Chapter 41 Wave Mechanics

Partly success: Bohr's theory was successful in explaining the spectrum of hydrogen. However, it could not predict the relative intensities of spectral lines or explain why, with increased resolution, some lines were found to consist of two or more finer lines.

More findings: Sommerfeld refined Bohr's theory by incorporating special relativity and the possibility of elliptical orbits. With the addition of two new quantum numbers, the Bohr-Sommerfeld theory accounted for many features of spectra and showed how the periodic table is built up in a systematic way.

Proper foundation: The rules that were used had no proper foundation and had limited explanatory power. Radical reform was needed in quantum theory.

41.1 De Broglie Waves

De Broglie put forward an astounding proposition that "**nature is symmetrical**".

Einstein had shown that a complete description of cavity radiation requires both the particle and wave aspects of cavity radiation.

De Broglie guessed that a similar wave-particle duality might apply to material particles. That is, *matter may also display wave nature*.

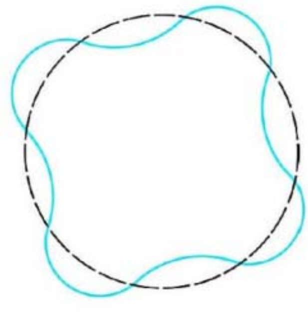
He used a combination of quantum theory and special relativity to propose that the wavelength, λ, associated with a particle is related to its linear momentum, $p=mv$, by

$$\lambda = \frac{h}{p}$$

41.1 De Broglie Waves (II)

The physical significance of the "matter wave" was not clear, but he gained courage from the following demonstration. In the Bohr's model, **the angular momentum of the electron is quantized**:

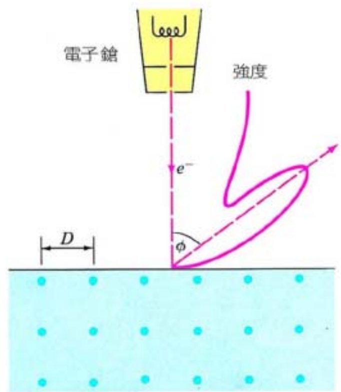
$$mvr = \frac{nh}{2\pi} \Rightarrow 2\pi r = n\lambda$$



This looks like the condition for a standing wave!

Stationary orbits: Only those orbits that can fit an integral number of wavelengths around the circumference are allowed.

41.2 Electron Diffraction



Davisson studied the scattering of electrons off nickel surface, reported the curious result that the reflected intensity depends on the orientation of the sample. Why? Matter wave.

Electrons were produced by a heated filament, accelerated by a potential difference, V, and then directed at the Ni target.

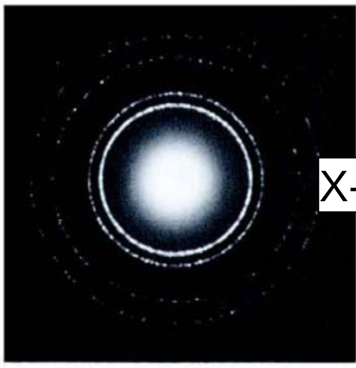
X-ray diffraction like: If the electrons had interacted with the atoms on a one-to-one basis, this would have produced random scattering. The pronounced reflections implied that the electrons were interacting with an array of atoms.

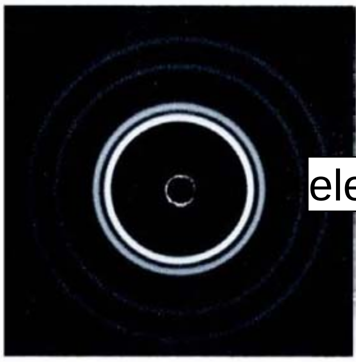
41.2 Electron Diffraction (II)

When a particle of mass *m* and charge *q* is accelerated from rest by a potential difference *V*, its kinetic energy is given by $K=p^2/2m=qV$. The de Broglie wavelength takes the form

$$p = \sqrt{2mgV}$$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mgV}}$$





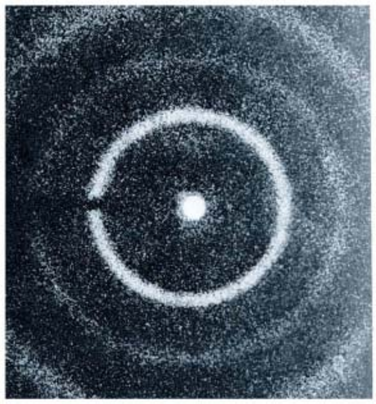
41.2 Electron Diffraction (III)

By an analysis similar to that for X-ray, it is found that the angular positions of the diffraction maxima are given by

$$D \sin\phi = n\lambda$$

Where D is the spacing between atoms, which in the case of nickel is 0.215 nm.

