangle)^2 \psi\, dx$ in the equation (21) is the expectation value of $(\hat{x} - \langle x\rangle)^2$ which has been defined as $(\Delta x)^2$.

Therefore,

$$N^* N \int e^{\,-(x-\langle x\rangle)^2/\delta\hbar}\, (\hat{x} - \langle x\rangle)^2 dx = (\Delta x)^2 \qquad (28)$$

Or, $(\pi\delta\hbar)^{-\frac{1}{2}} \cdot \frac{1}{2}\sqrt{\pi(\delta\hbar)^3} = (\Delta x)^2$

$$[\because \int_{-\infty}^{\infty} e^{-\alpha x^2}\, x^2\, dx = \frac{1}{2}\sqrt{\frac{\pi}{\alpha^3}}\,]$$

Or, $\frac{1}{2}\delta\hbar = (\Delta x)^2$

Or, $\delta = \frac{2(\Delta x)^2}{\hbar}$. (29)

Hence the form of the minimum wave packet is

$$\psi(x) = [2\pi(\Delta x)^2]^{-\frac{1}{4}}\, e^{\left[-\frac{(x-\langle x\rangle)^2}{4(\Delta x)^2} + \frac{i\langle p\rangle x}{\hbar}\right]} \quad (30)$$

This function has the form of Gaussian error function; actually this is the envelope of oscillations represented by the exponential term $e^{\frac{i\langle p\rangle x}{\hbar}}$. The width of the wave packet Δx is given in terms of standard deviation (σ) as

$(2\Delta x)^2 = 2\sigma^2$

Or, $\sigma = \sqrt{2}\,\Delta x$. (31)

The spread of a wave packet can be measured in terms of the uncertainty expressed by the following relation:

$$\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{\langle x^2\rangle}\,, \quad (32)$$

where, $\langle x\rangle$ stands for expectation value.

Now, at time $t = 0$; we get, $|\psi(x,0)|^2 = \frac{1}{\sigma\sqrt{\pi}}\, e^{-\frac{x^2}{\sigma^2}}$ and hence

$$(\Delta x)^2|_{t=0} = \langle x^2\rangle - \langle x\rangle^2$$

$$= \langle x^2\rangle \qquad [\because \text{ at } t = 0,\ \langle x\rangle = 0]$$

$$= \int_{-\infty}^{\infty} x^2\, |\psi(x,0)|^2\, dx$$

$$= \frac{1}{\sigma\sqrt{\pi}} \int_{-\infty}^{\infty} x^2\, e^{-\frac{x^2}{\sigma^2}} dx$$

$$= \frac{1}{\sigma\sqrt{\pi}} \cdot \frac{1}{2}\sqrt{\frac{\pi}{(\sigma^2)^3}} \qquad [\because \int_{-\infty}^{\infty} e^{-\alpha x^2}\, x^2\, dx = \frac{1}{2}\sqrt{\frac{\pi}{\alpha^3}}\,]$$

and thus,

$$(\Delta x)^2|_{t=0} = \frac{\sigma^2}{2}. \quad (33)$$

RESULTS AND DISCUSSION

To find the change with time of minimum packet, let us consider for simplicity that the wave packet has the form with $\langle x \rangle$ and/or $\langle p \rangle$. In terms of the standard deviation (σ), the wave function of the wave packet centered at origin at time $t = 0$, can be written as the following:

$$\psi(x,0) = \frac{1}{\sqrt{\sigma\sqrt{\pi}}}\, e^{[-\frac{x^2}{2\sigma^2}]}\, e^{[\frac{i}{\hbar}\langle p \rangle x]}. \quad (34)$$

Then, the Fourier transforms (Arfken and Weber, 2005) of the wave function $\psi(x,0)$ at the time $t = 0$ is given by

$$\varphi(p,0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x,0)\, e^{[-\frac{i}{\hbar} p\, x]}\, dx \quad (35)$$

