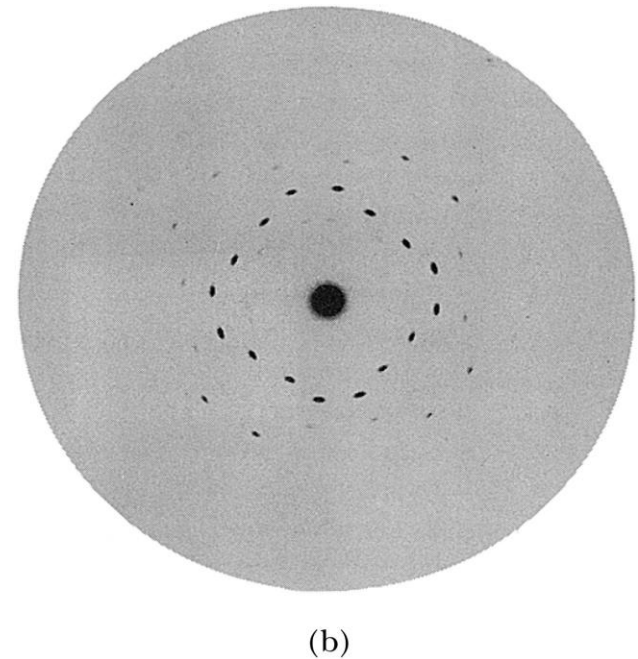
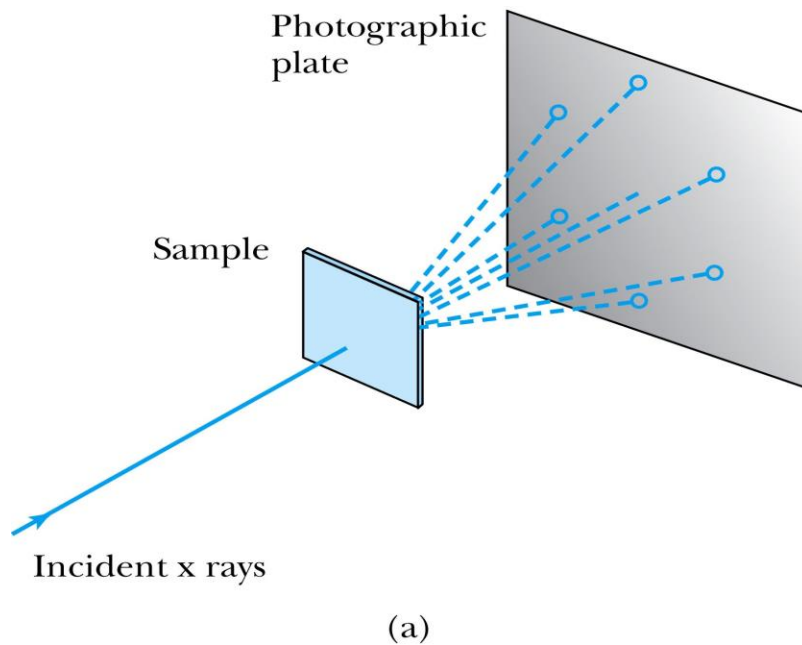

CHAPTER 5

Wave Properties of Matter and Quantum Mechanics

- 5.1 X-Ray Scattering
 - 5.2 De Broglie Waves
 - 5.3 Electron Scattering
 - 5.4 Wave Motion
 - 5.5 Waves or Particles?
 - 5.6 Uncertainty Principle
 - 5.7 Probability, Wave Functions, and the Copenhagen Interpretation
 - 5.8 Particle in a Box
-

5.1: X-Ray Scattering

- Max von Laue suggested that if x rays were a form of electromagnetic radiation, interference effects should be observed.
- Crystals act as three-dimensional gratings, scattering the waves and producing observable interference effects.

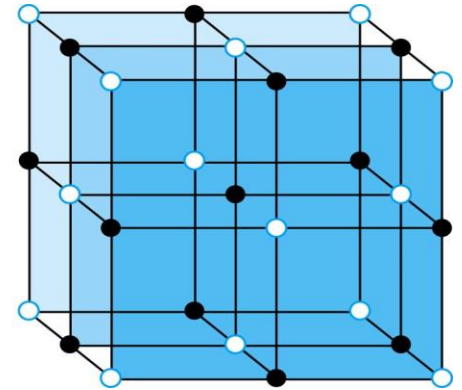
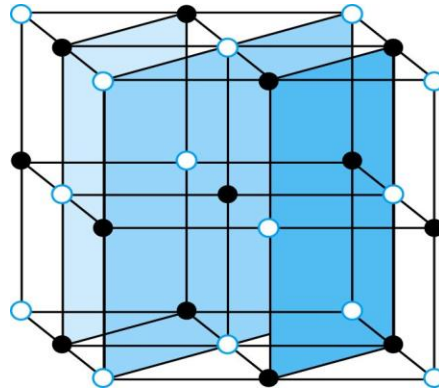


Lattice spacing d is about 0.1 nm

Bragg's Law

- William Lawrence Bragg interpreted the x-ray scattering as the reflection of the incident x-ray beam from a unique set of planes of atoms within the crystal.
- There are two conditions for constructive interference of the scattered x rays:

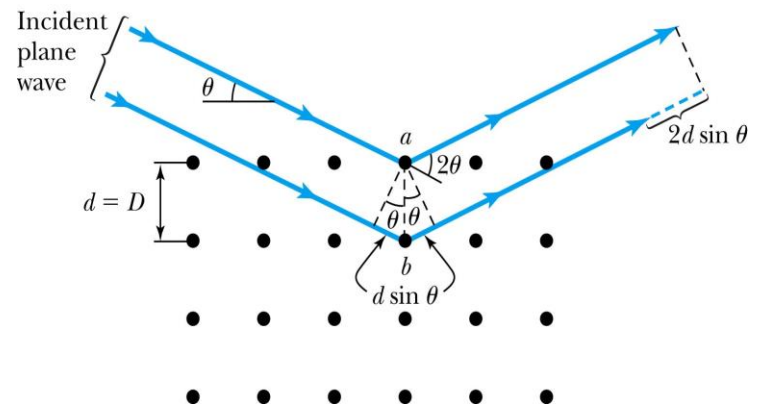
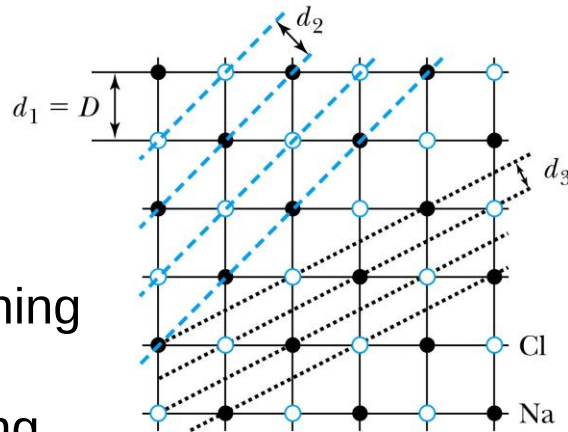
- 1) The angle of incidence must equal the angle of reflection of the outgoing wave.
- 2) The difference in path lengths must be an integral number of wavelengths.



- **Bragg's Law**
$$n\lambda = 2d \sin \theta$$

($n = \text{integer}$)

Used for determining wavelength or interplanar spacing





EXAMPLE 5.1

X rays scattered from rock salt (NaCl) are observed to have an intense maximum at an angle of 20° from the incident direction. Assuming $n = 1$ (from the intensity), what must be the wavelength of the incident radiation?

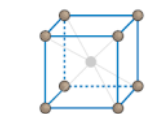
Strategy We will use Equation (5.1) to find λ , but we need to know d , the lattice spacing, and the angle θ . Notice that the angle between the incident beam and scattered wave for constructive interference is always 2θ (see Figures 5.4 and 5.5), and because $2\theta = 20^\circ$, we have $\theta = 10^\circ$. We can use the density of NaCl to help find d , because the volume taken up by one atom is d^3 .

Solution In Section 4.1 we showed that

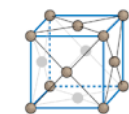
$$\frac{\text{Number of molecules}}{\text{Volume}} = \frac{N_A \rho}{M}$$

where N_A is Avogadro's number, ρ is the density, and M is the gram-molecular weight. For NaCl, $\rho = 2.16 \text{ g/cm}^3$ and $M = 58.5 \text{ g/mol}$.