Wavelike behavior is exhibited by all elementary particles.



A diffraction pattern produced by 0.07-eV neutrons passing through a polycrystal-line sample of iron.

Example 41.1

What is the de Broglie wavelength of (a) an electron accelerated from rest by a potential difference of 54 V, and (b) a 10 g bullet moving at 400 m/s?

Solution:

$$\text{(a) } \lambda = \frac{h}{p} = \frac{h}{\sqrt{2meV}} = \frac{6.626\times10^{-34}}{\sqrt{(2\times9.11\times10^{-31}\times1.6\times10^{-19}\times54}} = 0.167\ \text{nm}$$

$$\text{(b) } \lambda = \frac{h}{p} = \frac{6.626\times10^{-34}}{0.01\times400} = 1.66\times10^{-34}\ \text{m}$$

There is no chance of observing wave phenomena, such as diffraction, with macroscopic objects.

41.3 Schrodinger's Equation

When Schrodinger realized that Einstein took the matter wave seriously, he decided to look for an equation to describe these matter waves.

The derivation of Schrodinger's equation is not straight forward. A simplified discussion can be based on the wave equation.

wave equation $\quad \dfrac{\partial^2 y}{\partial x^2} - \dfrac{1}{v^2}\dfrac{\partial^2 y}{\partial t^2} = 0$

general solution $\quad y(x,t) = \psi(x)\sin\omega t$

time-independent $\quad \dfrac{\partial^2 \psi}{\partial x^2} + \dfrac{\omega^2}{v^2}\psi = 0$

matter wave $\quad \dfrac{\omega^2}{v^2} = \dfrac{p^2}{\hbar^2} = \dfrac{2m(E-U)}{\hbar^2}$

Schrodinger's Eq. $\quad \dfrac{\partial^2 \psi}{\partial x^2} + \dfrac{2m(E-U)}{\hbar^2}\psi = 0$

41.3 Schrodinger's Equation (II)

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m(E-U)}{\hbar^2}\psi = 0$$

This is the one-dimension **time-independent Schrodinger wave equation**. The wave function ψ(x) represents stationary states of an atomic system for which E is constant in time.

How can a *continuous* description lead to *discrete* quantities, such as the energy level of the hydrogen atom?

The boundary condition.

41.4 The Wave Function

Schroding's success in tackling several problems confirmed that the wave mechanics was an important advance. But how was the "wave associated with the particle" to be interpreted.

De Broglie suggested that the wave might represent the particle itself. Schrodinger believed that a particle is really a group of waves, **a wave packet**.

Einstein though the intensity of a light wave at a given point is a measure of the number of photons that arrive at the point. In other word, the wave function for the electromagnetic field determines the probability of finding a photon.

By analogy, Born suggested that the square of the wave function tells us the probability per unit volume of finding the particle. Born's interpretation of the wave function has now been generally accepted.

41.4 The Wave Function (II)

The square of the wave function tells us the probability per unit volume of finding the particle.

$$\psi^2 dV = \text{probability of finding a particle with a volume dV}$$

The quantity ψ2 is called the probability density.

Normalization: Since the particle has to be found somewhere, the sum of all the probabilities along the x axis has to be one:

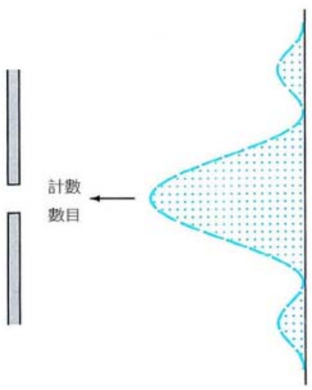
$$\int_{-\infty}^{\infty} \psi^2(x)dx = 1$$

A wave function that satisfies this condition is said to be normalized.