Or, $\varphi(p,0) = \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{\sqrt{\sigma\sqrt{\pi}}} \int_{-\infty}^{\infty} e^{[-\frac{x^2}{2\sigma^2}]}\, e^{[\frac{i}{\hbar}\langle p \rangle x]}\, e^{[-\frac{i}{\hbar} p\, x]}\, dx$

Or, $\varphi(p) = \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{\sqrt{\sigma\sqrt{\pi}}} \int_{-\infty}^{\infty} e^{-\frac{x^2}{2\sigma^2}}\, e^{-\frac{i}{\hbar}(p - \langle p \rangle)x}\, dx$

Or, $\varphi(p) = \sqrt{\frac{\sigma}{\hbar\sqrt{\pi}}}\, e^{-\frac{\sigma^2}{2\hbar^2}(p - \langle p \rangle)^2}$. (36)

Therefore, the wave packet at a later instant of time 't' can be obtained by Fourier transforms as the following:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \varphi(p)\, e^{\frac{i}{\hbar}(p\,x - E\,t)}\, dp\,, \quad (37)$$

where, $E = \frac{p^2}{2m}$ is the energy for a free particle wave function.

$$\therefore \psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \sqrt{\frac{\sigma}{\hbar\sqrt{\pi}}} \int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2\hbar^2}(p - \langle p \rangle)^2}\, e^{\frac{i}{\hbar}(p\,x - \frac{p^2}{2m} t)} dp$$

(38)

Or, $\psi(x,t) = \sqrt{\frac{\sigma}{2\pi\hbar \cdot \hbar\sqrt{\pi}}} \int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2\hbar^2}(p - \langle p \rangle)^2}\, e^{\frac{i}{\hbar}(p\,x - \frac{p^2}{2m} t)} dp$

$$= C \int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2\hbar^2}(p - \langle p \rangle)^2}\, e^{\frac{i}{\hbar}(p\,x - \frac{p^2}{2m} t)} dp \quad (39)$$

where, $C = \sqrt{\frac{\sigma}{2\pi\hbar \cdot \hbar\sqrt{\pi}}}$. (40)

$$\therefore \psi(x,t) = C \int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2\hbar^2}(p - \langle p \rangle)^2}\, e^{\frac{i}{\hbar}(p\,x - \frac{p^2}{2m} t)} dp \quad (41)$$

Let, $p - \langle p \rangle = k$ (42)

$\therefore p = k + \langle p \rangle$ and $(p - \langle p \rangle)^2 = k^2$ (43)

Also, $px = kx + \langle p \rangle x$ and $dp = dk$ (44)

Substituting the values of the equations from (42) to (44) in the expression of $\psi(x,t)$, the equation (39) takes the form as

$$\psi(x,t) = C\int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2\hbar^2}k^2}\, e^{\frac{i}{\hbar}[\,kx+\langle p\rangle x-\frac{(k+\langle p\rangle)^2}{2m}t]}dk \qquad (45)$$

$$= C\, e^{\frac{i}{\hbar}\langle p\rangle x} e^{-\frac{i}{\hbar}\frac{\langle p\rangle^2 t}{2m}} \int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2\hbar^2}k^2}\, e^{\frac{i}{\hbar}kx} e^{-\frac{i}{\hbar}\frac{(k^2+2k\langle p\rangle)t}{2m}} dk$$

Let, $A = C\, e^{\frac{i}{\hbar}\langle p\rangle x} e^{-\frac{i}{\hbar}\frac{\langle p\rangle^2 t}{2m}}$ (46)

and $I = \int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2\hbar^2}k^2}\, e^{\frac{i}{\hbar}kx} e^{-\frac{i}{\hbar}\frac{(k^2+2k\langle p\rangle)t}{2m}} dk$, (47)

such that $\psi(x,t) = A\cdot I$.

