Fourier Transform in Quantum Mechanics

The fundamental equation in quantum mechanics is the Schrodinger equation

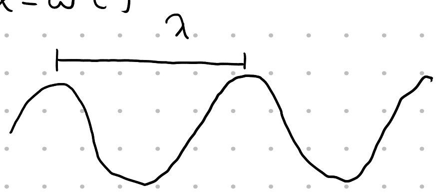
$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x,t)\psi(x,t)$$

Assuming $V(x,t)=0$, free particle

The solution of this equation is a wave,

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

$$k = \frac{2\pi}{\lambda}$$



From De broglie waves, we have that,

$$p = \frac{h}{\lambda} = \hbar k \rightarrow k = \frac{p}{\hbar}$$

$$\psi(x,t) = e^{i\left(\frac{p}{\hbar}x - \omega t\right)}$$

For simplicity let's take the wave profile a $t=0$

$$\psi(x) = e^{i\left(\frac{p}{\hbar}x\right)}$$

which is a solution of the time-independent Schrodinger equation,

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

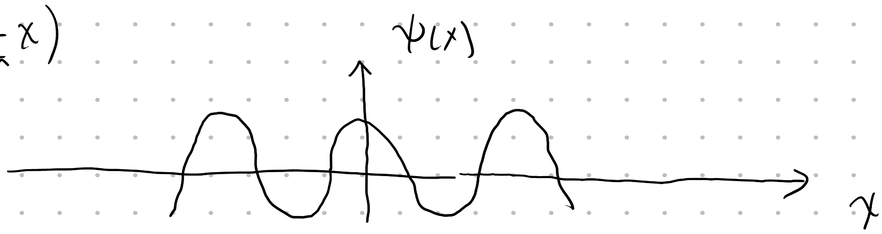
Proof:

$$-\frac{\hbar^2}{2m}\frac{p^2}{\hbar^2}(-1)\psi(x) = E\psi(x)$$

$$E = \frac{p^2}{2m} \leftarrow \text{as in the classical case,}$$

Hence, we have

$$\psi(x) = e^{i\left(\frac{p}{\hbar}x\right)}$$



And, $\psi(x)\,\psi^*(x) = P(x)$ ← is the probability density of the particle at x.

Now, the wavefunction $\psi(x)$ represents the probability in position space,

We can represent the wavefunction in the momentum space, by transforming $\psi(x)$ to $\phi(p)$ via the Fourier transform,

$$\begin{tikzcd} \psi(x) \arrow[r, bend left, "F.T"] & \phi(p) \arrow[l, bend left, "I.F.T"] \end{tikzcd}$$

$$\phi(p) = \int_{-\infty}^{\infty} \psi(x)\, e^{-ipx/\hbar}\, dx \quad ; \quad \psi(x) = e^{ip_0x/\hbar}, \quad p_0 \text{ fixed}$$

$$= \int_{-\infty}^{\infty} e^{ip_0x/\hbar}\, e^{-ipx/\hbar}\, dx$$

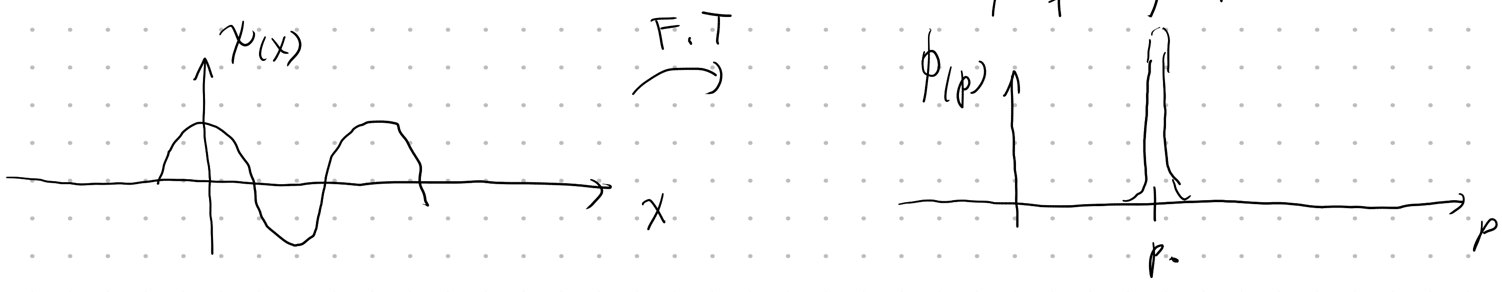
$$= \int_{-\infty}^{\infty} \left(\cos\left(\frac{p_0x}{\hbar}\right) + i\sin\left(\frac{p_0x}{\hbar}\right)\right)\left(\cos\left(\frac{px}{\hbar}\right) - i\sin\left(\frac{px}{\hbar}\right)\right) dx$$

