PHYS-3301

Lecture 7

Sep. 12, 2024

Chapter. 4
Wave & Particles II

"Matter" behaving as "Waves"

Outline:

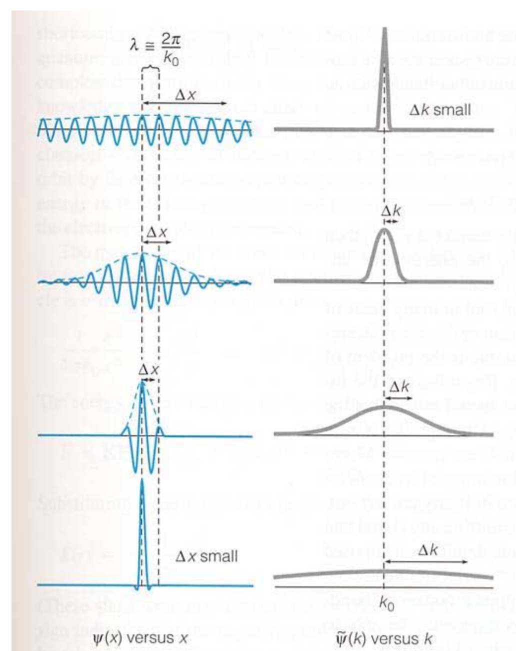
- A Double-Slit Experiment (watch "video")
- Properties of Matter Waves
- The Free-Particle Schrödinger Equation
- **Uncertainty Principle**
- **The Bohr Model of the Atom**
- **Mathematical Basis of the Uncertainty Principle – The Fourier Transform**

The Uncertainty Relations and the Fourier Transform

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

$$f(x) = \int_{-\infty}^{+\infty} \tilde{f}(k) e^{ikx}\, dk \qquad \text{(3-11)} \qquad \tilde{f}(k) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} f(x) e^{-ikx}\, dx$$

Inverse Fourier transform $(k \rightarrow x)$ Fourier transform $(x \rightarrow k)$



Fourier Transform

$$\psi(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\tilde{\psi}(k)e^{ikx}\,dk$$

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

Fourier Transform

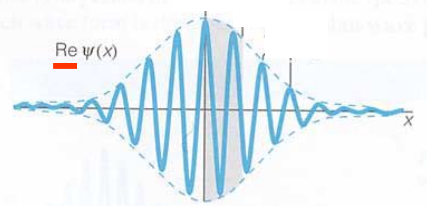
Spectral Content

$$\psi(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\tilde{\psi}(k)e^{ikx}\,dk$$

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

Gaussian Wave Packet

$$\psi(x) = Ae^{-(x/2\varepsilon)^2}e^{ik_0x}$$



Probability Density:

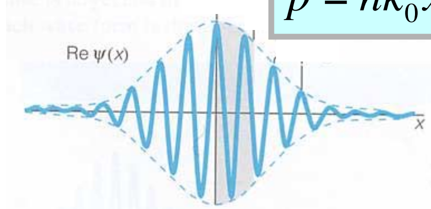
$$|\psi(x)|^2 = A^2e^{-(x/\varepsilon)^2}$$

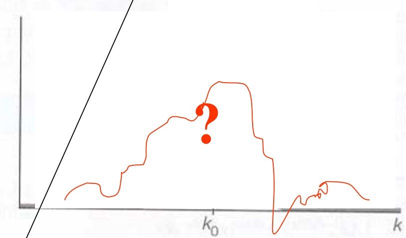
Gaussian Wave Packet

$$\psi(x) = Ae^{-(x/2\varepsilon)^2}e^{ik_0x}$$

$$\tilde{\psi}(k) = ?$$

$$\vec{p} = \hbar k_0\hat{x}$$





Find the *"Spectral Content"*:

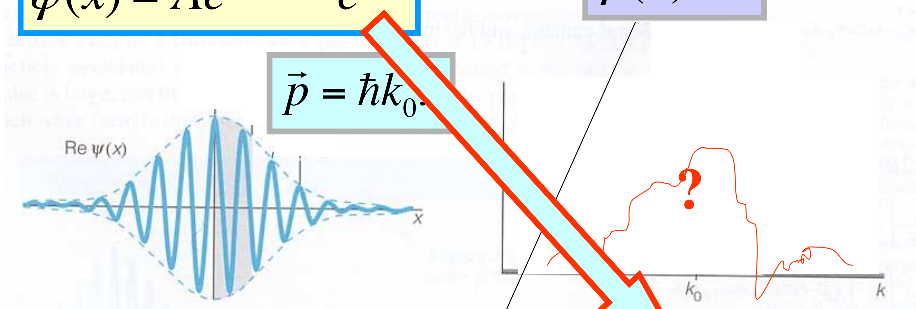
$$\tilde{\psi}(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\psi(x)e^{-ikx}\,dx$$