The integral in the equation (47) can be calculated as follows:

$$I = \int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2\hbar^2}k^2}\, e^{\frac{i}{\hbar}kx} e^{-\frac{i}{\hbar}\frac{(k^2+2k\langle p\rangle)t}{2m}} dk$$

$$= \int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2\hbar^2}k^2}\, e^{\frac{i2\hbar\sigma^2}{2\hbar^2\sigma^2}kx} e^{-\frac{i\hbar\sigma^2}{2\hbar^2 m\sigma^2}(k^2 t+2k\langle p\rangle t)} dk$$

$$= \int_{-\infty}^{\infty} e^{\frac{\sigma^2}{2\hbar^2}[-k^2\left(1+\frac{i\hbar t}{m\sigma^2}\right)+\frac{2i\hbar k}{\sigma^2}(x-\frac{\langle p\rangle t}{m})]} dk$$

$$= \int_{-\infty}^{\infty} e^{\frac{\sigma^2}{2\hbar^2}[\frac{-k^2\sigma^2\left(1+\frac{i\hbar t}{m\sigma^2}\right)+2i\hbar k(x-\frac{\langle p\rangle t}{m})}{\sigma^2}]} dk$$

$$= \int_{-\infty}^{\infty} e^{\frac{\sigma^2}{2\hbar^2}[\frac{-k^2\left(\sigma^2+\frac{i\hbar t}{m}\right)+2i\hbar k(x-\frac{\langle p\rangle t}{m})}{\sigma^2}]} dk \qquad (48)$$

Now, let us assume the term, $\left(\sigma^2 + \frac{i\hbar t}{m}\right) = \gamma^2$ (49)

$$\therefore I = \int_{-\infty}^{\infty} e^{\frac{\sigma^2}{2\hbar^2}[\frac{-k^2\gamma^2+2i\hbar k(x-\frac{\langle p\rangle t}{m})}{\sigma^2}]} dk$$

$$= \int_{-\infty}^{\infty} e^{\frac{\gamma^2}{2\hbar^2}\cdot[(\frac{i\hbar\left(x-\frac{\langle p\rangle t}{m}\right)}{\gamma^2})^2-\{k-\frac{i\hbar\left(x-\frac{\langle p\rangle t}{m}\right)}{\gamma^2}\}^2]} dk$$

$$= \int_{-\infty}^{\infty} e^{-\frac{1}{2\gamma^2}(x-\frac{\langle p\rangle t}{m})^2}\cdot e^{-\frac{\gamma^2}{2\hbar^2}\cdot\{k-\frac{i\hbar\left(x-\frac{\langle p\rangle t}{m}\right)}{\gamma^2}\}^2} dk \qquad (50)$$

Again, let the term, $\{k - \frac{i\hbar\left(x-\frac{\langle p\rangle t}{m}\right)}{\gamma^2}\} = z$ and by the use of the standard integral $\int_{-\infty}^{\infty} e^{-\alpha x^2}dx = \sqrt{\frac{\pi}{\alpha}}$; we have Integral '$I$' as

$$I = e^{-\frac{1}{2\gamma^2}(x-\frac{\langle p\rangle t}{m})^2}\int_{-\infty}^{\infty} e^{-\frac{\gamma^2}{2\hbar^2}z^2} dz$$

$$= e^{-\frac{1}{2\gamma^2}(x-\frac{\langle p\rangle t}{m})^2} \cdot \sqrt{\frac{\pi}{\frac{\gamma^2}{2\hbar^2}}}$$

Or, $I = e^{-\frac{(x-\frac{\langle p\rangle t}{m})^2}{2\gamma^2}} \cdot \sqrt{\frac{\pi \cdot 2\hbar^2}{\gamma^2}}$ (51)

Substituting the values of 'A' and 'I' respectively from the equations (46) and (51) in the expression for $\psi(x,t)$ we get,

