

ENGINEERING PHYSICS

[SUBJECT CODE: PHY1051]

COMMON COURSE MATERIAL FOR FIRST YEAR BTech STUDENTS



DEPARTMENT OF PHYSICS
MANIPAL INSTITUTE OF TECHNOLOGY

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Reference book:

Physics for Scientists and Engineers with Modern Physics by Raymond Serway and John Jewett (Cengage Learning, Seventh Edition 2012)

1 INTERFERENCE OF LIGHT WAVES

OBJECTIVES

- To understand the principles of interference.
- To explain the intensity distribution in interference under various conditions.
- To explain the interference from thin films.

Wave optics (Physical Optics): It is the study of interference, diffraction, and polarization of light. These phenomena cannot be adequately explained with the ray optics.

1.1 YOUNG'S DOUBLE-SLIT EXPERIMENT

Light waves also interfere with one another like mechanical waves. Fundamentally, all interference associated with light waves arises when the electromagnetic fields that constitute the individual waves combine.

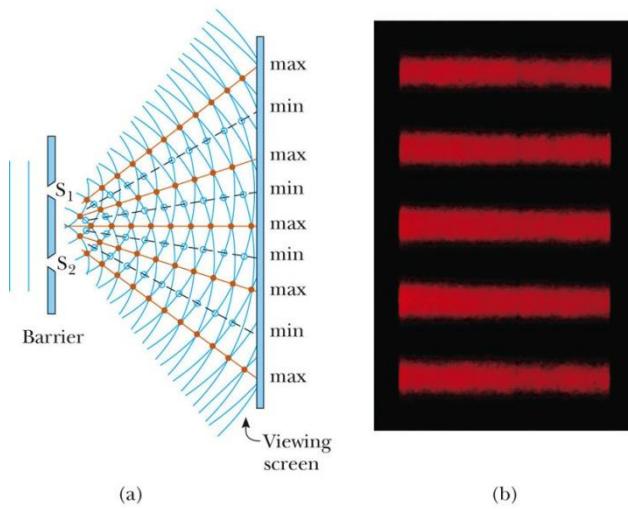


Figure 1.1 (a) Schematic diagram of Young's double-slit experiment. Slits S_1 and S_2 behave as coherent sources of light waves that produce an interference pattern on the viewing screen (drawing not to scale). (b) An enlargement of the center of a fringe pattern formed on the viewing screen.

Interference in light waves from two sources was first demonstrated by Thomas Young in 1801. A schematic diagram of the apparatus Young used is shown Fig. 1.1a. Plane light waves arrive at a barrier that contains two slits S_1 and S_2 . The light from S_1 and S_2 produces on a viewing screen a visible pattern of bright and dark parallel bands called **fringes** (Fig. 1.1b). When the light from S_1 and that from S_2 both arrive at a point on the screen such that constructive interference occurs at that location,

a bright fringe appears. When the light from the two slits combines destructively at any location on the screen, a dark fringe results.

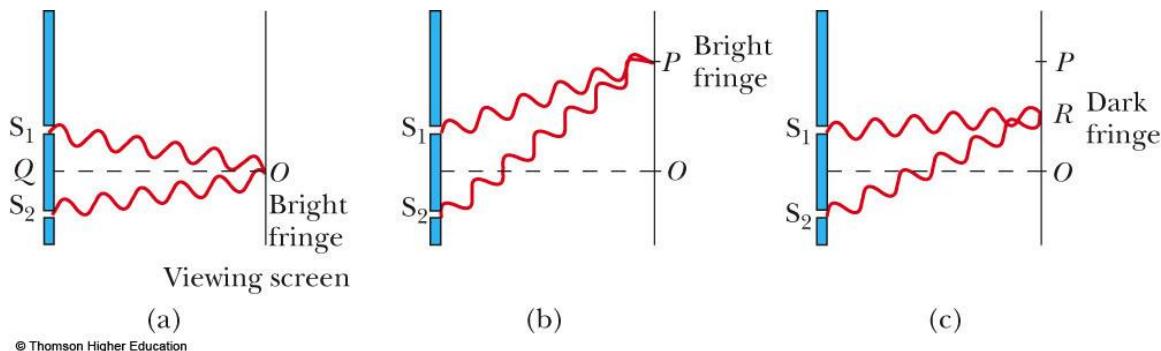


Figure 1.2 Waves leave the slits and combine at various points on the viewing screen.

Fig. 1.2 shows different ways in which two waves can combine at the screen. In Fig. 1.2a, the two waves, which leave the two slits in phase, strike the screen at the central point O . Because both waves travel the same distance, they arrive at O in phase. As a result, constructive interference occurs at this location and a bright fringe is observed. In Fig. 1.2b, the two waves leave the slits in phase, but the wave leaving from S_2 has to travel longer distance compare to wave from S_1 . However, the difference in the path is exactly one wavelength and they arrive in phase at P and a second bright fringe appears at this location. At point R in Fig. 1.2c, wave from S_2 has fallen half a wavelength behind the wave from S_1 and a crest of the upper wave overlaps a trough of the lower wave, giving rise to destructive interference at point R .

If two lightbulbs are placed side by side so that light from both bulbs combines, no interference effects are observed because the light waves from one bulb are emitted independently of those from the other bulb. The emissions from the two lightbulbs do not maintain a constant phase relationship with each other over time. Therefore, the conditions for constructive interference, destructive interference, or some intermediate state are maintained only for short time intervals. Since the eye cannot follow such rapid changes, no interference effects are observed. Such light sources are said to be **incoherent**.

To observe interference of waves from two sources, the following conditions must be met:

- The sources must be **coherent**; that is, they must maintain a constant phase with respect to each other.
- The sources should be **monochromatic**; that is, they should be of a single wavelength.

A common method for producing two coherent light sources is to use a monochromatic source to illuminate a barrier containing two small openings,

usually in the shape of slits, as in the case of Young's experiment illustrated in Fig. 1. The light emerging from the two slits is coherent because a single source produces the original light beam and the two slits serve only to separate the original beam into two parts. Any random change in the light emitted by the source occurs in both beams at the same time. As a result, interference effects can be observed when the light from the two slits arrives at a viewing screen.