Gaussian Wave Packet

$$\psi(x) = Ae^{-(x/2\varepsilon)^2} e^{ik_0 x}$$

$$\tilde{\psi}(k) = ?$$

$$\vec{p} = \hbar k_0$$



Find the *"Spectral Content"*:

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

$$\tilde{\psi}(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} (Ae^{-(x/2\varepsilon)^2} e^{-ik_0 x}) e^{ik\,x} dx$$

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

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

$$a = 1/4\varepsilon^2$$

$$b = i(k_0 - k)$$

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

$$\tilde{\psi}(k) = \frac{A}{2\pi} e^{-\varepsilon^2 (k_0 - k)^2} \sqrt{4\varepsilon^2 \pi}$$

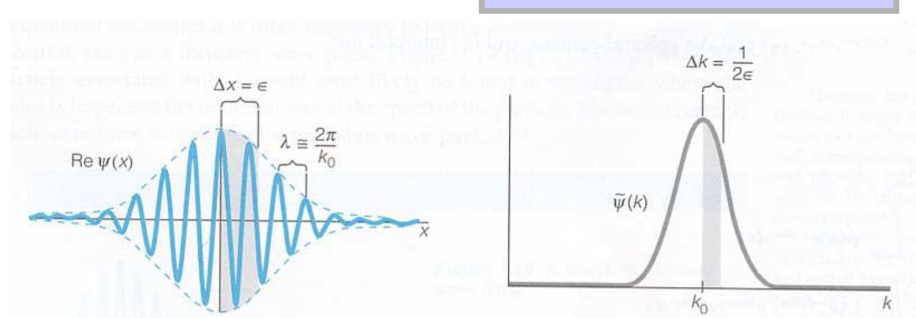
$$\tilde{\psi}(k) = \frac{A\varepsilon}{\sqrt{\pi}} e^{-\varepsilon^2 (k - k_0)^2}$$

Not a complex function

"Spectral Content" is* a Gaussian function *!

$$\psi(x) = Ae^{-(x/2\varepsilon)^2} e^{ik_0 x}$$

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



$$\psi(x) = Ae^{-(x/2\varepsilon)^2} e^{ik_0 x}$$

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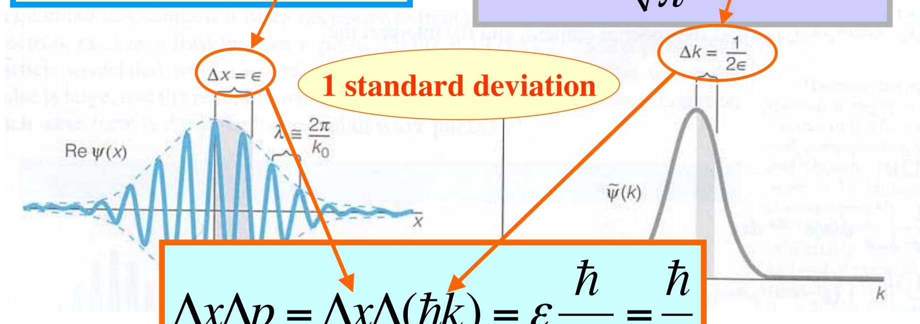
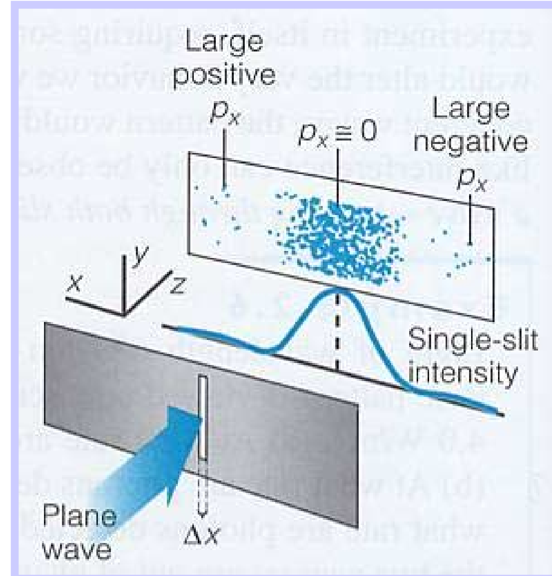


$$\Delta x \Delta p = \Delta x \Delta(\hbar k) = \varepsilon \frac{\hbar}{2\varepsilon} = \frac{\hbar}{2}$$