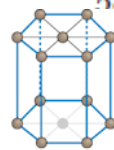
$$\frac{N_A \rho}{M} = \frac{\left(6.02 \times 10^{23} \frac{\text{molecules}}{\text{mol}}\right) \left(2.16 \frac{\text{g}}{\text{cm}^3}\right)}{58.5 \frac{\text{g}}{\text{mol}}}$$



Cubic body centered (bcc)
Fe, V, Nb, Cr



Cubic face centered (fcc)
Al, Ni, Ag, Cu, Au



Hexagonal
Ti, Zn, Mg, Cd

$$\begin{aligned} \frac{N_A \rho}{M} &= 2.22 \times 10^{22} \frac{\text{molecules}}{\text{cm}^3} \\ &= 4.45 \times 10^{22} \frac{\text{atoms}}{\text{cm}^3} \\ &= 4.45 \times 10^{28} \frac{\text{atoms}}{\text{m}^3} \end{aligned}$$

Because NaCl has a cubic array, we take d as the distance between Na and Cl atoms, so we have a volume of d^3 per atom.

$$\frac{1}{d^3} = 4.45 \times 10^{28} \frac{\text{atoms}}{\text{m}^3}$$

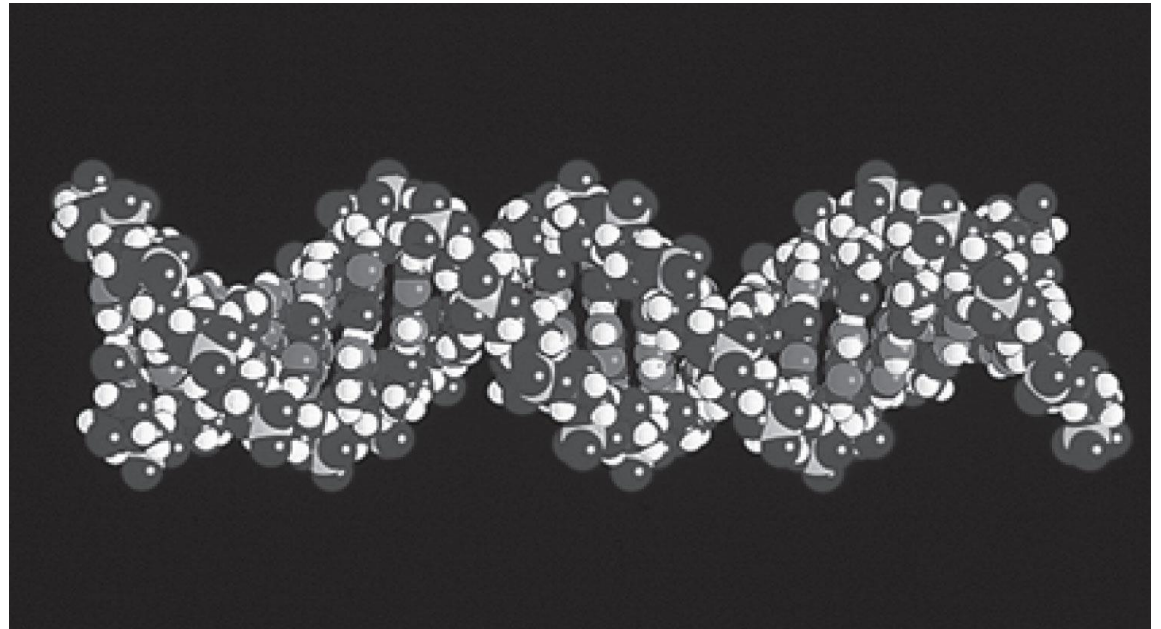
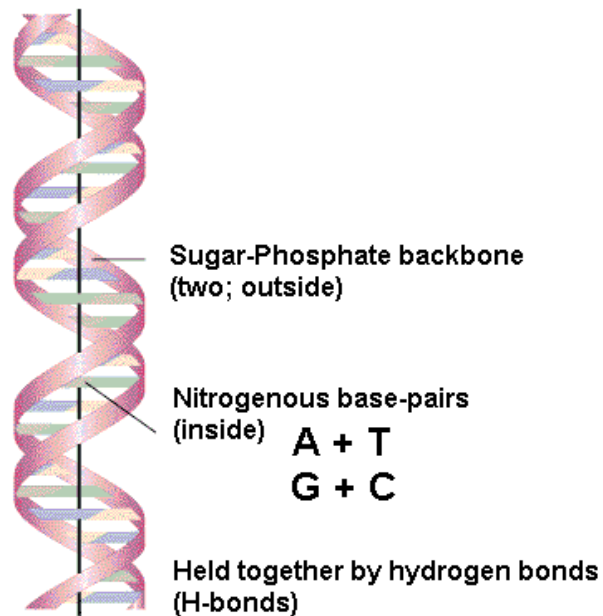
$$d = 2.82 \times 10^{-10} \text{ m} = 0.282 \text{ nm}$$

This technique of calculating the lattice spacing works for only a few cases because of the variety of crystal structures, many of which are noncubic.

We use Equation (5.1) to find λ .

$$\lambda = \frac{2d \sin \theta}{n} = \frac{(2)(0.282 \text{ nm})(\sin 10^\circ)}{1} = 0.098 \text{ nm}$$

which is a typical x-ray wavelength. NaCl is a useful crystal for determining x-ray wavelengths and for calibrating experimental apparatus.

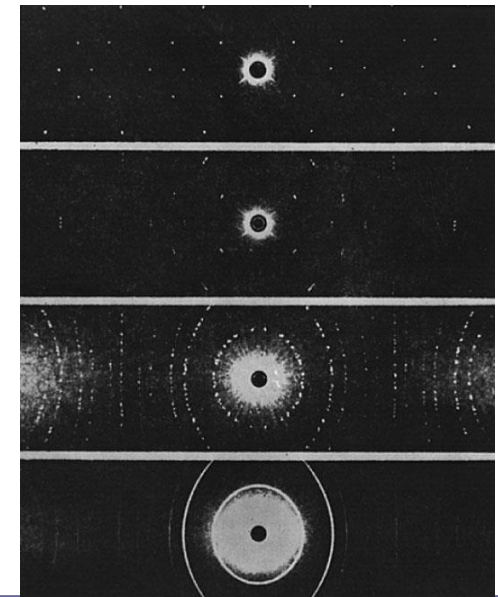
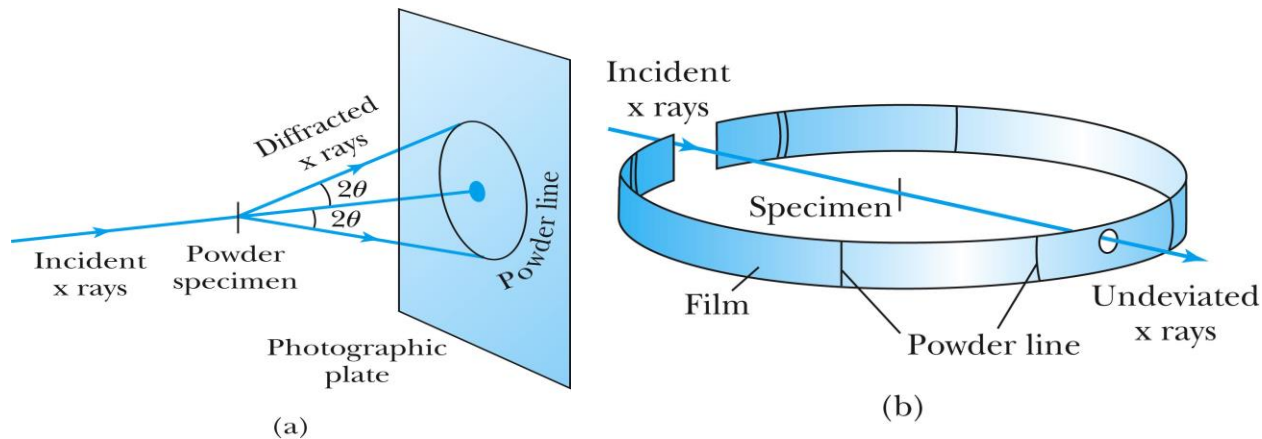
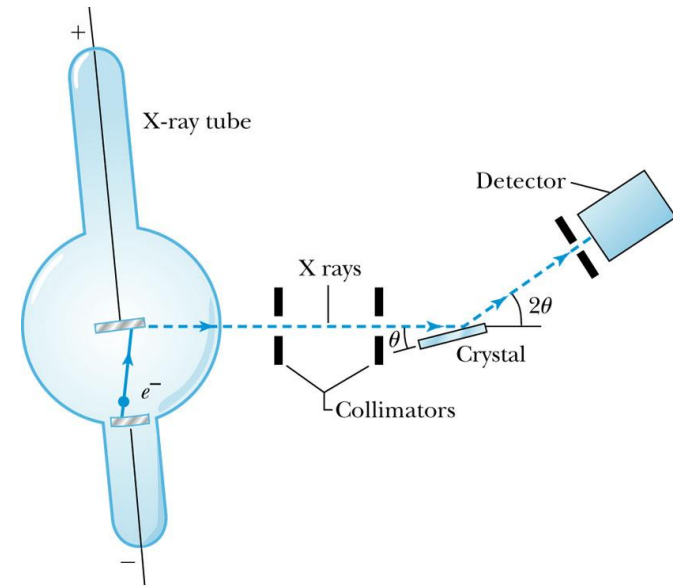


(a)

structure of DNA-double-helix by x-ray diffraction (Watson and Crick)

The Bragg Spectrometer

- A Bragg spectrometer scatters x rays from several crystals. The intensity of the diffracted beam is determined as a function of scattering angle by rotating the crystal and the detector.
- When a beam of x rays passes through the powdered crystal, the dots become a series of rings.

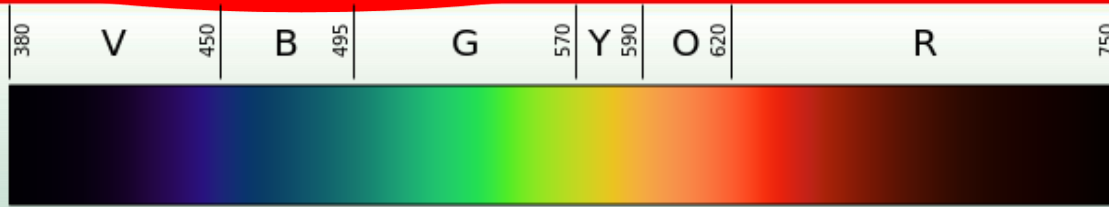


(c)

Quiz question

- Which of the following is true about Bragg planes?
 - a. There is only one Bragg plane for any given crystal structure.
 - b. They are especially useful for detecting transitions between energy levels in the crystals' atoms.
 - c. They are used to scatter alpha particles in gold and other materials.
 - d. They are evenly spaced planes within crystal structures of atoms.
 - e. All of the above.
-

Clicker - Questions



11) The color of visible light are listed in increasing order of frequency.