1.2 ANALYSIS MODEL: WAVES IN INTERFERENCE

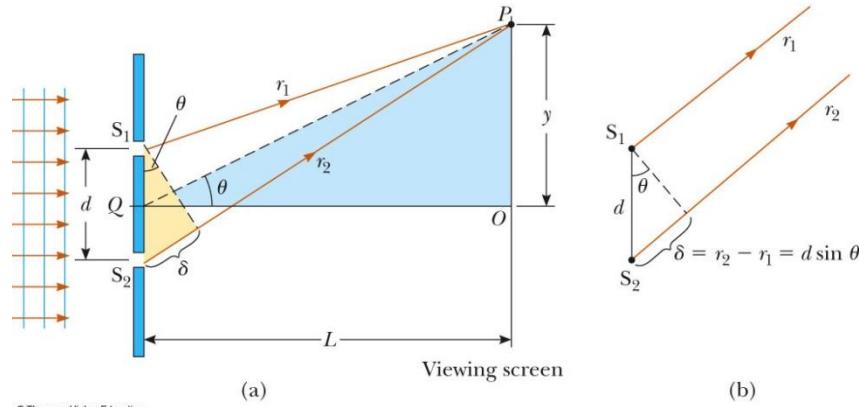


Figure 1.3 (a) Geometric construction for describing Young's double-slit experiment (not to scale). (b) The slits are represented as sources, and the outgoing light rays are assumed to be parallel as they travel to P .

The viewing screen is located a perpendicular distance L from the barrier containing two slits, S_1 and S_2 (Fig. 1.3a). These slits are separated by a distance d , and the source is monochromatic. To reach any arbitrary point P in the upper half of the screen, a wave from the lower slit must travel farther than a wave from the upper slit by a distance $d \sin \theta$ (Fig. 1.3b). This distance is called the **path difference** δ . If we assume the rays labeled r_1 and r_2 are parallel, which is approximately true if L is much greater than d , then δ is given by

$$\delta = r_2 - r_1 = d \sin \theta \quad (1.1)$$

The value of δ determines whether the two waves are in phase when they arrive at point P .

Angular positions of bright and dark fringes: If δ is either zero or some integer multiple of the wavelength, the two waves are in phase at point P and constructive interference results. Therefore, the condition for bright fringes, or **constructive interference**, at point P is,

$$d \sin \theta_{\text{bright}} = m\lambda ; \quad (m = 0, \pm 1, \pm 2, \dots) \quad (1.2)$$

The number m is called the **order number**.

When d is an odd multiple of $\lambda/2$, the two waves arriving at point P are 180° out of phase and give rise to destructive interference. Therefore, the condition for dark fringes, or **destructive interference**, at point P is,

$$d \sin \theta_{\text{dark}} = \left(m + \frac{1}{2} \right) \lambda ; \quad (m = 0, \pm 1, \pm 2, \dots) \quad (1.3)$$

Linear positions of bright and dark fringes: From the triangle OPQ in Fig. 1.3a,

$$\tan \theta = \frac{y}{L} \quad (1.4)$$

Using this result, the linear positions of bright and dark fringes are given by

$$y_{\text{bright}} = L \tan \theta_{\text{bright}} \quad (1.5)$$

$$y_{\text{bright}} = L \frac{m\lambda}{d} \quad (\text{small angle approximation}) \quad (1.6)$$

$$y_{\text{dark}} = L \tan \theta_{\text{dark}} \quad (1.7)$$

$$y_{\text{dark}} = L \frac{\left(m + \frac{1}{2} \right) \lambda}{d} \quad (\text{small angle approximation}) \quad (1.8)$$

1.3 INTENSITY DISTRIBUTION OF THE DOUBLE-SLIT INTERFERENCE PATTERN

Consider two coherent sources of sinusoidal waves such that they have same angular frequency ω and phase difference ϕ . The total magnitude of the electric field at point P on the screen in Fig. 1.3a is the superposition of the two waves. Assuming that the two waves have same amplitude E_0 , we can write the magnitude of electric field at point P due to each source as

$$E_1 = E_0 \sin \omega t \quad \text{and} \quad E_2 = E_0 \sin(\omega t + \phi) \quad (1.9)$$

Although the waves are in phase at the slits, their phase difference ϕ at P depends on the path difference $\delta = r_2 - r_1 = d \sin \theta$. A path difference of λ (for constructive interference) corresponds to a phase difference of 2π radians.

$$\phi = \frac{2\pi}{\lambda} \delta = \frac{2\pi}{\lambda} d \sin \theta \quad (1.10)$$

Using the superposition principle and Equation (1.9), we obtain the following expression for the magnitude of the resultant electric field at point P :

$$E_p = E_1 + E_2 = E_0 \left[\sin \omega t + \sin (\omega t + \phi) \right] \quad (1.11)$$

$$E_p = 2E_0 \cos\left(\frac{\phi}{2}\right) \sin\left(\omega t + \frac{\phi}{2}\right) \quad (1.12)$$

This result indicates that the electric field at point P has the same frequency ω as the light at the slits but that the amplitude of the field is multiplied by the factor $2 \cos(\phi/2)$. If $\phi = 0, 2\pi, 4\pi, \dots$, the magnitude of the electric field at point P is $2E_0$, corresponding to the condition for maximum constructive interference. Similarly, if $\phi = \pi, 3\pi, 5\pi, \dots$, the magnitude of the electric field at point P is zero.

Intensity of a wave is proportional to the square of the resultant electric field magnitude at that point. Using Equation 1.12, we can express the light intensity at point P as

$$I \propto E_p^2 = 4E_0^2 \cos^2\left(\frac{\phi}{2}\right) \sin^2\left(\omega t + \frac{\phi}{2}\right) \quad (1.13)$$

Most light-detecting instruments measure time-averaged light intensity, and the time averaged value of $\sin^2\left(\omega t + \frac{\phi}{2}\right)$ over one cycle is $1/2$. Therefore, we can write the average light intensity at point P as,

$$I = I_{\max} \cos^2\left(\frac{\phi}{2}\right) \quad (1.14)$$

where I_{\max} is the maximum intensity on the screen. Substituting the value for ϕ from Equation 1.10;

$$I = I_{\max} \cos^2\left(\frac{\pi d \sin \theta}{\lambda}\right) \quad (1.15)$$

Alternatively, since $\sin \theta \approx \frac{y}{L}$ for small values of θ , we can write;

$$I = I_{\max} \cos^2\left(\frac{\pi d}{\lambda L} y\right) \quad (1.16)$$

A plot of light intensity versus $d \sin \theta$ is given in Fig. 1.4. The interference pattern consists of equally spaced fringes of equal intensity.