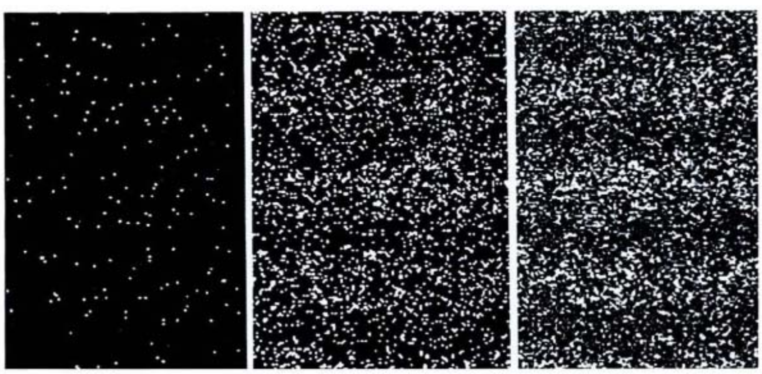
41.4 The Wave Function (III)

The classical physics and special relativity are based on the principle of determinism.

Quantum mechanics correctly predicts average value of physical quantities, not the result of individual measurements.



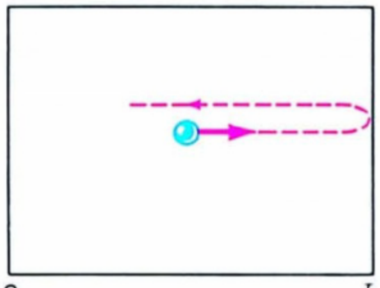
diffraction



interference

41.5 Application of Wave Mechanics: Particle is a box

Consider a particle of mass *m* that bounces back and forth in a one-dimensional box of side *L*. The potential *U* is zero within the box and infinite at the wall.



wave equation $$\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0, \text{ where } k = \sqrt{2mE}/\hbar$$

solutions $$\psi(x) = A\sin(kx + \phi)$$

boundary condition $$\psi(x) = A\sin(\frac{n\pi x}{L}), \ n = 1, \ 2, \ 3, ...$$

41.5 Application of Wave Mechanics: Particle is a box (II)

The wave length has to satisfy standing wave condition

$$k = 2\pi / \lambda = n\pi / L, \quad \lambda = 2L / n$$

From de Broglie's equation, we can derive the momentum and find out the velocity.

$$p = mv = \frac{h}{\lambda} = \frac{nh}{2L} \Rightarrow v = \frac{nh}{2mL}$$

The particle's energy, which is purely kinetic, $K=1/2mv^2$, is thus also quantized.

$$E_n = \frac{n^2 h^2}{8mL^2} \qquad n = 1, 2, 3, ..$$

41.5 Application of Wave Mechanics: Particle is a box (III)

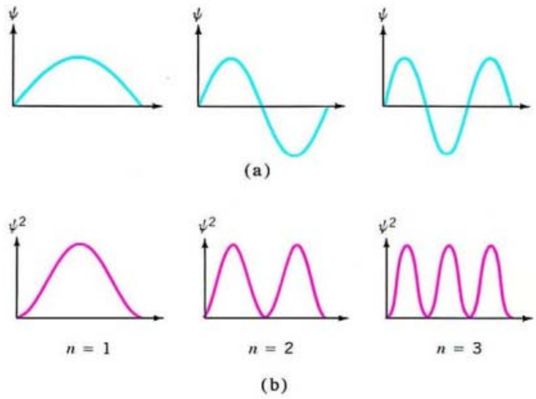
The quantized energy level:

$$E_n = \frac{n^2 h^2}{8mL^2} \qquad n = 1, 2, 3,..$$

The first three wave functions and probability densities

$$\psi(x) = A\sin(\frac{n\pi x}{L}), \; n = 1, \; 2, \; 3,...$$

$$\psi^2(x) = A^2 \sin^2(\frac{n\pi x}{L}), \; n = 1, \; 2, \; 3,...$$



Example 41.2

An electron is trapped within an infinite potential well of length 0.1 nm. What are the first three energy levels?

