Lecture 11 - Chapter. 4
Wave & Particles II

“Matter” behaving as “Waves”

Outline:
• A Double-Slit Experiment (watch “video”)
• Properties of Matter Waves
• The Free-Particle Schrödinger Equation
• Uncertainty Principle
• The Bohr Model of the Atom
• Mathematical Basis of the Uncertainty Principle – The Fourier Transform

The Schrödinger equation is based upon energy. The simplest solution is a plane wave, a complex exponential with two sinusoidal parts. The wave’s magnitude and the probability density vary neither in time nor in position.

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

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

$$frac{\hbar^2}{2m} = \frac{p^2}{2m} = E$$

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

$$|\Psi(x, t)|^2 = \Psi^*(x, t)\Psi(x, t) = |Ae^{-i(kx - \omega t)}| [Ae^{+i(kx - \omega t)}] = A^2$$

$$|\Psi(x, t)| = A = \text{constant (x,t)}$$
Uncertainty Principle

If a phenomenon has a wave nature, it is theoretically impossible to know precisely the position along an axis and the component of momentum along that axis simultaneously; \( \Delta x \) and \( \Delta p_x \) cannot be simultaneously zero. Rather, there is a strict theoretical lower limit on their product:

\[
\Delta p_x \Delta x \geq \frac{\hbar}{2}
\]  

(3-9)

Gaussian Wave form

\[ \Psi(x, 0) = A e^{-\left(x/2b\right)^2} \cos(kx) \]

\( x \)

\( A \)

The Uncertainty Relations in 3 Dimensions

\[
\Delta p_x \Delta x \geq \frac{\hbar}{2} \quad \Delta p_y \Delta y \geq \frac{\hbar}{2} \quad \Delta p_z \Delta z \geq \frac{\hbar}{2}
\]

\[
\Delta E \Delta t \geq \frac{\hbar}{2}
\]
The Uncertainty Relations and the Fourier Transform

Any wave may be expressed mathematically as a superposition of plane waves of different wavelengths and amplitudes.

\[ f(x) = \int_{-\infty}^{\infty} \tilde{f}(k) e^{ikx} \, dk \quad (3-11) \]
\[ \tilde{f}(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x) e^{-ikx} \, dx \]

Inverse Fourier transform (k→x)  Fourier transform (x→k)

Fourier Transform

\[ \psi(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{\psi}(k) e^{ikx} \, dk \]
\[ \tilde{\psi}(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \psi(x) e^{-ikx} \, dx \]
Gaussian Wave Packet

\[ \psi(x) = Ae^{-(x/2\epsilon)^2} e^{ik_0x} \]

Probability Density:

\[ |\psi(x)|^2 = A^2 e^{-(x/\epsilon)^2} \]

Gaussian Wave Packet

\[ \psi(x) = Ae^{-(x/2\epsilon)^2} e^{ik_0x} \]

\[ \vec{p} = \hbar k_0 \hat{x} \]

Find the “Spectral Content”:

\[ \tilde{\psi}(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \psi(x) e^{-ikx} dx \]

\[ \tilde{\psi}(k) = \frac{A}{2\pi} \int_{-\infty}^{\infty} e^{-(1/4\epsilon^2)x^2 + i(k_0 - k)x} dx \]

\[ \int_{-\infty}^{\infty} e^{-az^2 + bz} dz = e^{b^2/4a} \sqrt{\frac{\pi}{a}} \]

\[ a = 1/4\epsilon^2 \]

\[ b = i(k_0 - k) \]
\[ \tilde{\psi}(k) = \frac{A}{2\pi} \int_{-\infty}^{\infty} e^{-\frac{1}{4\varepsilon^2}x^2 + i(k_0 - k)x} dx \]

\[ \tilde{\psi}(k) = \frac{A}{2\pi} e^{-\frac{\varepsilon^2}{2}(k_0 - k)^2} \]

\[ \tilde{\psi}(k) = \frac{A\varepsilon}{\sqrt{\pi}} e^{-\frac{\varepsilon^2}{2}(k_0 - k)^2} \]

Not a complex function

“Spectral Content” is a Gaussian function!

\[ \psi(x) = A e^{-\frac{(x/2\varepsilon)^2}{2}} e^{ik_0x} \]

\[ \tilde{\psi}(k) = \frac{A\varepsilon}{\sqrt{\pi}} e^{-\frac{\varepsilon^2}{2}(k_0 - k)^2} \]

\[ \Delta x = \varepsilon \]

1 standard deviation

\[ \Delta x \Delta p = \Delta x \Delta (\hbar k) = \varepsilon \frac{\hbar}{2\varepsilon} = \frac{\hbar}{2} \]

Gaussian Wave Packet

Minimal Uncertainty

A Single-Slit

\[ \psi(x) = A e^{-\frac{(x/2\varepsilon)^2}{2}} e^{ik_0x} \]

\[ \tilde{\psi}(k) = \frac{A\varepsilon}{\sqrt{\pi}} e^{-\frac{\varepsilon^2}{2}(k_0 - k)^2} \]

\[ \Delta x = \varepsilon \]

1 standard deviation

\[ \Delta k = \frac{1}{2\varepsilon} \]

\[ \Delta x \Delta p = \Delta x \Delta (\hbar k) = \varepsilon \frac{\hbar}{2\varepsilon} = \frac{\hbar}{2} \]

Gaussian Wave Packet

Minimal Uncertainty

A Single-Slit

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Gaussian Wave Packet

Minimal Uncertainty
A Single-Slit

\[ \tilde{\psi}(k) = \frac{C}{\pi} \frac{\sin(ka/2)}{ka/2} \]

Spectral Content