$\psi(x,t) = A \cdot I$

$$= C\, e^{\frac{i}{\hbar}\langle p\rangle x} e^{-\frac{i}{\hbar}\frac{\langle p\rangle^2 t}{2m}} \cdot e^{-\frac{(x-\frac{\langle p\rangle t}{m})^2}{2\gamma^2}} \cdot \sqrt{\frac{\pi \cdot 2\hbar^2}{\gamma^2}}$$

$$= \sqrt{\frac{\sigma}{2\pi\hbar \cdot \hbar\sqrt{\pi}}} \cdot e^{\frac{i}{\hbar}\langle p\rangle x} \cdot e^{-\frac{i}{\hbar}\frac{\langle p\rangle^2 t}{2m}} \cdot e^{-\frac{(x-\frac{\langle p\rangle t}{m})^2}{2\gamma^2}} \cdot \sqrt{\frac{\pi \cdot 2\hbar^2}{\gamma^2}}$$

$$= \frac{1}{\sqrt{\sigma\sqrt{\pi}}} \cdot \frac{\sigma}{\gamma} \cdot e^{-\frac{\{x-\frac{\langle p\rangle t}{m}\}^2}{2\gamma^2}} e^{\frac{i}{\hbar}\langle p\rangle\,(x-\frac{\langle p\rangle t}{2m})} \quad (52)$$

Finally the expression for the wave function of the wave packet at later instant of time 't' can be written as follows:

$$\therefore \psi(x,t) = \frac{1}{\sqrt{\sigma\sqrt{\pi}}} \cdot \frac{\sigma}{\gamma} \cdot e^{-\frac{\{x-\frac{\langle p\rangle t}{m}\}^2}{2\gamma^2}} e^{\frac{i}{\hbar}\langle p\rangle\,(x-\frac{\langle p\rangle t}{2m})} \quad (53)$$

where, $\gamma^2 = \left(\sigma^2 + \frac{i\hbar t}{m}\right)$.

The equation (53) reveals that $\psi(x,t)$ simultaneously contains an amplitude factor $[\frac{1}{\sqrt{\sigma\sqrt{\pi}}} \cdot \frac{\sigma}{\gamma} \cdot e^{-\frac{\{x-\frac{\langle p\rangle t}{m}\}^2}{2\gamma^2}}]$ and a phase factor $[e^{\frac{i}{\hbar}\langle p\rangle\,(x-\frac{\langle p\rangle t}{2m})}]$.

The phase velocity 'v_p' is the velocity with which a particular phase of the wave moves. This is given by

$$\frac{d}{dt}[\frac{i}{\hbar}\langle p\rangle\left(x - \frac{\langle p\rangle t}{2m}\right)] = 0$$

$$v_p = \frac{\langle p\rangle}{2m} = \frac{v_g}{2}, \quad (54)$$

when the group velocity (or the particle velocity) of the wave is $v_g = \frac{\langle p\rangle}{m}$. (55)

The amplitude factor is also function of time, the position x changing with time according to the following:

$$(x)_t = x - \frac{\langle p\rangle t}{m} = x - v_g t. \quad (56)$$

This shows that packet travels with group velocity 'v_g'.

If, initially, $\langle p\rangle = 0$ [i.e. when value of the phase factor, $e^{\frac{i}{\hbar}\langle p\rangle\,(x-\frac{\langle p\rangle t}{2m})} = 1$], then packet remains stationary but the width of the packet increases with time.

$$\because \gamma^2 = \left(\sigma^2 + \frac{i\hbar t}{m}\right) = \sigma^2\left(1 + \frac{i\hbar t}{m\sigma^2}\right);$$

$$\therefore 2\gamma^2 = 2\sigma^2\left(1 + \frac{i\hbar t}{m\sigma^2}\right).$$

Since, γ^2 is a complex number (quantity), we can write γ^2 in terms of its modulus values along with the phase factor as follows:

$$\gamma^2 = \sigma^2(1 + \frac{\hbar^2 t^2}{m^2\sigma^4})^{\frac{1}{2}} e^{i\theta}\ , \qquad (57)$$