- a) violet, blue, yellow, green, orange, red
- b) red, yellow, orange, violet, blue, green
- c) blue, violet, green, yellow, red
- d) red, orange, yellow, green, blue, violet

5.2: De Broglie Waves = matter waves

- Prince Louis V. de Broglie suggested that mass particles should have wave properties similar to electromagnetic radiation.
- Thus the wavelength of a matter wave is called the de Broglie wavelength:

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

- Since for a photon, $E = pc$ and $E = hf$, the energy can be written as

$$hf = pc = p\lambda f$$



EXAMPLE 5.2

Calculate the de Broglie wavelength of (a) a tennis ball of mass 57 g traveling 25 m/s (about 56 mph) and (b) an electron with kinetic energy 50 eV.

Strategy The calculation for both of these wavelengths is a straightforward application of Equation (5.2).

Solution (a) For the tennis ball, $m = 0.057$ kg, so

$$\lambda = \frac{h}{p} = \frac{6.63 \times 10^{-34} \text{ J} \cdot \text{s}}{(0.057 \text{ kg})(25 \text{ m/s})} = 4.7 \times 10^{-34} \text{ m}$$

(b) For the electron, it is more convenient to use eV units, so we rewrite the wavelength λ as

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mK}} = \frac{hc}{\sqrt{2(mc^2)K}}$$

$$\lambda = \frac{1240 \text{ eV} \cdot \text{nm}}{\sqrt{(2)(0.511 \times 10^6 \text{ eV})(50 \text{ eV})}} = 0.17 \text{ nm}$$

Note that because the kinetic energy of the electron is so small, we have used a nonrelativistic calculation. Calculations in modern physics are normally done using eV units, both because it is easier and also because eV values are more appropriate for atoms and nuclei (MeV, GeV) than are joules. The values of hc and some masses can be found inside the front cover.

$$\begin{aligned} hc &= 4.1357 \times 10^{-15} \text{ eV} \cdot \text{s} \times 3 \times \frac{10^8 \text{ m}}{\text{s}} \\ &= 1240 \text{ eV} \cdot \text{nm} \end{aligned}$$

Clicker - Questions

14) Compute the De Broglie wavelength of

- i. A 2000 kg car traveling at 100m/sec.
- ii. A smoke particle of mass 10^{-6} g moving at 1cm/sec
- iii. An electron with kinetic energy of 1eV
- iv. A proton with kinetic energy of 1eV

- a) 3.3×10^{-41} m, 6.6×10^{-25} m, 1.2nm, 0.3nm
- b) 3.3×10^{-25} m, 6.6×10^{-24} m, 1.2nm, 0.3nm
- c) 3.3×10^{-39} m, 6.6×10^{-23} m, 12Å, 0.028nm
- d) 5.5×10^{-25} m, 6.6×10^{-23} m, 1.2Å, 500Å
- e) None of the above

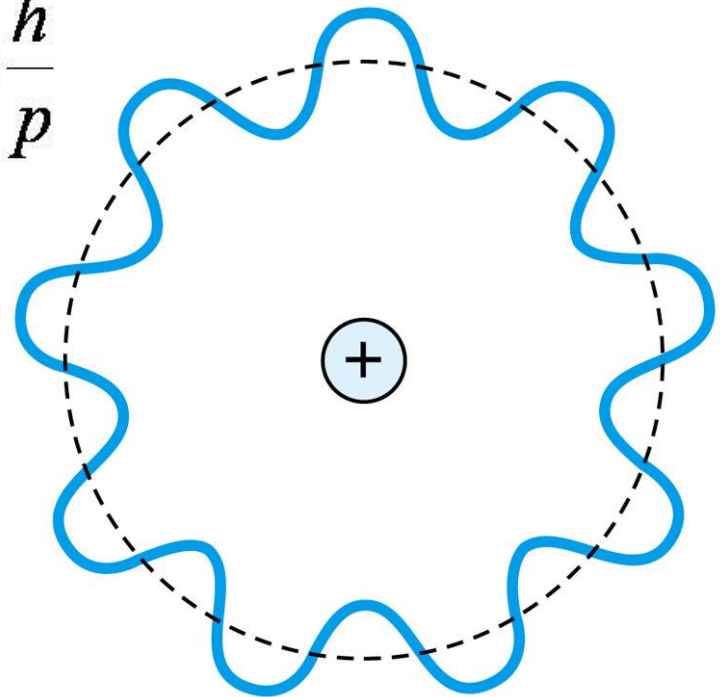
Bohr's Quantization Condition

- One of Bohr's assumptions concerning his hydrogen atom model was that the angular momentum of the electron-nucleus system in a stationary state is an integral multiple of $h/2\pi$.
- The electron is a standing wave in an orbit around the proton. This standing wave will have nodes and be an **integral** number of wavelengths.

$$2\pi r = n\lambda = n \frac{h}{p}$$

- The angular momentum becomes:

$$L = rp = \frac{nh}{2\pi} = n\hbar$$



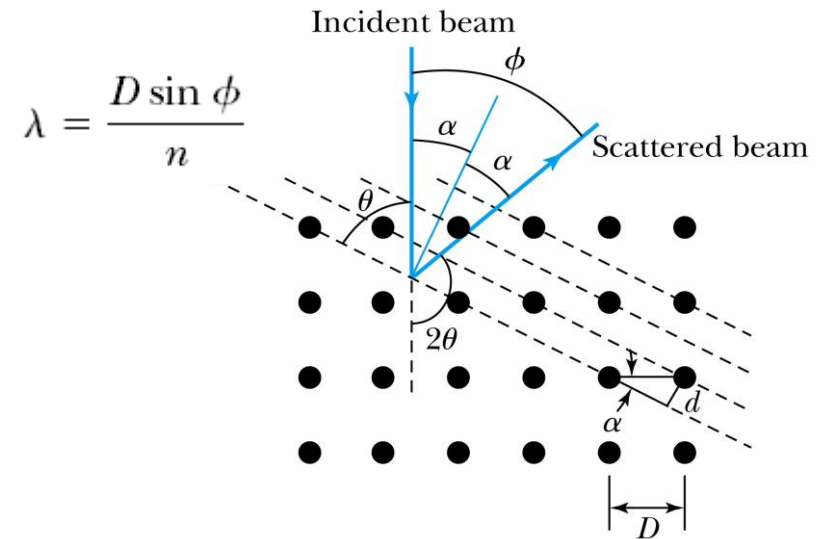
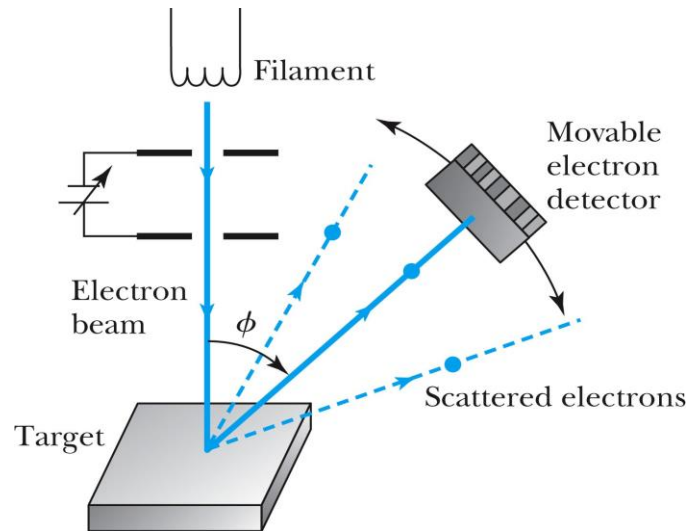
Apply the deBroglie wavelength of the electron in the Bohr atom as a standing wave

When de Broglie's matter waves are applied to electrons in the Bohr atom, which of the following occurs?

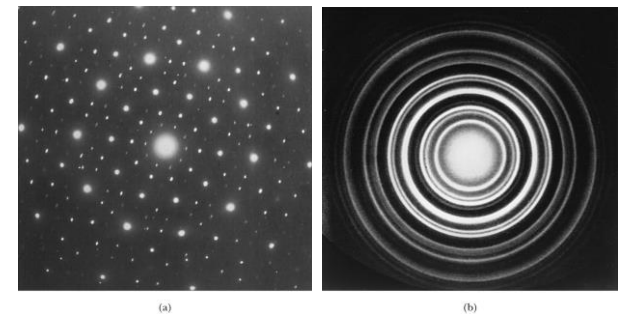
- a. The electron is found to have in its orbit an integral number of half-wavelengths.
 - b. Bohr's quantization assumption for electron orbits is modified to incorporate the wave properties of the electron.
 - c. de Broglie's results allow an integral number of wavelengths in the electron orbits.
 - d. The angular momentum of the electron in the atom is constant, with longer wavelengths at larger quantum numbers.
-

5.3: Electron Scattering

- Davisson and Germer experimentally observed that electrons were diffracted much like x rays in nickel crystals.



- George P. Thomson (1892–1975), son of J. J. Thomson, reported seeing the effects of electron diffraction in transmission experiments. The first target was celluloid, and soon after that gold, aluminum, and platinum were used. The randomly oriented polycrystalline sample of SnO_2 produces rings as shown in the figure at right.



The Spallation Neutron Source at Oakridge



EXAMPLE 5.4

In introductory physics, we learned that a particle (ideal gas) in thermal equilibrium with its surroundings has a kinetic energy of $3kT/2$. Calculate the de Broglie wavelength for (a) a neutron at room temperature (300 K) and (b) a “cold” neutron at 77 K (liquid nitrogen).

Strategy In both of these cases we will use Equation (5.2) to find the de Broglie wavelength. First, we will need to determine the momentum, and we note in both cases the energies of the particles will be so low that we can perform a nonrelativistic calculation. Neutrons have a rest energy of almost 1000 MeV, and their kinetic energies at these temperatures will be quite low (0.026 eV at 300 K).