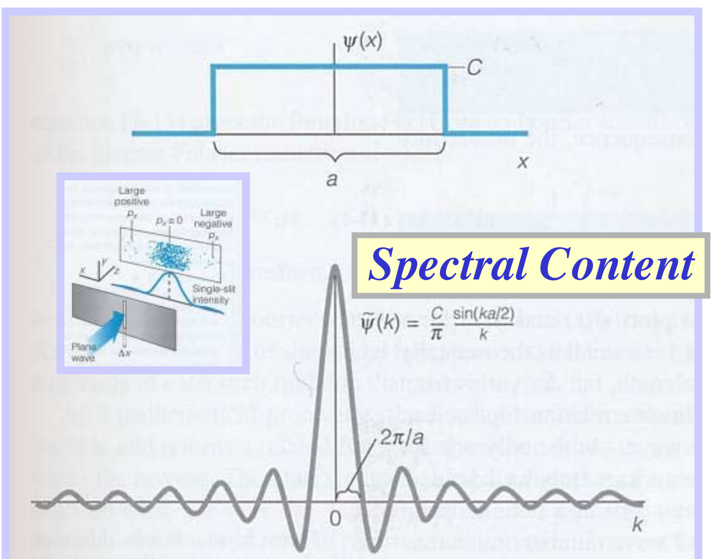
Gaussian Wave Packet

Minimal Uncertainty

A Single-Slit



A Single-Slit



Chapter. 5
Bound States: Simple Case

Purpose:

- **To make QM useful in real application,**
- **we must have a way to account for the effects of external forces****

Let's start with the Schrödinger eq. to include these effects.

**** interaction of object with its surrounding**

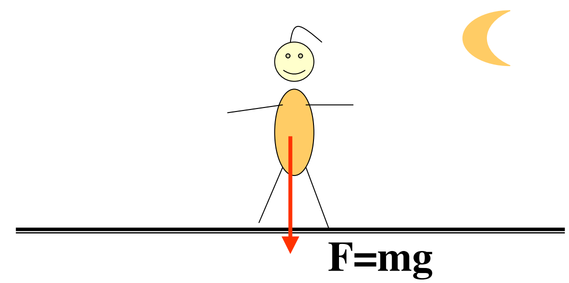
Chapter. 5
Bound States: Simple Case

Outline:

- The Schrödinger Equation (for interacting particles)
- Stationary States
- Physics Conditions: Well-Behaved Functions
- A Review of Classical Bound States
- Case 1: Particles in a Box – The Infinite Well
- Case 2: The Finite Well
- Case 3: The Simple Harmonic Oscillator
- Expectation Values, Uncertainties, and Operators

The Schrodinger Equation for Interacting Particles

A Particle Interacting With What?



The Schrodinger Equation for Interacting Particles

A Particle Interacting With What?

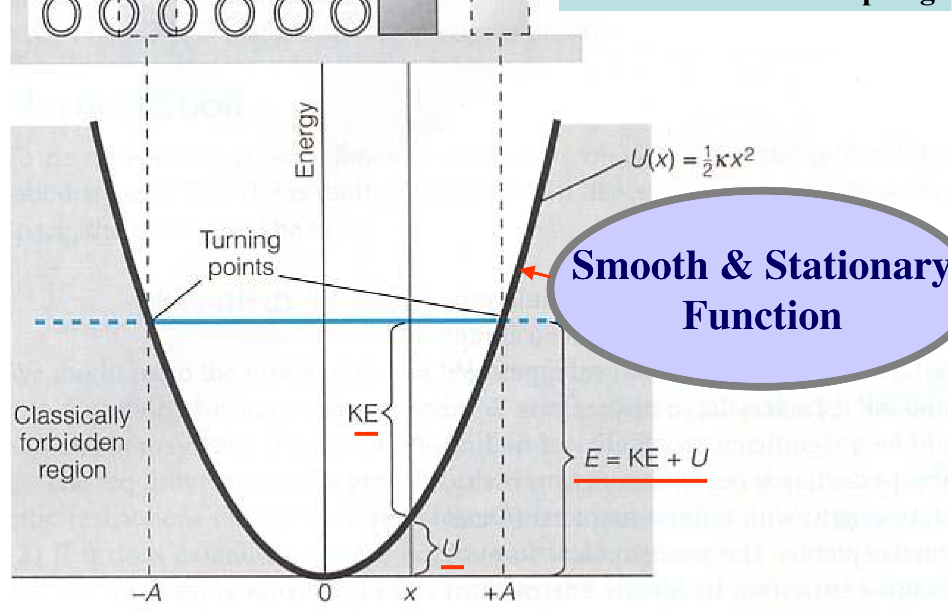
Simplification:

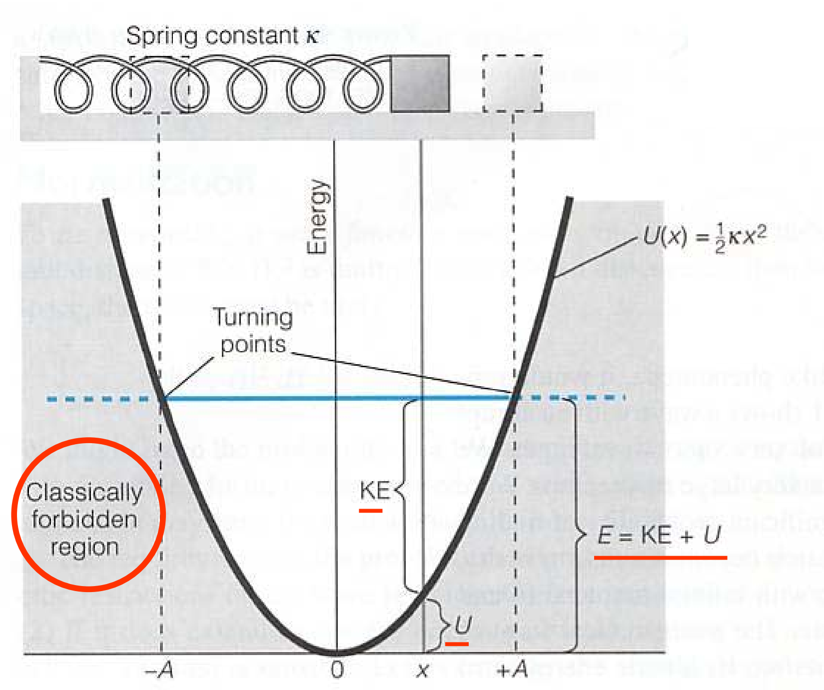
The Concept of Potential

(replaces all individual particle-particle interactions with a single smooth potential)

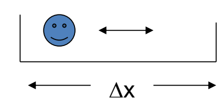
Why? – see next page

Energy vs. Position for a mass connected to a spring





Bound Systems

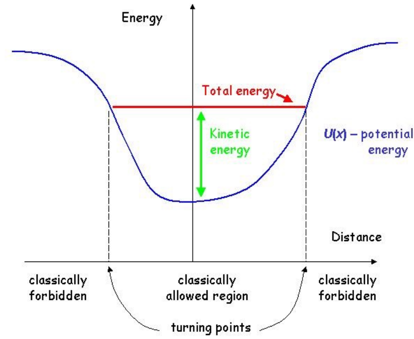


A bound system: any system of interacting particles where the nature of the interactions between the particles keeps their relative separation limited. Classical example: the solar system.

In general, the problem is very difficult.

Simplification: motion of a single particle that moves in a fixed potential energy field $U(x)$. The mass of the particle is small compared to the total mass of the system (e.g. heavy nucleus - light electron).

Classical bound system: $E(x)=K(x)+U(x)$



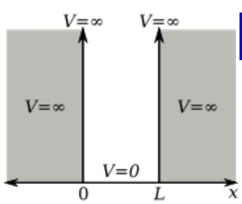
$E(x)=U(x)$

Classically allowed region:

$E(x)>U(x) \qquad K(x)>0$

Classically forbidden region:

$E(x)<U(x)$



The Infinite Square Well

a particle in the potential is completely free, except at the two ends where an infinite force prevents it from escaping

Outside the well: $\psi(x)=0$ - the probability of finding the particle =0

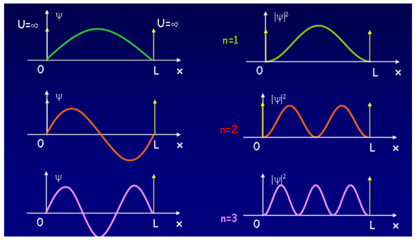
Inside the well: $-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}=E\psi(x)$

$\frac{d^2\psi(x)}{dx^2}=-k^2\psi(x) \qquad k\equiv\frac{\sqrt{2mE}}{\hbar}$ - the harmonic oscillator equation

General solution: $\psi(x)=A\sin kx+B\cos kx$ - constants *A* and *B* are fixed by boundary conditions

Continuity of the wave function: $\psi(0)=\psi(L)=0 \qquad \psi(0)=A\sin k0+B\cos k0=B=0$

Thus, $\psi(x)=A\sin kx \qquad \psi(L)=A\sin kL=0 \qquad kL=0,\pm\pi,\pm 2\pi,\ldots$



$$k_n=\frac{n\pi}{L},\ n=1,2,\ldots$$

n – ***quantum number*** (1D motion is characterized by a single q.n., for 2D motion we need two quantum numbers, etc.)

See later for details