where, $\theta = \tan^{-1}(\frac{\hbar t}{m\sigma^2})$. (58)

$$\therefore \frac{1}{\gamma^2} = \frac{e^{-i\theta}}{\sigma^2(1+\frac{\hbar^2 t^2}{m^2\sigma^4})^{\frac{1}{2}}}$$

$$\text{Or, } \frac{1}{\gamma} = \frac{e^{-\frac{i\theta}{2}}}{\sigma(1+\frac{\hbar^2 t^2}{m^2\sigma^4})^{\frac{1}{4}}} = \frac{1}{\sigma}(1 + \frac{\hbar^2 t^2}{m^2\sigma^4})^{-\frac{1}{4}} \cdot\ e^{-\frac{i\theta}{2}}. \qquad (59)$$

$$\because \psi(x,t) = \frac{1}{\sqrt{\sigma\sqrt{\pi}}} \cdot \frac{\sigma}{\gamma} e^{\frac{i}{\hbar}\langle p\rangle\,(x-\frac{\langle p\rangle t}{2m})} \cdot e^{-\frac{\{x-\frac{\langle p\rangle t}{m}\}^2}{2\gamma^2}}$$

Substituting the modulus values along with the phase factor in the expression of $\psi(x,t)$ we have,

$$\psi(x,t) = \frac{1}{\sqrt{\sigma\sqrt{\pi}}} \cdot \frac{\sigma}{1} \cdot \frac{1}{\sigma}(1 + \frac{\hbar^2 t^2}{m^2\sigma^4})^{-\frac{1}{4}} \cdot\ e^{-\frac{i\theta}{2}} \cdot e^{\frac{i}{\hbar}\langle p\rangle\,(x-\frac{\langle p\rangle t}{2m})} \cdot\ e^{-\frac{\{x-\frac{\langle p\rangle t}{m}\}^2}{(2\sigma^2+\frac{2i\hbar t}{m})}}$$

$$= \frac{1}{\sqrt{\sigma\sqrt{\pi}}} \cdot (1 + \frac{\hbar^2 t^2}{m^2\sigma^4})^{-\frac{1}{4}} \cdot\ e^{-\frac{i\theta}{2}} \cdot e^{\frac{i}{\hbar}\langle p\rangle\,(x-\frac{\langle p\rangle t}{2m})} \cdot\ e^{-\frac{\{x-\frac{\langle p\rangle t}{m}\}^2}{(2\sigma^2+\frac{2i\hbar t}{m})}} \qquad (60)$$

Therefore, the probability density (Das and Sengupta, 2002) of the wave packet in position space now can be expressed as the square absolute of $\psi(x,t)$ as following:

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

$$\frac{1}{\sigma\sqrt{\pi}} \cdot (1 + \frac{\hbar^2 t^2}{m^2\sigma^4})^{-\frac{1}{2}} \cdot |e^{-\frac{\{x-\frac{\langle p\rangle t}{m}\}^2}{\left(2\sigma^2+\frac{2i\hbar t}{m}\right)}}|^2 \cdot \quad \{e^{-\frac{i\theta}{2}} e^{\frac{i}{\hbar}\langle p\rangle\left(x-\frac{\langle p\rangle t}{2m}\right)} \cdot e^{\frac{i\theta}{2}}\, e^{-\frac{i}{\hbar}\langle p\rangle\left(x-\frac{\langle p\rangle t}{2m}\right)}\}$$

$$= \frac{1}{\sigma\sqrt{\pi}} \cdot (1 + \frac{\hbar^2 t^2}{m^2\sigma^4})^{-\frac{1}{2}} \cdot |e^{-\frac{\{x-\frac{\langle p\rangle t}{m}\}^2}{(2\sigma^2+\frac{2i\hbar t}{m})}}|^2$$