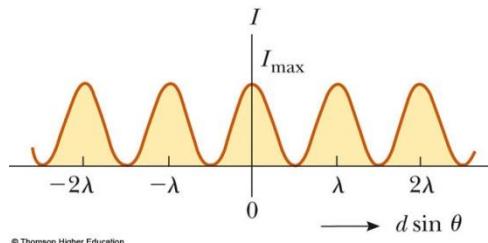
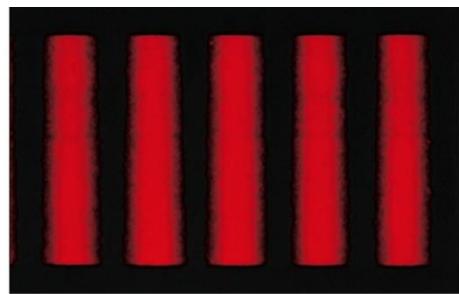


Figure 1.4 Light intensity versus $d \sin \theta$ for a double-slit interference pattern when the screen is far from the two slits ($L \gg d$).

1.4 CHANGE OF PHASE DUE TO REFLECTION

Young's method for producing two coherent light sources involves illuminating a pair of slits with a single source. Another simple arrangement for producing an interference pattern with a single light source is known as *Lloyd's mirror* (Fig. 1.5).

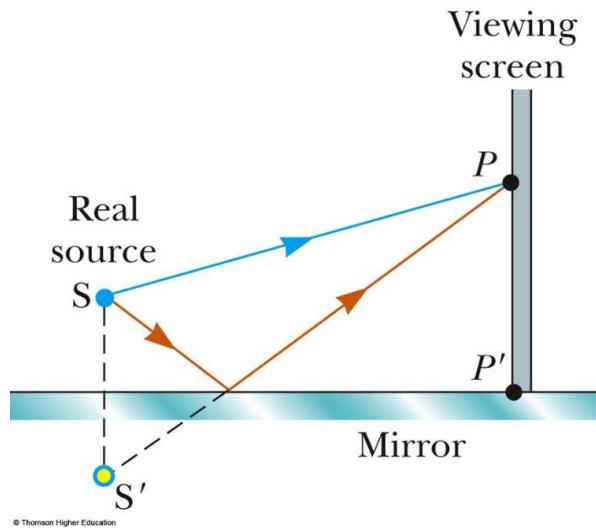


Figure 1.5 Lloyd's mirror. The reflected ray undergoes a phase change of 180° .

A point light source S is placed close to a mirror, and a viewing screen is positioned some distance away and perpendicular to the mirror. Light waves can reach point P on the screen either directly from S to P or by the path involving reflection from the mirror. The reflected ray can be treated as a ray originating from a virtual source S' . As a result, we can think of this arrangement as a double slit source where the

distance d between sources S and S' in Fig. 1.5 is analogous to length d in Fig. 1.3a. Hence, at observation points far from the source ($L \gg d$), waves from S and S' form an interference pattern exactly like the one formed by two real coherent sources. But, the positions of the dark and bright fringes, however, are reversed relative to the pattern created by two real coherent sources (Young's experiment). Such a reversal can only occur if the coherent sources S and S' differ in phase by 180° .

In general, an electromagnetic wave undergoes a phase change of 180° upon reflection from a medium that has a higher index of refraction than the one in which the wave is traveling. Analogy between reflected light waves and the reflections of a transverse pulse on a stretched string is shown in Fig. 1.6.

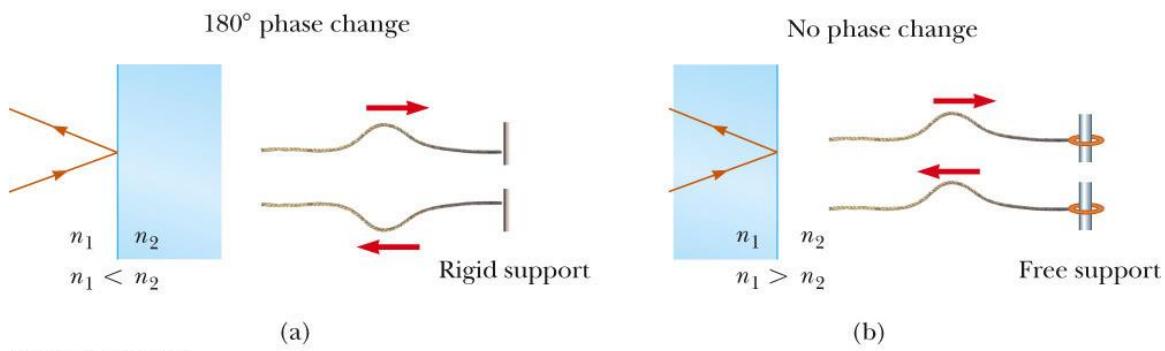


Figure 1.6 Comparisons of reflections of light waves and waves on strings.

The reflected pulse on a string undergoes a phase change of 180° when reflected from the boundary of a denser string or a rigid support, but no phase change occurs when the pulse is reflected from the boundary of a less dense string or a freely-supported end. Similarly, an electromagnetic wave undergoes a 180° phase change when reflected from a boundary leading to an optically denser medium, but no phase change occurs when the wave is reflected from a boundary leading to a less dense medium.

1.5 INTERFERENCE IN THIN FILMS

Interference effects are commonly observed in thin films, such as thin layers of oil on water or the thin surface of a soap bubble. The varied colors observed when white light is incident on such films result from the interference of waves reflected from the two surfaces of the film. Consider a film of uniform thickness t and index of refraction n . Assume light rays traveling in air are nearly normal to the two surfaces of the film as shown in Fig. 1.7. If λ is the wavelength of the light in free space and n is the index of refraction of the film material, then the wavelength of light λ_n in the film is $\lambda_n = \frac{\lambda}{n}$.

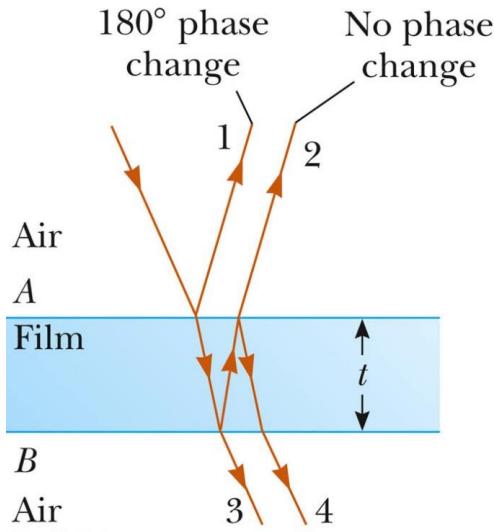


Figure 1.7 Light paths through a thin film.