From orthogonality,

$$\phi(p) = \frac{1}{2}\left[\delta\left(\frac{p_0}{\hbar} - \frac{p}{h}\right) + \delta\left(\frac{p_0}{\hbar} + \frac{p}{\hbar}\right)\right]$$

$$+ \frac{1}{2}\left[\delta\left(\frac{p_0}{\hbar} - \frac{p}{\hbar}\right) - \delta\left(\frac{p_0}{\hbar} + \frac{p}{\hbar}\right)\right]$$

$$= \delta\left(\frac{p_0}{\hbar} - \frac{p}{\hbar}\right) = \delta(p_0 - p_0)$$ ← It peaks at the frequency p_0.



Total uncertainty of position leads to total certainty of momentum.

An interesting solution of the T-I-S-E is the Gaussian wave packet,

$$\psi(x) = e^{i\left(\frac{px}{\hbar}\right)} e^{-x^2/2\sigma^2} \qquad P(x) = e^{-x^2/2(\sigma^2/2)} \leftarrow \text{prob}$$

this is a wave modulated with a Gaussian,

Its Fourier transform is given by,

$$\phi(p) = \int e^{i\left(\frac{p_0 x}{\hbar}\right)} e^{-x^2/4\sigma^2} e^{\frac{-ipx}{\hbar}} dx$$

$$= \exp\left[\frac{-(p-p_0)^2\sigma^2}{2\hbar^2}\right] = \exp\left[\frac{-(p-p_0)^2}{2(\hbar^2/\sigma^2)}\right]$$

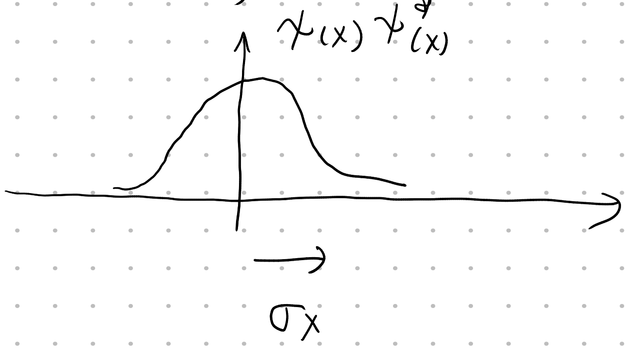
the probability of momentum is

$$Q(p) = \phi(p)\phi^*(p) = e^{-(p-p_0)^2/2(\hbar^2/2\sigma^2)} = e^{-(p-p_0)^2/2\sigma_p^2}$$

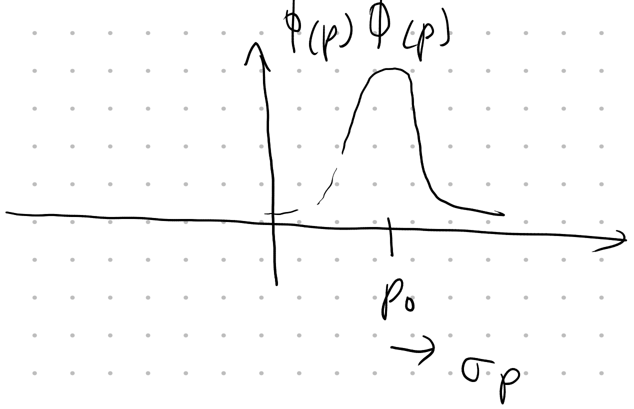
Hence $\sigma_x \sigma_p = \frac{\sigma}{\sqrt{2}} \frac{\hbar}{\sqrt{2}\sigma} = \frac{\hbar}{2}$

$\sigma_x \sigma_p \geq \frac{\hbar}{2} \leftarrow$ uncertainty principle,

Pictorially,



$\xrightarrow{\text{F.T}}$



If σ_x is large σ_p is small, and viceversa.