Solution:

$$E_n = \frac{n^2 h^2}{8mL^2} \qquad n = 1, 2, 3,.. \qquad L = 0.1\,\text{nm} = 1\times 10^{-10}\,\text{m}$$

$$E_n = \frac{n^2 (6.626\times 10^{-34})^2}{8(9.1\times 10^{-31})\times 10^{-20}} = n^2 (6.03\times 10^{-18})\text{J} = 37.7n^2 \text{ eV}$$

$$E_1 = 37.7\,\text{eV}, \; E_2 = 151\,\text{eV}, \; E_3 = 339\,\text{eV}$$

Example 41.3

Consider a 10^{-7} kg dust particle confined to a 1-cm box. (a) What is the minimum speed possible? (b) What is the quantum number n if the particle's speed is 10^{-3} mm/s?

Solution:

$$\text{(a) } E_n = \frac{n^2 h^2}{8mL^2} \qquad n = 1, 2, 3,.. \qquad L = 1\,\text{cm} = 1\times 10^{-2}\,\text{m}$$

$$E_n = \frac{n^2 (6.626\times 10^{-34})^2}{8(1\times 10^{-7})\times 10^{-4}} = \frac{1}{2}mv^2 \Rightarrow v_1 = 3.32\times 10^{-25}\ \text{m/s}$$

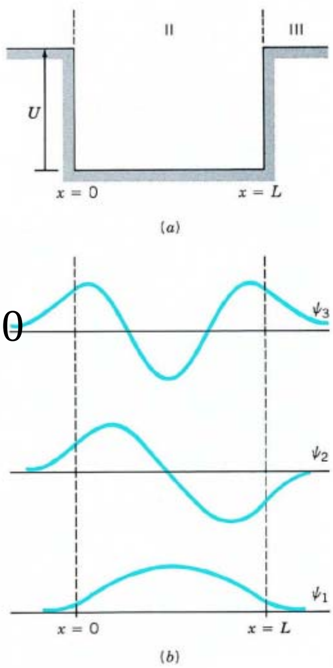
$$\text{(b) If } v_n = 0.001\,\text{mm/s}, n = ?$$

$$n = \frac{2\times(1\times 10^{-7})\times 10^{-6}}{(6.626\times 10^{-34})} \approx 10^{23}$$

The corresponding principle resolves the zero-energy and uniform probability problems.

41.5 Application of Wave Mechanics: Finite potential well

Consider a particle of mass *m* that bounces back and forth in a one dimensional box of side *L*. The potential *U* is zero within the box and infinite at the wall.



$$\text{wave equation } \frac{\partial^2\psi}{\partial x^2} + k^2\psi = 0, \text{or } \frac{\partial^2\psi}{\partial x^2} + K^2\psi = 0$$

$$\text{where } k = \sqrt{2mE}/\hbar \text{ or } K = \sqrt{2m(U-E)}/\hbar$$

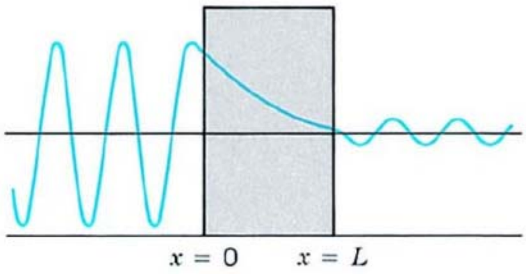
$$\psi(x)\begin{cases} = A\exp(Kx) & x \le 0 \\ = B\exp(ikx) + C\exp(-ikx) & 0 \le x \le L \\ = D\exp(-Kx) & L \le x \end{cases}$$

What is the boundary conditions?

41.5 Application of Wave Mechanics: Barrier Penetration: Tunneling

When a particle with energy *E* encounters a potential energy barrier of height *U (>E),* what would happens?

Partly reflected and partly transmitted (tunneling).



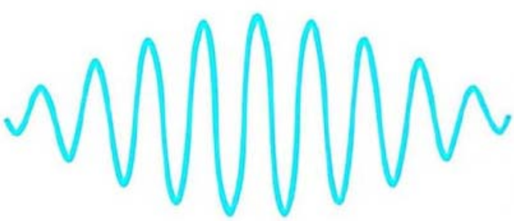
Examples: Tunnel diode, Josepheson junction, and scanning tunneling electron microscope.