Reflected ray 1, which is reflected from the upper surface (A) in Fig. 1.7, undergoes a phase change of 180° with respect to the incident wave. Reflected ray 2, which is reflected from the lower film surface (B), undergoes no phase change because it is reflected from a medium (air) that has a lower index of refraction. Therefore, ray 1 is 180° out of phase with ray 2, which is equivalent to a path difference of $\lambda_n/2$. We must also consider that ray 2 travels an extra distance $2t$ before the waves recombine in the air above surface A. (Remember that we are considering light rays that are close to normal to the surface. If the rays are not close to normal, the path difference is larger than $2t$). If $2t = \lambda_n/2$, rays 1 and 2 recombine in phase and the result is constructive interference. In general, the condition for **constructive** interference in thin film is,

$$2t = \left(m + \frac{1}{2}\right)\lambda_n \quad (m = 0, 1, 2, \dots) \quad (1.17)$$

Or,

$$2nt = \left(m + \frac{1}{2}\right)\lambda_n \quad (m = 0, 1, 2, \dots) \quad (1.18)$$

If the extra distance $2t$ traveled by ray 2 corresponds to a multiple of λ_n the two waves combine out of phase and the result is destructive interference. The general equation for **destructive** interference in thin films is

$$2nt = m\lambda \quad (m = 0, 1, 2, \dots) \quad (1.19)$$

1.6 NEWTON'S RINGS

When a plano-convex lens is placed on top of a flat glass surface as shown in Fig. 1.8a, interference fringes are formed, and these fringes can be seen under the

traveling microscope. With this arrangement, the air film between the glass surfaces varies in thickness from zero at the point of contact to some value t at point P . If the radius of curvature R of the lens is much greater than the distance r and the system is viewed from above, a pattern of light and dark rings is observed as shown in Fig. 1.8b. These circular fringes, discovered by Newton, are called **Newton's rings**.

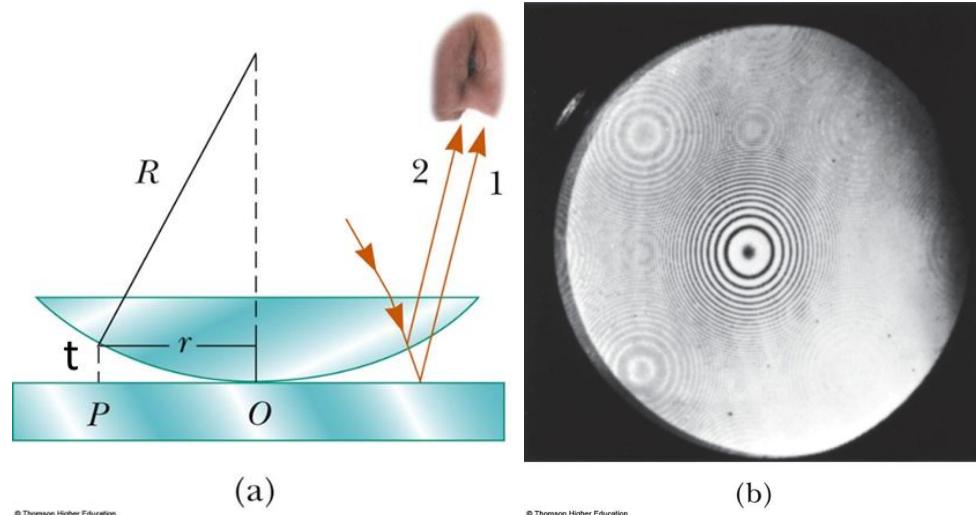


Figure 1.8 (a) The combination of rays reflected from the flat plate and the curved lens surface gives rise to an interference pattern known as Newton's rings. (b) Photograph of Newton's rings.

Expressions for radii of the bright and dark rings:

Using the geometry shown in Fig. 1.8a, we can obtain expressions for the radii of the bright and dark rings in terms of the radius of curvature R and wavelength λ . For the thin air film trapped between the two glass surfaces as shown in the figure above, the conditions for constructive (bright rings) and destructive (dark rings) interference are given by equations (1.18) and (1.19).

Consider the dark rings (destructive interference)

$$2nt = m\lambda, \quad m = 0, 1, 2, 3\dots$$

For air film, $n \approx 1$, $\therefore 2t = m\lambda$

From the above figure, $t = R - \sqrt{R^2 - r^2}$

$$t = R - R \left[1 - \left(\frac{r}{R} \right)^2 \right]^{1/2}$$

Binomial theorem is, $(1+y)^n = 1 + ny + \frac{n(n-1)}{2!} y^2 + \dots$

If $r/R \ll 1$, using binomial theorem and neglecting higher order terms,

$$t = R - R \left[1 - \frac{1}{2} \left(\frac{r}{R} \right)^2 + \dots \right] \approx \frac{r^2}{2R} \quad (1.20)$$

Substituting the value of t from equation (1.20) into equation (1.19), we get

$$r_{dark} \approx \sqrt{mR\lambda} \quad (m = 0, 1, 2, \dots) \quad (1.21)$$

In general, for any thin film of refractive index n_{film} , the expression for the radii of the dark rings is given by $r_{dark} \approx \sqrt{\frac{mR\lambda}{n_{film}}} \quad (m = 0, 1, 2, \dots)$ (1.22)

Similarly, the expression for the radii of the bright rings is given by,

$$r_{bright} \approx \sqrt{\frac{\left(m + \frac{1}{2}\right)R\lambda}{n_{film}}} \quad (m = 0, 1, 2, \dots) \quad (1.23)$$

That is, the diameters of Newton's dark rings are proportional to square root of the natural numbers and the diameters of Newton's bright rings are proportional to square root of natural odd numbers.

1.7 MICHELSON INTERFEROMETER

The **interferometer**, invented by American physicist A. A. Michelson (1852–1931), splits a light beam into two parts and then recombines the parts to form an interference pattern. A schematic diagram of the interferometer is shown in Fig. 1.9. A ray of light from a monochromatic source is split into two rays by mirror M_o , which is inclined at 45° to the incident light beam. Mirror M_o , called a *beam splitter*, transmits half the light incident on it and reflects the rest. One ray is reflected from M_o to the right toward mirror M_1 , and the second ray is transmitted vertically through M_o toward mirror M_2 . Hence, the two rays travel separate paths L_1 and L_2 . After reflecting from M_1 and M_2 , the two rays eventually recombine at M_o to produce an interference pattern, which can be viewed through a telescope.