$$= \frac{1}{\sigma\sqrt{\pi}} \cdot (1 + \frac{\hbar^2 t^2}{m^2\sigma^4})^{-\frac{1}{2}} \cdot [e^{-\frac{\{x - \frac{\langle p \rangle t}{m}\}^2}{\left(2\sigma^2 + \frac{2i\hbar t}{m}\right)}} \cdot e^{-\frac{\{x - \frac{\langle p \rangle t}{m}\}^2}{\left(2\sigma^2 - \frac{2i\hbar t}{m}\right)}}]$$

$$\therefore |\psi(x,t)|^2 == \frac{1}{\sigma\sqrt{\pi}} \cdot (1 + \frac{\hbar^2 t^2}{m^2\sigma^4})^{-\frac{1}{2}} \cdot e^{-\frac{\{x - \frac{\langle p \rangle t}{m}\}^2}{\sigma^2 (1+\frac{\hbar^2 t^2}{m^2\sigma^4})}}. \quad (61)$$

The width of the wave packet is described by as follows:

$$(\Delta x)^2 = \int_{-\infty}^{\infty} x^2 \, |\psi(x,t)|^2 \, dx$$

$$= \int_{-\infty}^{\infty} x^2 \, \frac{1}{\sigma\sqrt{\pi}} \cdot (1 + \frac{\hbar^2 t^2}{m^2\sigma^4})^{-\frac{1}{2}} \cdot e^{-\frac{\{x - \frac{\langle p \rangle t}{m}\}^2}{\sigma^2 (1+\frac{\hbar^2 t^2}{m^2\sigma^4})}} dx$$

$$= \frac{1}{\sigma\sqrt{\pi}} \cdot (1 + \frac{\hbar^2 t^2}{m^2\sigma^4})^{-\frac{1}{2}} \int_{-\infty}^{\infty} x^2 \, \cdot e^{-\frac{\{x - \frac{\langle p \rangle t}{m}\}^2}{\sigma^2 (1+\frac{\hbar^2 t^2}{m^2\sigma^4})}} dx$$

$$= \frac{\sigma^2}{2} \cdot (1 + \frac{\hbar^2 t^2}{m^2\sigma^4})^{-\frac{1}{2}} \cdot \frac{1}{2} \cdot \sqrt{\frac{\pi}{\{\sigma^2 \, (1+\frac{\hbar^2 t^2}{m^2\sigma^4})\}^3}}$$

$$= \frac{1}{\sigma\sqrt{\pi}} \cdot (1 + \frac{\hbar^2 t^2}{m^2\sigma^4})^{-\frac{1}{2}} \cdot \frac{1}{2} \cdot \sqrt{\pi} \cdot \sigma^3 \, \{(1 + \frac{\hbar^2 t^2}{m^2\sigma^4})\}^{\frac{3}{2}}$$

$$= \frac{\sigma^2}{2} \cdot (1 + \frac{\hbar^2 t^2}{m^2\sigma^4})$$

$$\therefore (\Delta x)^2 = \frac{\sigma^2}{2} \cdot (1 + \frac{\hbar^2 t^2}{m^2\sigma^4})$$

$$= (\Delta x)^2_{t=0}(1 + \frac{\hbar^2 t^2}{m^2\sigma^4}); \qquad [\because \; (\Delta x)^2_{t=0} = \frac{\sigma^2}{2}] \quad (62)$$

Or, $(\Delta x) = (\Delta x)_{t=0}\sqrt{1 + \frac{\hbar^2 t^2}{m^2\sigma^4}}$ (63)

Let, $\frac{m\sigma^2}{\hbar} = T$, then the equation (62) leads to the following as:

$(\Delta x)^2 = (\Delta x)^2_{t=0}(1 + \frac{t^2}{T^2});$ (64)

Or, $(\Delta x) = (\Delta x)_{t=0}[1 + (\frac{t}{T})^2]^{\frac{1}{2}};$ (65)

where, $T = \frac{m\sigma^2}{\hbar} = \frac{2m(\Delta x)^2_{t=0}}{\hbar}$ (66)

The expression of the equation (66) represents a time constant (T) that characterizes the rate at which the wave packet spreads.

