Gaussian Wave Packets

Consider a free particle whose wave function is a Gaussian at $t=0$.

$$\psi(x,0) = \underbrace{\left(\frac{2}{a^2\pi}\right)^{1/4}}_{A} e^{-x^2/a^2} \quad \text{(Normalized)}$$

Find $\phi(k)$

$$\phi(k) = \frac{A}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-x^2/a^2} e^{-ikx}\, dx$$

$$= \frac{A}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{1}{a^2}\left(x^2 + ika^2x\right)}\, dx$$

Complete the Square in the Exponent

$$x^2 + ika^2x + \left(\frac{ika^2}{2}\right)^2 - \left(\frac{ika^2}{2}\right)^2$$

$$= \left(x + \frac{ika^2}{2}\right)^2 - \left(\frac{ika^2}{2}\right)^2$$

$$\phi(k) = \frac{A}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{1}{a^2}\left(x + \frac{ika^2}{2}\right)^2} e^{\frac{1}{a^2}\left(\frac{ika^2}{2}\right)^2}$$

$$= \frac{A}{\sqrt{2\pi}} e^{-\frac{k^2a^2}{4}} \int_{-\infty}^{\infty} e^{-\frac{1}{a^2}\left(x + i\frac{ka^2}{2}\right)^2} dx$$

u-substitution

$$u = x + \frac{ika^2}{2} \qquad du = dx$$

$$\phi(k) = \frac{A}{\sqrt{2\pi}} e^{-\frac{k^2a^2}{4}} \underbrace{\int_{-\infty}^{\infty} e^{-u^2/a^2} du}_{\sqrt{\pi}\, a}$$

$$= \frac{a}{\sqrt{2}} \left(\frac{2}{a^2\pi}\right)^{1/4} e^{-k^2a^2/4}$$

Fourier transform of a Gaussian is a Gaussian.

Uncertainty

If $\quad \psi(x,0) = \left(\frac{2\lambda}{\pi}\right)^{1/4} e^{-\lambda x^2}$

$$\Rightarrow \quad \langle x \rangle = 0$$

$$\langle x^2 \rangle = \frac{1}{4\lambda}$$

$$\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \frac{1}{2\sqrt{\lambda}}$$

~~For~~ For our wave function, $\lambda = 1/a^2$

$$\sigma_x = \frac{a}{2}$$

Our "k" space wave function is also a Gaussian

$$\langle k \rangle = 0 \qquad \langle k^2 \rangle = \frac{1}{4\lambda}$$

$$\sigma_k = \frac{1}{2\sqrt{\lambda}} = \frac{1}{a}$$

$$\lambda = a^2/4$$

Momentum Uncertainty $\quad \sigma_p = \hbar \sigma_k = \frac{\hbar}{a}$

Uncertainty Relation

$$\sigma_x \sigma_p = \left(\frac{a}{2}\right)\left(\frac{\hbar}{a}\right) = \frac{\hbar}{2}$$

$\Rightarrow$ The Gaussian is the minimum uncertainty wave packet.

Time Evolution of the Wave Packet

For a free particle

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

$$\psi(x,t) = \frac{A}{\sqrt{2\pi}}\left(\frac{a}{\sqrt{2}}\right)\int_{-\infty}^{\infty} dk\, e^{-\frac{k^2 a^2}{4}} e^{-i\omega t} e^{ikx}$$

$$= \frac{A}{\sqrt{2\pi}}\left(\frac{a}{\sqrt{2}}\right)\int_{-\infty}^{\infty} dk\, e^{-\frac{k^2 a^2}{4}} e^{ikx} e^{-\frac{i\hbar k^2 t}{2m}}$$

We would like to compute the wave speed of this wave packet to determine if the wave moves as $\frac{d\langle x\rangle}{dt} = \frac{\langle p\rangle}{m}$.

Unfortunately, the average speed of the wave is zero, $\langle k\rangle = 0 \longrightarrow \hbar\langle k\rangle = \langle p\rangle = 0$

We need to change the wave packet to move the average momentum away from zero. We know how to do this with a Gaussian, try the wave packet.

$$\psi(x,0) = \frac{A}{\sqrt{2\pi}}\frac{a}{\sqrt{2}}\int_{-\infty}^{\infty} dk\; e^{-\frac{(k-k_0)^2 a^2}{4}} e^{ikx}$$

We know from the homework that this will yield

$$\langle k\rangle = k_0 \longrightarrow \langle p\rangle = \hbar k_0$$

We can perform the transform by completing the square again

$$\psi(x,0) = A e^{-x^2/a^2} e^{ik_0 x}$$

The net effect of the change is we pick up a factor of $e^{ik_0 x} = e^{ipx/\hbar}$ the solution for a free particle moving with momentum p.

Now calculate the full time evolution

$$\psi(x,t) = \left(\frac{2a^2}{\pi}\right)^{1/4} \frac{e^{i\phi} e^{ik_0 x}}{\left(a^4 + \frac{4\hbar^2 t^2}{m^2}\right)^{1/4}} \exp -\left[\frac{\left(x - \frac{\hbar k_0}{m} t\right)^2}{a^2 + \frac{2i\hbar t}{m}}\right]$$

$$\phi = -\theta - \frac{\hbar k_0^2}{2m} t \qquad \tan 2\theta = \frac{2\hbar t}{ma^2}$$

$$= \frac{A}{\sqrt{2\pi}} \left(\frac{a}{\sqrt{2}}\right) \int_{-\infty}^{\infty} e^{-\frac{a^2}{4}(k-k_0)^2} e^{-i\frac{\hbar k^2}{2m}t} e^{ikx} \, dk$$

Properties

I. Wave moves with speed $\frac{\hbar k_0}{m} = v_{group}$

II The width of the wavepacket increases as

$$\Delta x = \frac{a}{2}\sqrt{1 + \frac{4\hbar^2 t^2}{m^2 a^4}}$$

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Jon requested some additional steps.

$$p(x) = \psi^* \psi = \left(\frac{2a^2}{\pi}\right)^{1/2} \frac{1}{\sqrt{a^4 + \frac{4\hbar^2 t^2}{m^2}}}$$

$$\exp\left[- \frac{\left(x - \frac{\hbar k_0}{m} t\right)^2}{a^2 + \frac{2i\hbar t}{m}} + \frac{-\left(x - \frac{\hbar k_0}{m} t\right)^2}{a^2 - \frac{2i\hbar t}{2m}} \right]$$

Work on [ ]

$$[\;] = -\left(x - \frac{\hbar k_0}{m} t\right)^2 \left[\frac{a^2 - \frac{2i\hbar t}{m}}{a^4 + \frac{4\hbar^2 t^2}{m}} + \frac{a^2 + 2i\hbar t}{a^4 + \frac{4\hbar^2 t^2}{m}} \right]$$

$$= \frac{-2a^2\left(x - \frac{\hbar k_0}{m} t\right)^2}{a^4 + \frac{4\hbar^2 t^2}{m}} = \frac{-2\left(x - \frac{\hbar k_0}{m} t\right)^2}{a^2 + \frac{4\hbar^2 t^2}{m a^2}}$$