The interference condition for the two rays is determined by the difference in their path length. When the two mirrors are exactly perpendicular to each other, the interference pattern is a target pattern of bright and dark circular fringes. As M_1 is moved, the fringe pattern collapses or expands, depending on the direction in which M_1 is moved. For example, if a dark circle appears at the center of the target pattern (corresponding to destructive interference) and M_1 is then moved a distance $\lambda/4$ toward M_o , the path difference changes by $\lambda/2$. This replaces dark circle at center by bright circle. Therefore, the fringe pattern shifts by one-half fringe each time M_1 is moved a distance $\lambda/4$. The wavelength of light is then measured by counting the number of fringe shifts for a given displacement of M_1 . So it can also be used to

detect small change in path length as in the laser interferometer gravitational-wave observatory.

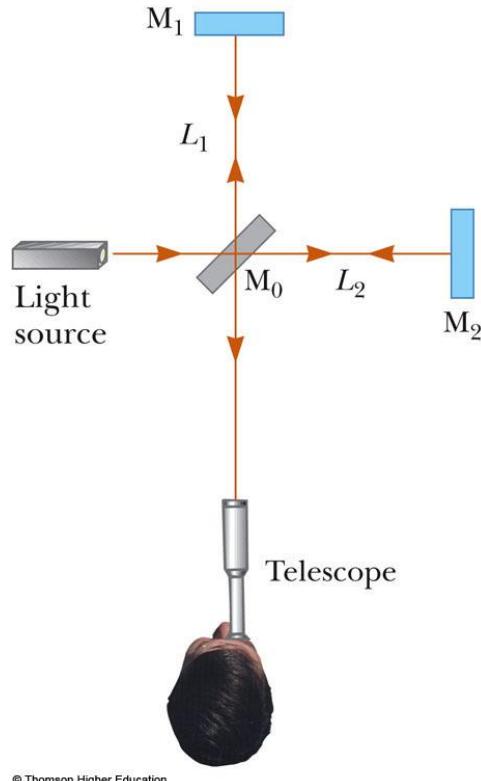


Figure 1.9 Schematic diagram of Michelson Interferometer

1.8 QUESTIONS

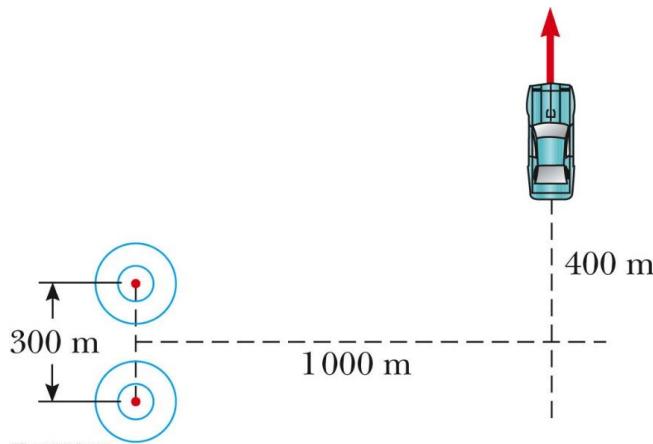
1. What is interference of light waves?
2. What is coherence? Mention its importance.
3. Write the necessary condition for the constructive and destructive interference of two light waves in terms of path/phase difference.
4. Obtain an expression for intensity of light in double-slit interference.
5. Write the conditions for constructive and destructive interference of reflected light from a thin soap film in air, assuming normal incidence.
6. Explain the formation of fringes in Michelson interferometer.

1.9 PROBLEMS

1. A viewing screen is separated from a double slit by 4.80 m. The distance between the two slits is 0.0300 mm. Monochromatic light is directed toward the double slit and forms an interference pattern on the screen. The first dark fringe is 4.50 cm from the center line on the screen. (A) Determine the

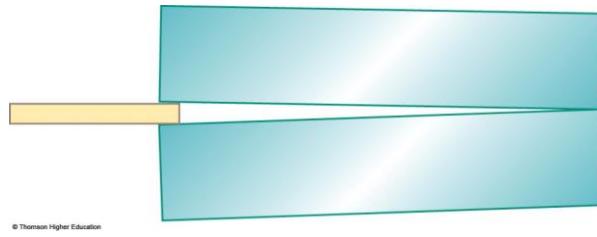
wavelength of the light. (B) Calculate the distance between adjacent bright fringes. Ans: 562 nm and 9 cm

2. A light source emits visible light of two wavelengths: $\lambda = 430 \text{ nm}$ and $\lambda' = 510 \text{ nm}$. The source is used in a double-slit interference experiment in which $L = 1.50 \text{ m}$ and $d = 0.025 \text{ mm}$. Find the separation distance between the third-order bright fringes for the two wavelengths. Ans: 1.44 cm
3. A laser beam ($\lambda = 632.8 \text{ nm}$) is incident on two slits 0.200 mm apart. How far apart are the bright interference fringes on a screen 5.00 m away from the double slits? Ans: 15.8 mm
4. A Young's interference experiment is performed with monochromatic light. The separation between the slits is 0.500 mm, and the interference pattern on a screen 3.30 m away shows the first side maximum 3.40 mm from the center of the pattern. What is the wavelength? Ans: 515 nm
5. Young's double-slit experiment is performed with 589-nm light and a distance of 2.00 m between the slits and the screen. The tenth interference minimum is observed 7.26 mm from the central maximum. Determine the spacing of the slits. Ans: 1.54 mm
6. Two radio antennas separated by $d = 300 \text{ m}$ as shown in figure simultaneously broadcast identical signals at the same wavelength. A car travels due north along a straight line at position $x = 1000 \text{ m}$ from the center point between the antennas, and its radio receives the signals. (a) If the car is at the position of the second maximum after that at point O when it has traveled a distance $y = 400 \text{ m}$ northward, what is the wavelength of the signals? (b) How much farther must the car travel from this position to encounter the next minimum in reception? Note: Do not use the small-angle approximation in this problem. Ans: 55.7 m and 124 m