International Journal of Physics and Mathematical Sciences ISSN: 2277-2111 (Online)
An Online, International Journal, Available at http://www.cibtech.org/jpms.htm
2022 Vol. 12, pp. 21-34/Sudin
Research Article (Open Access)

In terms of the uncertainty quantities (Δx and Δp), the equation (64) with the help of the equation (66) can be written as the following:

$$(\Delta x)^2 = (\Delta x)^2_{t=0} + \frac{t^2}{T^2}(\Delta x)^2_{t=0}$$

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

$$= (\Delta x)^2_{t=0} + (\Delta p)^2_{t=0}\frac{t^2}{m^2}. \qquad (67)$$

The graphical representation of the equation (63) is shown in Fig. 1 by the curve $\frac{(\Delta x)}{(\Delta x)_{t=0}}$ Or, $\sqrt{1+\frac{\hbar^2 t^2}{m^2\sigma^4}}$ versus t as follows:

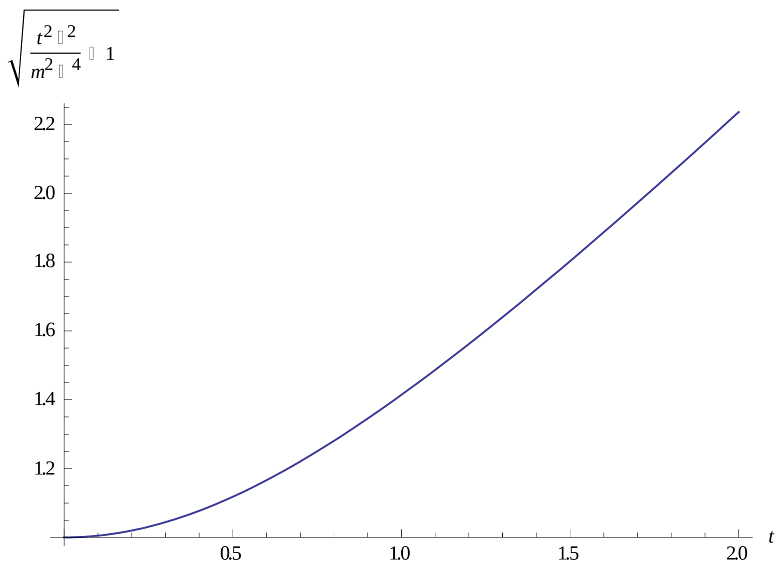

Fig. 1: $\frac{(\Delta x)}{(\Delta x)_{t=0}}$ Or $\sqrt{1+\frac{\hbar^2 t^2}{m^2\sigma^4}}$ versus t curve

From Fig. 1 it can be observed that the curve maintains its parabolic nature for smaller time limits ($t < 1$) and in the vicinity of the origin. The curve becomes linear when it tends to go away from the vicinity of the origin and for the larger time limits ($t > 1$). It can also be observed from the Fig. 1 that the shape of the wave packet changes inappreciably as longer as $t \ll T$ but when $t \gg T$, the original shape of the packet is completely changed indicating that the spreading is quadratic in time for small 't' and it becomes linear in time for large 't'.