Solution We begin by finding the de Broglie wavelength of the neutron in terms of the temperature.

$$\begin{aligned}\frac{p^2}{2m} &= \text{K.E.} = \frac{3}{2}kT \\ p &= \sqrt{3mkT}\end{aligned}\quad (5.8)$$

$$\begin{aligned}\lambda &= \frac{h}{p} = \frac{h}{\sqrt{3mkT}} = \frac{hc}{\sqrt{3(mc^2)kT}} \\ &= \frac{1}{T^{1/2}} \frac{1240 \text{ eV} \cdot \text{nm}}{\sqrt{3(938 \times 10^6 \text{ eV})(8.62 \times 10^{-5} \text{ eV/K})}}\end{aligned}$$

It again has been convenient to use eV units.

$$\begin{aligned}\lambda &= \frac{2.52}{T^{1/2}} \text{ nm} \cdot \text{K}^{1/2} \\ \lambda(300 \text{ K}) &= \frac{2.52 \text{ nm} \cdot \text{K}^{1/2}}{\sqrt{300 \text{ K}}} = 0.145 \text{ nm} \\ \lambda(77 \text{ K}) &= \frac{2.52 \text{ nm} \cdot \text{K}^{1/2}}{\sqrt{77 \text{ K}}} = 0.287 \text{ nm}\end{aligned}\quad (5.9)$$

These wavelengths are thus suitable for diffraction by crystals. “Supercold” neutrons, used to produce even larger wavelengths, are useful because extraneous electric and magnetic fields do not affect neutrons nearly as much as electrons.

5.4: Wave Motion

- De Broglie matter waves suggest a further description. The displacement of a wave is

$$\Psi(x, t) = A \sin \left[\frac{2\pi}{\lambda} (x - vt) \right]$$

- This is a solution to the wave equation

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 \Psi}{\partial t^2}$$

- Define the wave number k and the angular frequency ω as:

$$k \equiv \frac{2\pi}{\lambda} \quad \text{and} \quad \omega = \frac{2\pi}{T}$$

- The wave function is now: $\Psi(x, t) = A \sin (kx - \omega t)$
-

Wave Properties

- The phase velocity is the velocity of a point on the wave that has a given phase (for example, **the crest**) and is given by

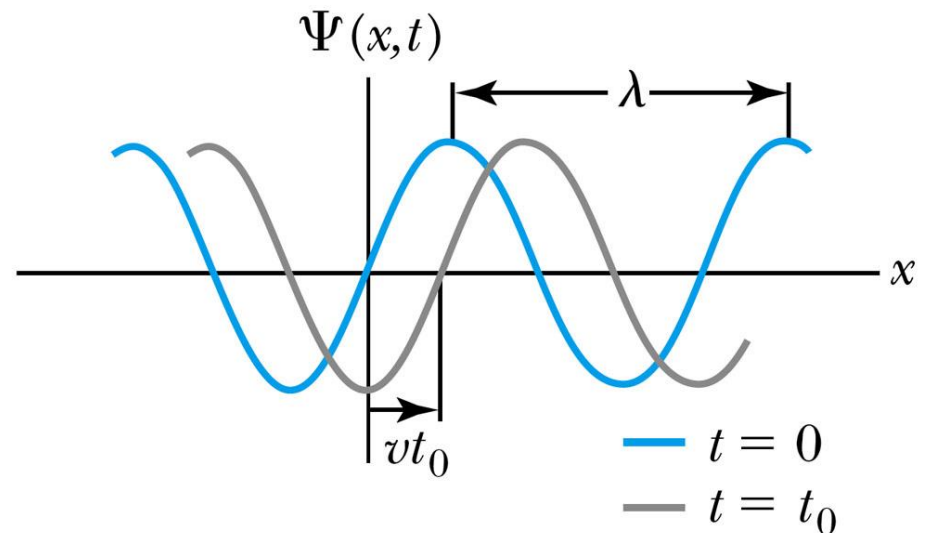
$$v_{\text{ph}} = \frac{\lambda}{T} = \frac{\omega}{k}$$

- A phase constant Φ shifts the wave:

$$\Psi(x, t) = A \sin(kx - \omega t + \phi).$$

$$\omega = \frac{2\pi}{T}$$

$$\Psi(x, t) = A \sin(kx - \omega t + \phi)$$



Wave motion

Quantum mechanics is linearly based on wave motion: wave particle duality.
Towards the wave equation:

Max (particle) velocity

$$y(x, t) = A \sin(\omega t - kx) \quad \text{wave function at fixed location 'x'}$$

$$v_y = \frac{\partial y}{\partial t} = \omega A \cos(\omega t - kx)$$

Max (particle) acceleration

$$a_y = \frac{\partial^2 y}{\partial t^2} = -\omega^2 A \sin(\omega t - kx) = -\omega^2 y(x, t) \quad \text{SHM } a_y = -\omega y$$

At fixed time **t**

$$\text{Slope: } \frac{dy}{dx} = -k A \cos(\omega t - kx)$$

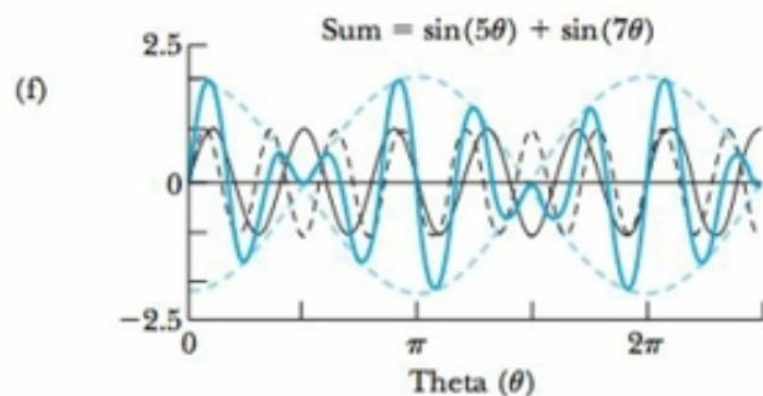
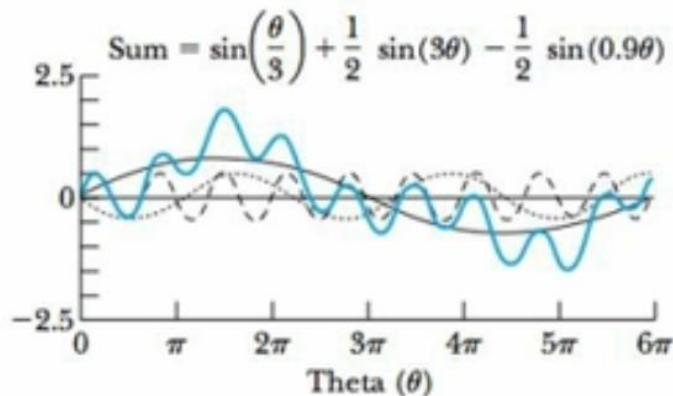
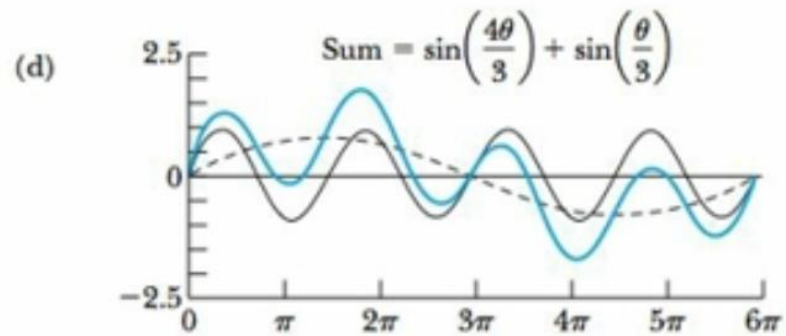
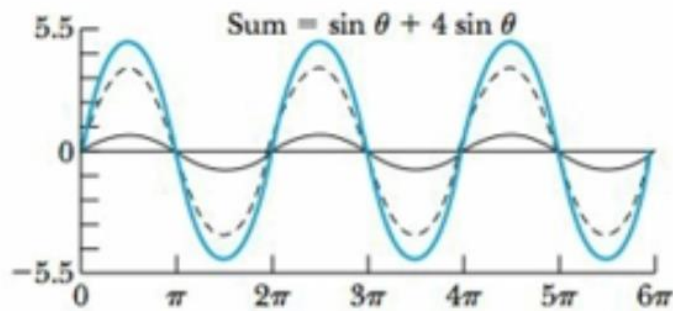
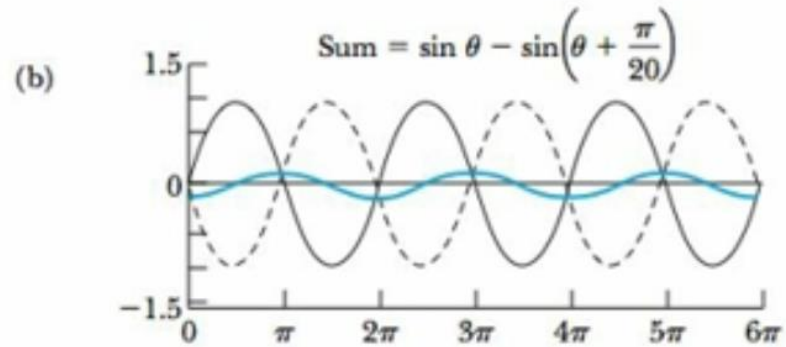
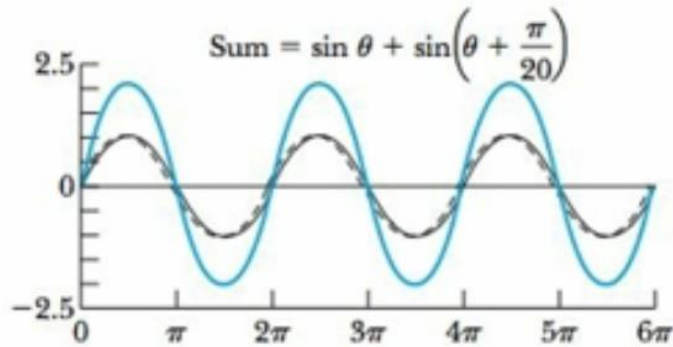
$$\frac{\partial^2 y(x, t)}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 y(x, t)}{\partial t^2}$$

$$\text{Curvature: } \frac{\partial^2 y}{\partial x^2} = -k^2 A \sin(\omega t - kx) = -k^2 y(x, t)$$

$$\text{Wave equation } \frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 y}{\partial t^2}$$

$$\frac{\frac{\partial^2 y}{\partial t^2}}{\frac{\partial^2 y}{\partial x^2}} = \frac{-\omega^2 y(x, t)}{-k^2 y(x, t)} = \frac{-\omega^2}{-k^2} = v^2$$