Can we reproduce such effect in classical electromagnetism?

41.6 Heisenberg Uncertainty Principle

The wavelength of a wave can be specified precisely only if the wave extends over many cycles. But if a matter wave is spread out in space, the position of the particle is poorly defined. Thus to reduce the uncertainty in position of the particle, Δx, one can propose many wave length to form a reasonably well-localized ***wave-packet***.

(*a*)



(*b*)

41.6 Heisenberg Uncertainty Principle (II)

From the de Broglie matter wave relation, we see that a spread in wavelengths, $\Delta\lambda$, means that the wave packet involves a spread in momentum, Δp. According to the Heisenberg uncertainty principle, the uncertainties in position and in momentum are related by

$$\Delta x \Delta p \geq h$$

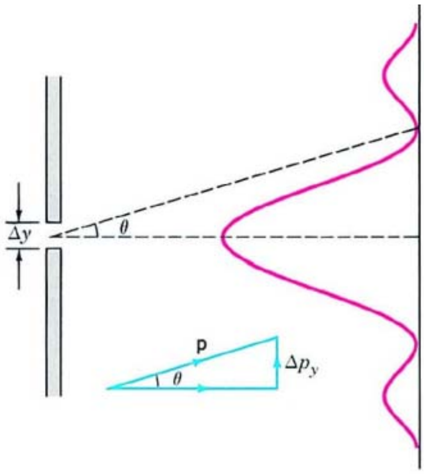
It is not possible to measure both the position of a particle and its linear momentum simultaneously to arbitrary precision.

For a wave packet, the uncertainty relation is an intrinsic property, independent of the measuring apparatus.

41.6 Heisenberg Uncertainty Principle (III) Another derivation

Consider the electron diffraction by a single slit.

We know that the position of the first minimum is given by



$$\begin{cases} \sin\theta = \dfrac{\lambda}{a} = \dfrac{\lambda}{\Delta y} \Rightarrow \Delta y = \dfrac{\lambda}{\sin\theta} \\ \Delta p_y = p \sin\theta \end{cases}$$

$$\Rightarrow \Delta y \Delta p_y \approx h$$

A finer slit would locate the particle more precisely but lead to a wider diffraction pattern---that is, to a greater uncertainty in the transverse momentum.

41.6 Heisenberg Uncertainty Principle (IV) other pair

The Heisenberg uncertainty principle also applies to other pairs of variables.

$$\Delta x \Delta p_x \geq h, \qquad \Delta y \Delta p_y \geq h, \qquad \Delta z \Delta p_z \geq h$$

Among the most important are energy and time:

$$\Delta E \Delta t \geq h$$

To minimize the uncertainty in measuring the energy of a system, one must observe it for as long as possible.

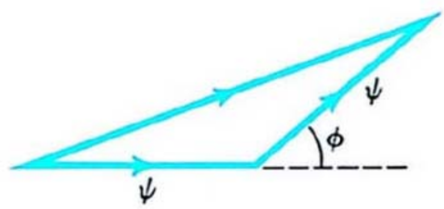
The energy of a system can fluctuate from the value set by the conservation of energy---provided the fluctuation occurs within the time interval specified by above Eq.

41.7 Wave-Particle Duality

Let's reconsider Young's double-slit experiment, but now conducted with electrons.

Let us say that ψ1 is the wave function that applies to the passage of an electron through slit S1 whereas ψ2 applies to slit S2. When both slits are open, the distribution will display the familiar interference fringes.

$$\psi^2 = |\boldsymbol{\psi}_1 + \boldsymbol{\psi}_2|^2 = \psi_1^2 + \psi_2^2 + 2\psi_1\psi_2 \cos\phi$$



41.7 Wave-Particle Duality (II)

Bohr noted that any given experiment reveals either the wave aspect or the particle aspect.

Complementarily principle: A complete description of matter and radiation requires both particle and wave aspects.

Exercises and Problems

Ch.41:

Ex. 13, 19, 27, 28

Prob. 1, 4, 5, 9, 11