CONCLUSION

The wave-packets and its dynamics have been a side issue in quantum mechanics for a long time. Their use in theory has been limited to simple textbook examples, which help the undergraduate students to understand how Fourier transforms connect the position and momentum representations and yield the Heisenberg uncertainty principle. Most of the scattering theory, however, has been based on the time-independent view of interfering plane and spherical waves, and in atomic and molecular physics, interactions of matter with light have been treated by finding the wave functions for all the quantum states of the system and calculating their static overlap integrals (Franck-Condon factors). In these systems the time evolution for each state has been assumed to be independent of the other states and unitary, thus only contributing to the phase of the wave function of the corresponding quantum state. In this present article, a localized wave packet of a free particle at its initial time '$t = 0$' is considered. A wave packet localized in a very small region can be regarded as a point and its motion may be described by the motion of a single particle. The wave functions [$\psi(x, 0)$ and $\psi(x, t)$] describing the motion of the wave packet at different intervals of time in position space are obtained mathematically. The widths of the wave functions $\psi(x, 0)$ and $\psi(x, t)$ are found to be 'Gaussian' in nature. At later instant of time 't' the wave packet moves with group velocity with having the spreading. However, in the absence of a potential this remains constant. The time-dependence of the spreading indicates that there is a characteristic time-scale known as 'dispersion-time-scale' over which the spreading takes place.

Further the change of minimum wave packet with time and the dynamical changes of the spread of the wave packet have been discussed theoretically. It can be observed that the amplitude factor of the wave function of the initial wave packet depends on the standard deviation (σ) but at later instant of time 't' when the wave packet starts spreading, the amplitude factor no longer remains dependent on the standard deviation (σ). Later, 'the measure of the rate at which the wave packet spreads' has been discussed in terms of the sizes of the uncertainties in position and momentum space. The spreading is quadratic in time, for small time 't', becoming linear in time for large 't'. The characteristic time-scale over which the spreading takes place is termed as dispersion-time-scale. The dispersion time-scale is important for setting the regime in which time-dependent wave-packet dynamics can be observed. However, the dispersive time-scale is still seen to play a role in determining spreading or dispersion in realistic potentials and is especially important during dissociation. Because of the landmark contributions of the wave packet dynamics, the significant advancements have taken place in the field of physics, atom optics, semiconductor physics and chemistry of laser interactions with atoms and molecules. It remains an interesting curiosity to investigate the efficacy of studying the dynamics of wave packet for the systems involving different types of potential.

ACKNOWLEDGEMENT

The author is sincerely thankful to the anonymous referees for providing their useful and constructive suggestions.

COMPETING INTERESTS

The author declares that there are no competing interests, financial or otherwise regarding the publication of this paper.

REFERENCES

Arfken GB and Weber HJ (2005). Mathematical Methods for Physicists, 6th Edition. *Elsevier Academic Press, New York, USA*, 938-941.

Das SK and Sengupta S (2002). Quantum and classical propagation of a Gaussian ensemble: Two examples. *Current Science* **83** (10) 1231-1234.

Ehrenfest P (1927). Bemerkungüber die angenäherte Gültigkeit der klassischen Mechanik innerhalb der Quantenmechanik. *Zeitschrift fuer Physik* **45** (7-8) 455-457. https://doi.org/10.1007/BF01329203

Garraway BM and Suominen K A (1995). Wave-packet dynamics: new physics and chemistry in femto-time. *Reports on Progress in Physics* **58** (4) 365-419.
DOI: 10.1088/0034-4885/58/4/001

Julienne PS, Smith AM and Burnett K (1992). Theory of Collisions between Laser Cooled Atoms. *Advances In Atomic, Molecular, and Optical Physics* **30** 141-198.
doi:10.1016/S1049-250X(08)60175-5

Merzbacher E (1970). Quantum Mechanics, 2nd Edition. *John Wiley and Sons Ltd., New York,USA*, 1-35.
Schiff LI (1968/2011). Quantum Mechanics, 3rd Edition. *Tata McGraw Hill Education Private Ltd., New Delhi, India*, 60-65.
Schrödinger E (1926). Quantisierung als Eigenwertproblem II. *Annalen der Physik* **79** (6) 489–527. https://doi.org/10.1002/andp.19263840602
Tsuru H (1991). Wave Packet Motion in Harmonic Potential. *Journal of the Physical Society of Japan* **60** (11) 3657-3663.
Zettili N (2009/2018). Quantum Mechanics Concepts and Applications, 2nd Edition. *Wiley India Pvt. Ltd., New Delhi, India*, 38-54.