Superposition of waves with different frequencies, phases, and amplitudes



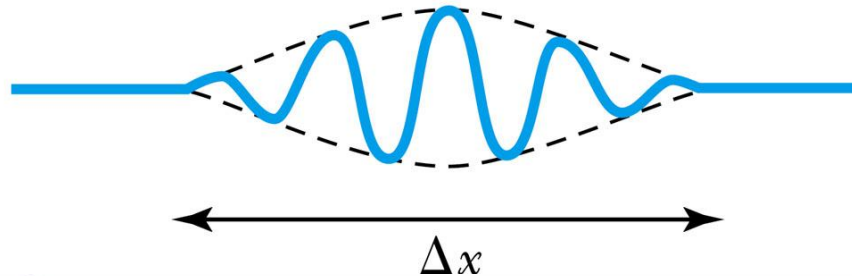
Principle of Superposition

- When two or more waves traverse the same region, they act independently of each other.
- Combining **two waves** yields:

$$Y(x, t) = Y_1(x, t) + Y_2(x, t) = 2A \cos\left(\frac{Dk}{2}x - \frac{D\omega}{2}t\right) \cos(k_{av}x - \omega_{av}t)$$

- The combined wave oscillates within an envelope that denotes the maximum displacement of the combined waves.
- When combining many waves with different amplitudes and frequencies, a pulse, or **wave packet**, is formed which moves at a **group velocity**:

$$u_{gr} = \frac{D\omega}{Dk}$$



$$\begin{aligned} \Psi(x, t) &= \Psi_1(x, t) + \Psi_2(x, t) \\ &= A \cos(k_1x - \omega_1t) + A \cos(k_2x - \omega_2t) \end{aligned} \quad (5.20)$$

$$= 2A \cos\left[\frac{1}{2}(k_1 - k_2)x - \frac{1}{2}(\omega_1 - \omega_2)t\right] \cos\left[\frac{1}{2}(k_1 + k_2)x - \frac{1}{2}(\omega_1 + \omega_2)t\right]$$

$$= 2A \cos\left(\frac{\Delta k}{2}x - \frac{\Delta \omega}{2}t\right) \cos(k_{av}x - \omega_{av}t) \quad (5.21)$$

Wave Packet Envelope(from two waves)

- The superposition of two waves yields a wave number and angular frequency of the wave packet envelope.

$$\frac{\Delta k}{2}x - \frac{\Delta \omega}{2}t$$

- The range of wave numbers and angular frequencies that produce the wave packet have the following relations:

$$\Delta k \Delta x = 2\pi \qquad \Delta \omega \Delta t = 2\pi$$

- A **Gaussian wave packet** has similar relations:

$$\Delta k \Delta x = \frac{1}{2} \qquad \Delta \omega \Delta t = \frac{1}{2}$$

- The localization of the wave packet over a small region to describe a particle requires a large range of wave numbers. Conversely, a small range of wave numbers cannot produce a wave packet localized within a small distance.

Wave packet : Fourier Series and Integral

- The sum of **many waves** that form a wave packet is called a **Fourier series**:

$$\Psi(x, t) = \sum_i A_i \cos(k_i x - \omega_i t)$$

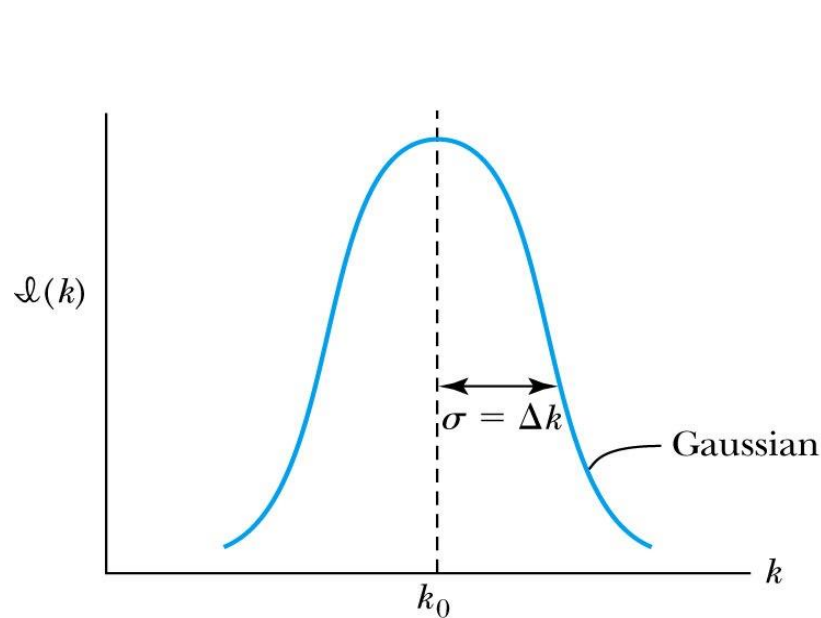
- Summing an **infinite number** of waves yields the Fourier integral:

$$\Psi(x, t) = \int \tilde{A}(k) \cos(kx - \omega t) dk$$

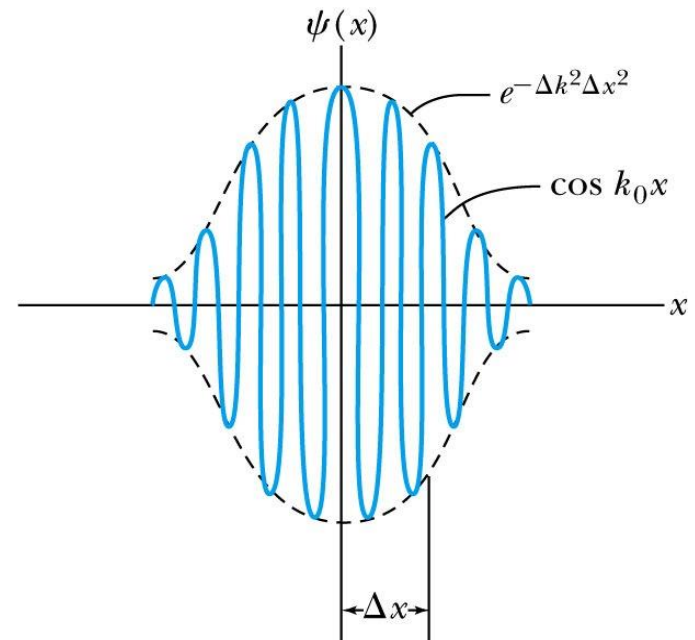
Gaussian Function

- A Gaussian wave packet describes the envelope of a pulse wave.

$$\Psi(x, 0) = \Psi(x) = Ae^{-\Delta k^2 x^2} \cos(k_0 x)$$



(a)



(b)

- The group velocity is $u_{\text{gr}} = \frac{d\omega}{dk}$

Group velocity of the wave packet = velocity of the particle described by the wavepacket

relate u_{gr} to de Broglie

$$u_g = \frac{d\omega}{dk}$$

$$\text{de Broglie wave } \begin{cases} E = hf = \hbar(2\pi f) = \hbar\omega \\ p = \frac{h}{\lambda} = \hbar \frac{2\pi}{\lambda} = \hbar k \end{cases}$$

$$u_{gr} = \frac{d\omega}{dk} = \frac{d(\hbar\omega)}{d(\hbar k)} = \frac{dE}{dp} = \frac{pc^2}{E}$$

use $E^2 = p^2 c^2 + m^2 c^4$ make derivative

$$2E dE = 2pc^2 dp$$

$$\frac{dE}{dp} = \frac{pc^2}{E}$$

group velocity of a wave packet
= velocity of a particle

$$mv c^2 / mc^2 = v$$

Dispersion causes group and phase velocities to be different

- Considering the group velocity of a de Broglie wave packet yields:

$$u_{\text{gr}} = \frac{dE}{dp} = \frac{pc^2}{E}$$

- The relationship between the phase velocity and the group velocity is

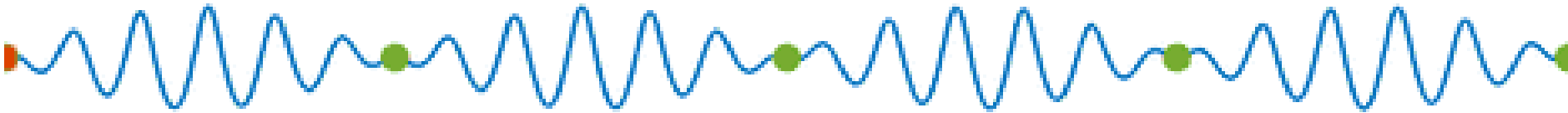
$$u_{\text{gr}} = \frac{d\omega}{dk} = \frac{d}{dk}(v_{\text{ph}}k) = v_{\text{ph}} + k \frac{dv_{\text{ph}}}{dk}$$