7. Two narrow parallel slits separated by 0.250 mm are illuminated by green light ($\lambda = 546.1 \text{ nm}$). The interference pattern is observed on a screen 1.20 m away from the plane of the slits. Calculate the distance (a) from the central maximum to the first bright region on either side of the central maximum and (b) between the first and second dark bands. Ans: 2.62 mm and 2.62 mm

8. In a Young's interference experiment, the two slits are separated by 0.150 mm and the incident light includes two wavelengths: $\lambda_1 = 540$ nm (green) and $\lambda_2 = 450$ nm (blue). The overlapping interference patterns are observed on a screen 1.40 m from the slits. Calculate the minimum distance from the center of the screen to a point where a bright fringe of the green light coincides with a bright fringe of the blue light. Ans: 2.52 cm
9. In a double slit experiment, let $L = 120$ cm and $d = 0.250$ cm. The slits are illuminated with coherent 600-nm light. Calculate the distance y above the central maximum for which the average intensity on the screen is 75.0% of the maximum. Ans: 48 micrometer
10. Show that the two waves with wave functions $E_1 = 6.00 \sin(100\pi t)$ and $E_2 = 8.00 \sin(100\pi t + \pi/2)$ add to give a wave with the wave function $E_R \sin(100\pi t + \phi)$. Find the required values for E_R and ϕ . Ans: 10 and 53.1°
11. Calculate the minimum thickness of a soap-bubble film that results in constructive interference in the reflected light if the film is illuminated with light whose wavelength in free space is $\lambda = 600$ nm. The index of refraction of the soap film is 1.33. (b) What if the film is twice as thick? Does this situation produce constructive interference? Ans: 113 nm and No
12. Solar cells—devices that generate electricity when exposed to sunlight—are often coated with a transparent, thin film of silicon monoxide (SiO , $n = 1.45$) to minimize reflective losses from the surface. Suppose a silicon solar cell ($n = 3.5$) is coated with a thin film of silicon monoxide for this purpose. Determine the minimum film thickness that produces the least reflection at a wavelength of 550 nm, near the center of the visible spectrum. Ans: 95 nm
13. A thin film of oil ($n = 1.25$) is located on smooth, wet pavement. When viewed perpendicular to the pavement, the film reflects most strongly red light at 640 nm and reflects no green light at 512 nm. How thick is the oil film? Ans: 512 nm.
14. An oil film ($n = 1.45$) floating on water is illuminated by white light at normal incidence. The film is 280 nm thick. Find (a) the wavelength and color of the light in the visible spectrum most strongly reflected and (b) the wavelength and color of the light in the spectrum most strongly transmitted. Explain your reasoning. Ans: 541 nm and 406 nm
15. An air wedge is formed between two glass plates separated at one edge by a very fine wire of circular cross section as shown in Figure 12. When the wedge is illuminated from above by 600-nm light and viewed from above, 30 dark fringes are observed. Calculate the diameter d of the wire. Ans: 8.7 micrometer



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16. When a liquid is introduced into the air space between the lens and the plate in a Newton's-rings apparatus, the diameter of the tenth ring changes from 1.50 to 1.31 cm. Find the index of refraction of the liquid. Ans: 1.31
17. A certain grade of crude oil has an index of refraction of 1.25. A ship accidentally spills 1.00 m³ of this oil into the ocean, and the oil spreads into a thin, uniform slick. If the film produces a first-order maximum of light of wavelength 500 nm normally incident on it, how much surface area of the ocean does the oil slick cover? Assume the index of refraction of the ocean water is 1.34. Ans: 5 km²
- 18.** In a Newton's-rings experiment, a plano-convex glass ($n = 1.52$) lens having radius $r = 5.00$ cm is placed on a flat plate as shown in Figure 1.8a. When light of wavelength 650 nm is incident normally, 55 bright rings are observed, with the last one precisely on the edge of the lens. (a) What is the radius R of curvature of the convex surface of the lens? (b) What is the focal length of the lens? Ans: 70.5 m and 138 m
19. Monochromatic light is beamed into a Michelson interferometer. The movable mirror is displaced 0.382 mm, causing the interferometer pattern to reproduce itself 1700 times. Determine the wavelength of the light. What color is it? Ans: 449 nm, Blue
- 20.** Mirror M_1 in Figure 1.9 is moved through a displacement ΔL . During this displacement, 250 fringe reversals (formation of successive dark or bright bands) are counted. The light being used has a wavelength of 632.8 nm. Calculate the displacement ΔL . Ans: 39.6 micrometer
21. One leg of a Michelson interferometer contains an evacuated cylinder of length L , having glass plates on each end. A gas is slowly leaked into the cylinder until a pressure of 1 atm is reached. If N bright fringes pass on the screen during this process when light of wavelength λ is used, what is the index of refraction of the gas? Ans: $n = 1 + (N\lambda)/(2L)$

2 DIFFRACTION PATTERNS AND POLARIZATION

OBJECTIVES

- To understand the principles of diffraction.
- To explain the intensity distribution in diffraction under various conditions.
- To explain the diffraction of light waves at single, multiple slits and circular apertures.
- To understand polarization phenomena and various techniques used to produce polarized light.

2.1 INTRODUCTION TO DIFFRACTION PATTERNS

Light of wavelength comparable to or larger than the width of a slit spreads out in all forward directions upon passing through the slit. This phenomenon is called *diffraction*. When light passes through a narrow slit, it spreads beyond the narrow path defined by the slit into regions that would be in shadow if light traveled in straight lines. Other waves, such as sound waves and water waves, also have this property of spreading when passing through apertures or by sharp edges.

A **diffraction pattern** consisting of light and dark areas is observed when a narrow slit is placed between a distant light source (or a laser beam) and a screen, the light produces a diffraction pattern like that shown in Figure 2.1 (a). The pattern consists of a broad, intense central band (called the **central maximum**) flanked by a series of narrower, less intense additional bands (called **side maxima** or **secondary maxima**) and a series of intervening dark bands (or **minima**).

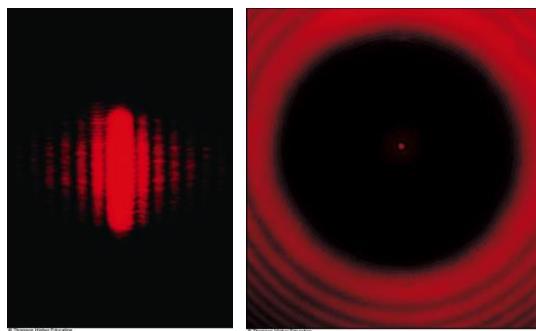


Figure 2.1 (a) The diffraction pattern that appears on a screen when light passes through a narrow vertical slit. (b) Diffraction pattern created by the illumination of a penny, with the penny positioned midway between the screen and light source.