- Hence the group velocity may be greater or less than the phase velocity. A medium is called **nondispersive** when the phase velocity is the same for all frequencies and equal to the group velocity.

$$v_{\text{ph}} = \lambda f = \frac{\omega}{k}$$

$$\omega = v_{\text{ph}} \cdot k$$

phase and group velocity



$$u_{\text{gr}} = \frac{D\omega}{Dk}$$

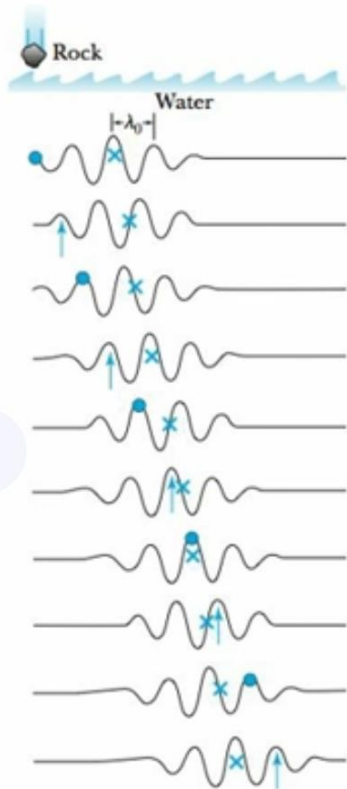


Figure 5.17 Progression with time of wave packet for which $u_{\text{gr}} = v_{\text{ph}}/2$. Note how the individual wave (arrow and dot alternately) moves through the wave packet (symbol X) with time.



EXAMPLE 5.5

We just saw that the speed of a nonrelativistic particle of mass m is not equal to its phase velocity. Show that the particle speed is equal to the group velocity.

Strategy We can use the relation for the group velocity in Equation (5.28) or (5.31). Either should work, and using both equations will be instructive.

Solution First, we look at Equation (5.31) for our nonrelativistic particle:

$$u_{\text{gr}} = \frac{pc^2}{E} = \frac{mvc^2}{mc^2} = v \quad (5.35)$$

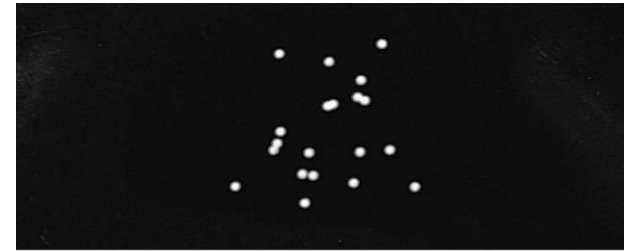
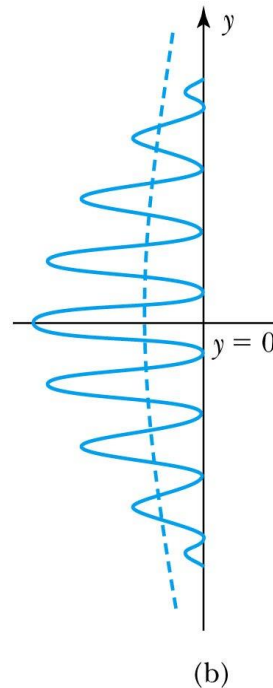
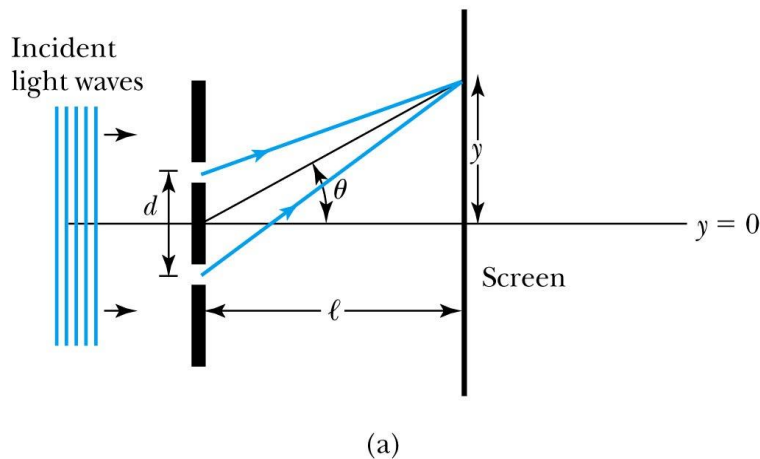
In order to use Equation (5.28) we utilize the results in Equations (5.29) and (5.30) for ω and k .

$$u_{\text{gr}} = \frac{d\omega}{dk} = \frac{d(E/\hbar)}{d(p/\hbar)} = \frac{dE}{dp} = \frac{d}{dp} \frac{p^2}{2m} = \frac{2p}{2m} = v$$

We agree that the particle, when acting as a wave, moves with the group velocity, not the phase velocity.

5.5: Waves or Particles?

- Young's double-slit diffraction experiment demonstrates the wave property of light.
- However, dimming the light results in single flashes on the screen representative of particles.



(a) 20 counts



(b) 100 counts



(c) 500 counts



(d) ~ 4000 counts

Which slit?

- To determine which slit the electron went through: We set up a light shining on the double slit and use a powerful microscope to look at the region. After the electron passes through one of the slits, light bounces off the electron; we observe the reflected light, so we know which slit the electron came through.
- Use a subscript “ph” to denote variables for light (photon). Therefore the momentum of the photon is

$$p_{\text{ph}} = \frac{h}{\lambda_{\text{ph}}} > \frac{h}{d}$$

- The momentum of the electrons will be on the order of $p_{\text{el}} = \frac{h}{\lambda_{\text{el}}} \sim \frac{h}{d}$.
- The difficulty is that the momentum of the photons used to determine which slit the electron went through is sufficiently great to strongly modify the momentum of the electron itself, thus changing the direction of the electron! The attempt to identify which slit the electron is passing through will in itself change the interference pattern.

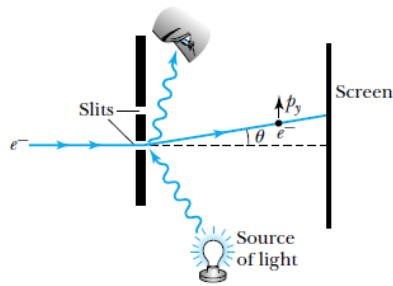


Figure 5.21 An attempt to determine which slit an electron passes through in the double-slit experiment. A powerful light source scatters a photon from the electron, and the scattered photon is observed. The motion of the electron is affected.

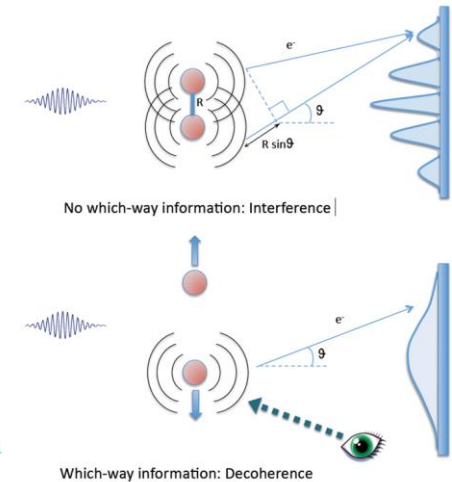
The difficulty is that the momentum of the photons used to determine which

The difficulty is that the momentum of the photons used to determine which slit the electron went through is sufficiently great to strongly modify the momentum of the electron itself, thus changing the direction of the electron! The attempt to identify which slit the electron is passing through will in itself change the interference pattern. We will take a closer look at this experiment in Section 5.6. In trying to determine which slit the electron went through, we are examining the particle-like behavior of the electron. When we are examining the interference pattern of the electron, we are using the wavelike behavior of the electron.

Bohr resolved this dilemma by pointing out that the particle-like and wave-like aspects of nature are *complementary*. Both are needed—they just can't be observed simultaneously.

Bohr's principle of complementarity: *It is not possible to describe physical observables simultaneously in terms of both particles and waves.*

Physical observables are those quantities such as position, velocity, momentum, and energy that can be experimentally measured. In any given instance we must use either the particle description or the wave description. Usually the choice is clear. The interference pattern of the double-slit experiment suggests that the light (or electron) had to go through both slits, and we must use the wave description. In our description of nature, we cannot describe phenomena by displaying both particle and wave behavior at the same time.

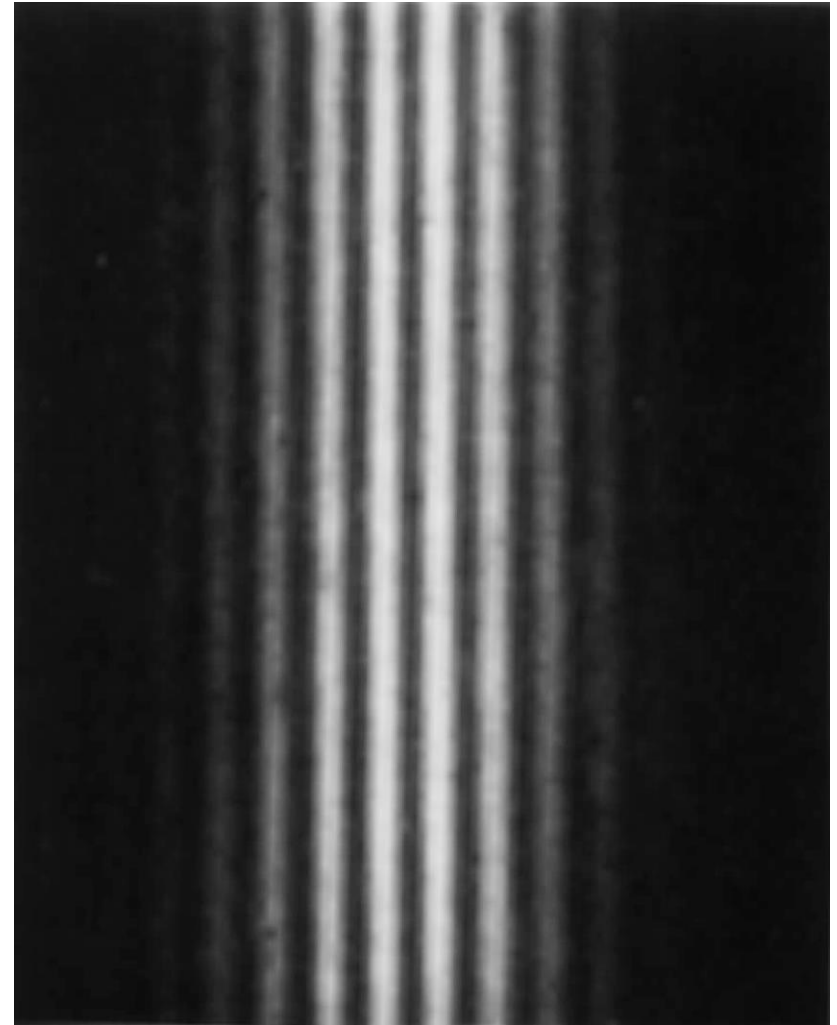


Principle of complementarity

Physical observables

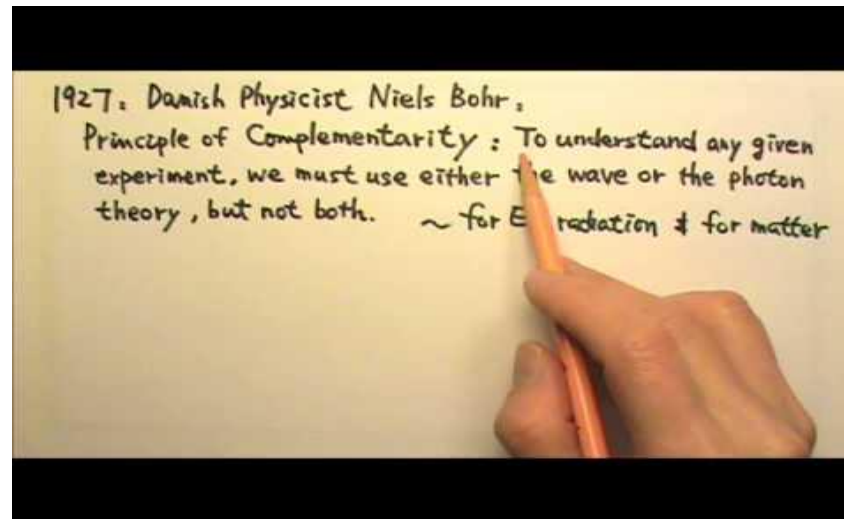
Electron Double-Slit Experiment

- C. Jönsson of Tübingen, Germany, succeeded in 1961 in showing double-slit interference effects for electrons by constructing very narrow slits and using relatively large distances between the slits and the observation screen.
- This experiment demonstrated that precisely the same behavior occurs for both light (waves) and electrons (particles).



Wave particle duality solution

- The solution to the wave particle duality of an event is given by the following principle.
- **Bohr's principle of complementarity:** It is not possible to describe physical observables simultaneously in terms of both particles and waves.
- **Physical observables** are those quantities such as position, velocity, momentum, and energy that can be experimentally measured. In any given instance we must use either the particle description or the wave description.



5.6: Uncertainty Principle

- It is impossible to measure simultaneously, with no uncertainty, the precise values of k and x for the same particle. The wave number k may be rewritten as

$$k = \frac{2\pi}{\lambda} = \frac{2\pi}{h/p} = p \frac{2\pi}{h} = \frac{p}{h}$$

- For the case of a Gaussian wave packet we have

$$\Delta k \Delta x = \frac{\Delta p}{h} \Delta x = \frac{1}{2}$$

Thus for a single particle we have Heisenberg's **uncertainty principle**:

$$\Delta p_x \Delta x \geq \frac{\hbar}{2}$$



Energy Uncertainty

- If we are uncertain as to the exact position of a particle, for example an electron somewhere inside an atom, the particle can't have zero kinetic energy.

$$K_{\min} = \frac{p_{\min}^2}{2m} \geq \frac{(\Delta p)^2}{2m} \geq \frac{\hbar^2}{2m\ell^2}$$

- The energy uncertainty of a Gaussian wave packet is

$$\Delta E = h \Delta f = h \frac{\Delta \omega}{2\pi} = \hbar \Delta \omega$$

combined with the angular frequency relation

$$\Delta \omega \Delta t = \frac{\Delta E}{\hbar} \Delta t = \frac{1}{2}$$

- Energy-Time Uncertainty Principle $\Delta E \Delta t \geq \frac{\hbar}{2}$.

Uncertainty principle

When localizing a wave packet over a small region we have
 $\Delta k \cdot \Delta x = 2\pi \rightarrow \Delta k$ must be large to have Δx small (good location)

It is better to use: $\Delta k \Delta x = \frac{1}{2}$ Gaussian wave packet

Uncertainty principle : It is impossible to measure with no uncertainty the precise values of k and x simultaneously for the same particles
Heisenberg

$$k = \frac{2\pi}{\lambda} = \frac{2\pi}{h/p} = p \frac{2\pi}{h} = \frac{p}{\hbar}$$

$$\left. \begin{array}{l} \Delta k = \frac{\Delta p}{\hbar} \\ \text{use Gaussian wave packet} \\ \Delta k \Delta x = \frac{1}{2} \end{array} \right\} \Delta p \Delta x = \frac{\hbar}{2}$$

This applies to
all three directions

$$\Delta p_x \Delta x \geq \frac{\hbar}{2}$$

so we put indices on it

$$\Delta E \cdot \Delta t \geq \frac{\hbar}{2}$$

Which of the following statements is most correct about the uncertainty principle?

- a) It is impossible to know exactly both the position and the momentum of a particle simultaneously.
- b) An electron with some momentum can be trapped into an arbitrarily small box.
- c) Our instruments will eventually be able to measure more precisely than the principle presently allows.
- d) On large length scales, the uncertainty principle dominates our understanding of the physical world.
- e) A particle limited in space can occupy any energy.



EXAMPLE 5.8

Calculate the momentum uncertainty of (a) a tennis ball constrained to be in a fence enclosure of length 35 m surrounding the court and (b) an electron within the smallest diameter of a hydrogen atom.

Strategy We will use Equation (5.40) to find Δp_x . The position uncertainty Δx is approximately half of the enclosure.

Solution (a) If we insert the uncertainty of the location of the tennis ball, $\Delta x = (35 \text{ m})/2$, into Equation (5.40), we have

$$\Delta p_x \geq \frac{1}{2} \frac{\hbar}{\Delta x} = \frac{1.05 \times 10^{-34} \text{ J} \cdot \text{s}}{2(35 \text{ m})/2} = 3 \times 10^{-36} \text{ kg} \cdot \text{m/s}$$

We will have no problem specifying the momentum of the tennis ball!

Not a large uncertainty

(b) The diameter of the hydrogen atom in its lowest energy state (smallest radius) is $2a_0$. We arbitrarily take the uncertainty Δx to be half the diameter or equal to the radius, $\Delta x = a_0$.

$$\begin{aligned} \Delta x &= a_0 = 0.529 \times 10^{-10} \text{ m} \\ \Delta p_x &\geq \frac{1}{2} \frac{\hbar}{\Delta x} = \frac{1.05 \times 10^{-34} \text{ J} \cdot \text{s}}{2(0.529 \times 10^{-10} \text{ m})} \\ &= 1 \times 10^{-24} \text{ kg} \cdot \text{m/s} \end{aligned}$$

This may seem like a small momentum, but for an electron with a mass of about 10^{-30} kg , it corresponds to a speed of about 10^6 m/s , which is not insignificant! Note that this is comparable to the speed of the electron in the first Bohr orbit [Equation (4.31)].

This is a large uncertainty

5.7: Probability, Wave Functions, and the Copenhagen Interpretation

- The wave function determines the likelihood (or probability) of finding a particle at a particular position in space at a given time.

$$P(y) dy = |\Psi(y,t)|^2 dy$$

- The total probability of finding the electron is 1. Forcing this condition on the wave function is called normalization.

$$\int_{-\infty}^{\infty} P(y) dy = \int_{-\infty}^{\infty} |\Psi(y,t)|^2 dy = 1$$

The Copenhagen Interpretation

- Bohr's interpretation of the wave function consisted of 3 principles:
 - 1) The uncertainty principle of Heisenberg
 - 2) The complementarity principle of Bohr
 - 3) The statistical interpretation of Born, based on probabilities determined by the wave function

 - Together these three concepts form a logical interpretation of the physical meaning of quantum theory. According to the Copenhagen interpretation, physics depends on the outcomes of measurement.
-

5.8: Particle in a Box

- A particle of mass m is trapped in a one-dimensional box of width l .
- The particle is treated as a wave.
- The box puts boundary conditions on the wave. The wave function must be zero at the walls of the box and on the outside.
- In order for the probability to vanish at the walls, we must have an integral number of **half wavelengths** in the box.

$$\frac{n\lambda}{2} = \ell \quad \text{or} \quad \lambda_n = \frac{2\ell}{n} \quad (n = 1, 2, 3, \dots)$$