Figure 2.1 (b) shows a diffraction pattern associated with the shadow of a penny. A bright spot occurs at the center, and circular fringes extend outward from the shadow's edge. From the viewpoint of ray optics (in which light is viewed as rays traveling in straight lines), we expect the center of the shadow to be dark because that part of the viewing screen is completely shielded by the penny. We can explain the central bright spot by using the wave theory of light, which predicts constructive interference at this point.

2.2 DIFFRACTION PATTERNS FROM NARROW SLITS

Let's consider light passing through a narrow opening modeled as a slit and projected onto a screen. To simplify our analysis, we assume the observing screen is far from the slit and the rays reaching the screen are approximately parallel. In laboratory, this situation can also be achieved experimentally by using a converging lens to focus the parallel rays on a nearby screen. In this model, the pattern on the screen is called a **Fraunhofer diffraction pattern**.

Until now, we have assumed slits are point sources of light. In this section, we abandon that assumption and see how the finite width of slits is the basis for understanding Fraunhofer diffraction. We can explain some important features of this phenomenon by examining waves coming from various portions of the slit as shown in Figure 2.2.

According to Huygens's principle, each portion of the slit acts as a source of light waves. Hence, light from one portion of the slit can interfere with light from another portion, and the resultant light intensity on a viewing screen depends on the direction θ . Based on this analysis, we recognize that a diffraction pattern is an interference pattern in which the different sources of light are different portions of the single slit.

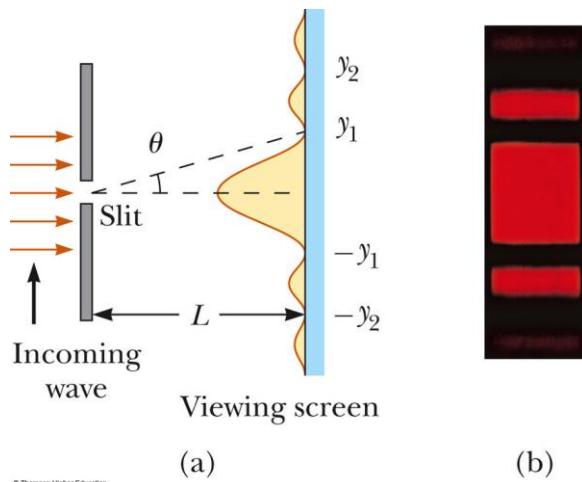


Figure 2.2(a) Geometry for analyzing the Fraunhofer diffraction pattern of a single slit. (b) Photograph of a single-slit Fraunhofer diffraction pattern.

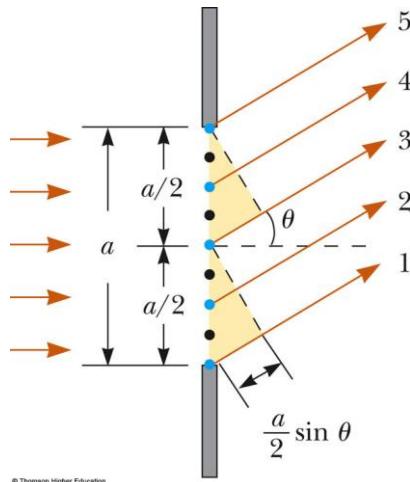


Figure 2.3 Paths of light rays that encounter a narrow slit of width a and diffract toward a screen in the direction described by angle θ .

To analyze the diffraction pattern, let's divide the slit into two halves as shown in Figure 2.3. Keeping in mind that all the waves are in phase as they leave the slit, consider rays 1 and 3. As these two rays travel toward a viewing screen far to the right of the figure, ray 1 travels farther than ray 3 by an amount equal to the path difference $(a/2) \sin \theta$, where a is the width of the slit. Similarly, the path difference between rays 2 and 4 is also $(a/2) \sin \theta$, as is that between rays 3 and 5. If this path difference is exactly half a wavelength (corresponding to a phase difference of 180°), the pairs of waves cancel each other and destructive interference results.

This cancellation occurs for any two rays that originate at points separated by half the slit width because the phase difference between two such points is 180° . Therefore, waves from the upper half of the slit interfere destructively with waves from the lower half when

$$\frac{a}{2} \sin \theta = \pm \frac{\lambda}{2}$$

Dividing the slit into four equal parts and using similar reasoning, we find that the viewing screen is also dark when

$$\sin \theta = \pm 2 \frac{\lambda}{a}$$

Likewise, dividing the slit into six equal parts shows that darkness occurs on the screen when

$$\sin \theta = \pm 3 \frac{\lambda}{a}$$

Therefore, the general condition for destructive interference is

$$\sin \theta_{\text{dark}} = m \frac{\lambda}{a} \quad m = \pm 1, \pm 2, \pm 3, \dots \quad (2.1)$$

2.3 INTENSITY OF SINGLE-SLIT DIFFRACTION PATTERNS

Analysis of the intensity variation in a diffraction pattern from a single slit of width ‘ a ’ shows that the intensity is given by

$$I = I_{\max} \left[\frac{\sin (\pi a \sin \theta / \lambda)}{\pi a \sin \theta / \lambda} \right]^2 \quad (2.2)$$

where I_{\max} is the intensity at $\theta = 0$ (the central maximum) and λ is the wavelength of light used to illuminate the slit. Intensity variation plot and photograph of the pattern are shown below.

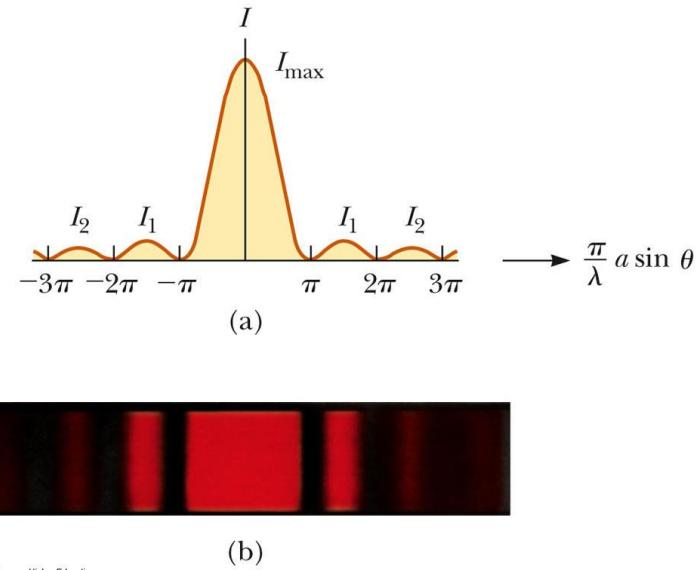


Figure 2.4 A plot of light intensity I versus $(\pi/\lambda)a \sin \theta$ for the single-slit Fraunhofer diffraction pattern. (b) Photograph of a single slit Fraunhofer diffraction pattern.