- The energy of the particle is $E = \text{K.E.} = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2}$.
- The possible wavelengths are quantized which yields the energy:

$$E_n = \frac{h^2}{2m} \left(\frac{n}{2\ell} \right)^2 = n^2 \frac{h^2}{8m\ell^2} \quad (n = 1, 2, 3, \dots)$$

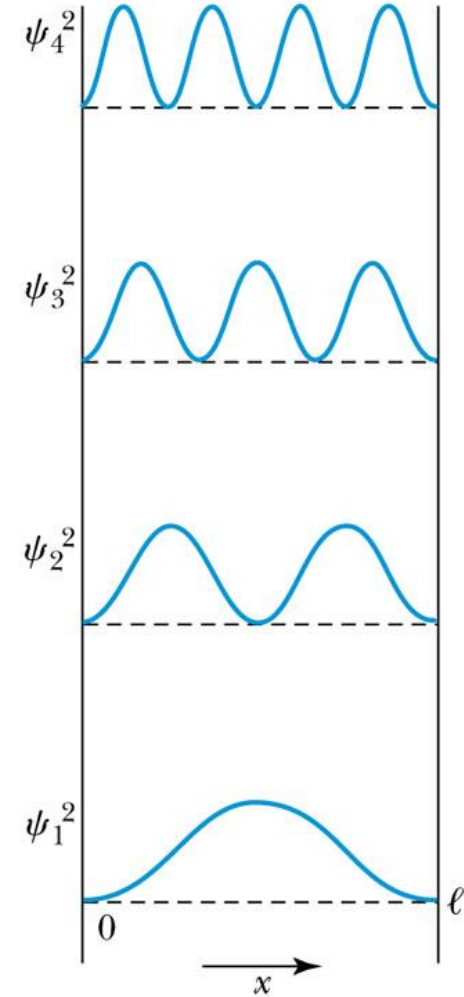
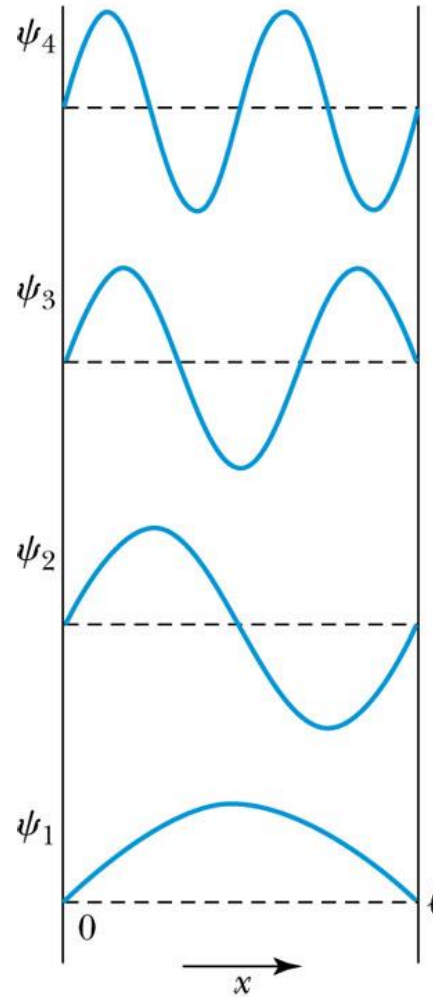
- The possible energies of the particle are quantized.

Probability of the Particle

- The probability of observing the particle between x and $x + dx$ in each state is

$$P_n dx \propto |\Psi_n(x)|^2 dx$$

- Note that $E_0 = 0$ is not a possible energy level.
- The concept of energy levels, as first discussed in the Bohr model, has surfaced in a natural way by using waves.





EXAMPLE 5.13

Find the quantized energy levels of an electron constrained to move in a one-dimensional atom of size 0.1 nm.

Strategy We previously found the minimum kinetic energy of an electron in a similar situation in Example 5.9. In the present case we want to use quantum theory, so we use Equation (5.51) for the energy levels.

Solution We use Equation (5.51) and insert the appropriate values for m and ℓ .

$$\begin{aligned} E_n &= n^2 \frac{h^2}{8m\ell^2} = n^2 \frac{h^2 c^2}{8mc^2 \ell^2} \\ &= n^2 \frac{(1239.8 \text{ eV} \cdot \text{nm})^2}{(8)(0.511 \times 10^6 \text{ eV})(0.1 \text{ nm})^2} \\ &= n^2(38 \text{ eV}) \end{aligned}$$

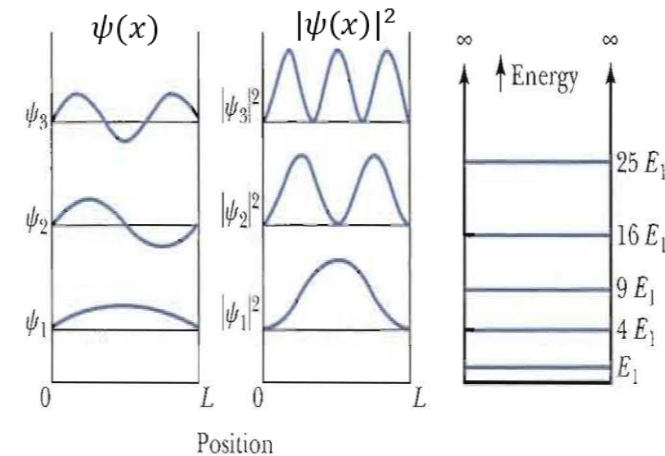
The first three energy levels are $E_1 = 38 \text{ eV}$, $E_2 = 152 \text{ eV}$, and $E_3 = 342 \text{ eV}$.

Particle in a box

Consider a particle trapped in a box to have wave behavior;

An integer number of half wavelengths must fit into the box. At the wall's the probability must be zero which means also the wave function must be zero.

$$n \frac{\lambda}{2} = l \quad \text{or} \quad \lambda = \frac{2l}{n} \quad (n = 1, 2, 3 \dots)$$



This condition leads to energy quantization only certain energies are possible

$$E = K = \frac{1}{2}mv^2 = \frac{p^2}{2m} \quad \text{and} \quad pc = hf \quad \text{So; } E = \frac{p^2}{2m} = \frac{h^2}{\lambda^2 2m} = \frac{h^2 n^2}{8ml^2}$$

$$E = \frac{h^2 n^2}{8ml^2} \quad (n = 1, 2, 3 \dots) \quad \text{or} \quad E_n = n^2 \frac{\hbar^2 \pi^2}{2ml^2}$$

Note: Bohr radius $a_0 = 0.53 \times 10^{-10}$ m and diameter $2a_0 = 0.1$ nm

5.13 Calculate the quantized energy levels of an electron in a one-dimensional H-atom ($l=0.1$ nm)

$$E_n = n^2 \frac{\hbar^2 \pi^2 c^2}{2ml^2 c^2} = n^2 \frac{(4 \times 10^{-16} \text{ eVs})^2 (3 \times 10^8 \frac{\text{m}}{\text{s}})^2 (\frac{10^9 \text{ mm}}{1 \text{ m}})^2}{8(0.5 \times 10^6 \text{ eV})^2 (0.1 \text{ nm})^2} = n^2 38 \text{ eV}$$

5.42 What is the minimum uncertainty in the speed of a bacterium.....

$$\Delta p \Delta x = m \Delta v \Delta x \geq \frac{\hbar}{2}$$

$$\Delta v = \frac{\hbar}{2m \Delta x} = \frac{1.054 \times 10^{-34} \text{ J} \cdot \text{s}}{2(3.0 \times 10^{-15} \text{ kg})(1.0 \times 10^{-6} \text{ m})} = 1.76 \times 10^{-14} \text{ m/s}$$

so

5.36 some physics theories indicate a lifetime of the proton of 10^{36} years. What does such a prediction say about the energy of a proton??

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

$$\Delta E \geq \frac{\hbar}{2\Delta t} = \frac{1.054 \times 10^{-34} \text{ J} \cdot \text{s}}{2(1 \times 10^{36} \text{ y})(3.16 \times 10^7 \text{ s/y})} = 1.67 \times 10^{-78} \text{ J}$$

Clicker - Questions

13) The energies of the excited states of a particle in a infinite square well are exact and have no energy uncertainty. What does this suggest about the lifetime of a particle in those excited states?

- a) The particle stays in its excited state forever.
- b) The particle decays immediately.
- c) The particle decays with an exponential decay law.
- d) The lifetime depends on whether the particle is an electron or a proton.

Clicker - Questions

15) An electron is trapped in a one-dimensional region of length $1 \times 10^{-10} \text{m}$. How much energy must be supplied to excite the electron from the ground state to the second excited state?

a) 38 eV

b) 114 eV

c) 304 eV

d) 342 eV

Infinite Square well

Divide the problem into 3 parts: two are outside the well and one is inside the well.

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = E\psi$$

OUTSIDE: $x < 0$ and $x > 0$; $\psi = 0$

INSIDE: $V = 0$ and $-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi$ with boundary condition $\psi = 0$ at $x = 0, L$

$$\frac{d^2\psi}{dx^2} = -k^2\psi; \quad \text{and} \quad k^2 = \frac{2mE}{\hbar^2} \quad \psi = A\sin kx + B\cos kx$$

At $x = 0$;

$$0 = A\sin 0 + B\cos 0 \quad \text{So; } B = 0$$

At $x = L$;

$$0 = A\sin kL \quad (n = 1, 2, 3 \dots)$$

$$kL = n\pi \quad (n = 1, 2, 3 \dots)$$

$$\text{So; } k = \frac{\pi n}{L}$$

$$\psi = A\sin kx = A\sin \frac{\pi n}{L} x$$

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$

Determine the only constant A : $\int_0^L A^2 \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$

$$A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx \} A^2 \frac{L}{2} = 1 \rightarrow A = \sqrt{\frac{2}{L}}$$

$$\text{and } \psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