2.4 INTENSITY OF TWO-SLIT DIFFRACTION PATTERNS

When more than one slit is present, we must consider not only diffraction patterns due to the individual slits but also the interference patterns due to the waves coming from different slits. Intensity due to combined effect is given by

$$I = I_{\max} \cos^2 \left(\frac{\pi d \sin \theta}{\lambda} \right) \left[\frac{\sin (\pi a \sin \theta / \lambda)}{\pi a \sin \theta / \lambda} \right]^2 \quad (2.3)$$

Above equation represents the single-slit diffraction pattern (the factor in square brackets) acting as an “envelope” for a two slit interference pattern (the cosine-squared factor).

We have seen that angular position of interference maxima is given by $d \sin \theta = m\lambda$, where d is the distance between the two slits. Also, the first diffraction minimum occurs when $a \sin \theta = \lambda$, where a is the slit width. Dividing interference equation by diffraction equation,

$$\frac{d}{a} = m$$

In this case, m^{th} interference maximum coincides with first diffraction minimum.

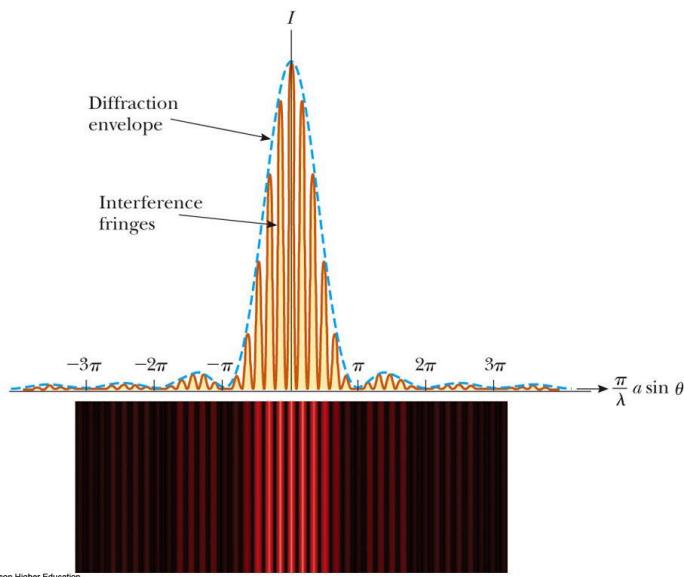


Figure 2.5 The combined effects of two-slit and single-slit interference.

2.5 RESOLUTION OF SINGLE-SLIT AND CIRCULAR APERTURES

The ability of optical systems to distinguish between closely spaced objects is limited because of the wave nature of light. To understand this limitation, consider Figure 2.6, which shows two light sources far from a narrow slit of width a . The sources can be two noncoherent point sources S_1 and S_2 ; for example, they could be two distant stars. If no interference occurred between light passing through different parts of the slit, two distinct bright spots (or images) would be observed on the viewing screen. Because of such interference, however, each source is imaged as a bright central region flanked by weaker bright and dark fringes, a diffraction pattern. What is observed on the screen is the sum of two diffraction patterns: one from S_1 and the other from S_2 .

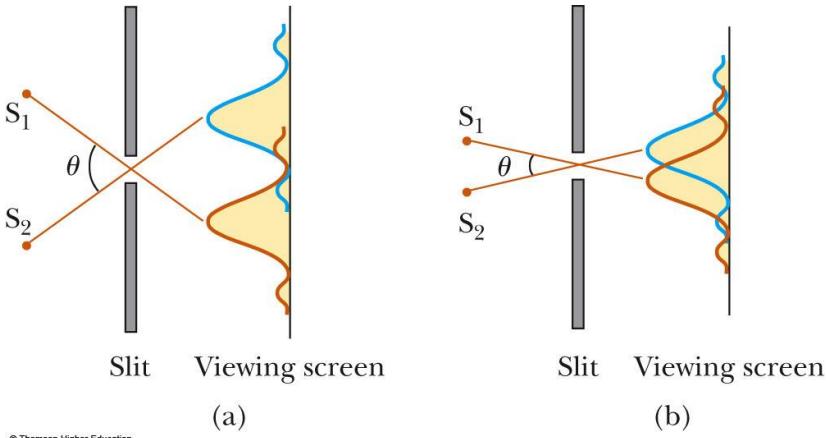


Figure 2.6 Two-point sources far from a narrow slit each produce a diffraction pattern. (a) The sources are separated by a large angle. (b) The sources are separated by a small angle.

When the central maximum of one image falls on the first minimum of another image, the images are said to be just resolved. This limiting condition of resolution is known as **Rayleigh's criterion**.

From Rayleigh's criterion, we can determine the minimum angular separation θ_{min} subtended by the sources at the slit in Figure 2.6 for which the images are just resolved. Equation 2.1 indicates that the first minimum ($m = 1$) in a single-slit diffraction pattern occurs at the angle for which

$$\sin \theta = \frac{\lambda}{a} \quad (2.4)$$

where a is the width of the slit. According to Rayleigh's criterion, this expression gives the smallest angular separation for which the two images are resolved. Because $\lambda \ll a$ in most situations, $\sin \theta$ is small and we can use the approximation $\sin \theta \approx \theta$. Therefore, the limiting angle of resolution for a slit of width a is

$$\theta_{min} = \frac{\lambda}{a} \quad (2.5)$$

where θ_{min} is expressed in radians. Hence, the angle subtended by the two sources at the slit must be greater than λ/a if the images are to be resolved.

Many optical systems use circular apertures rather than slits. The diffraction pattern of a circular aperture as shown in the photographs of Figure 2.7 consists of a central circular bright disk surrounded by progressively fainter bright and dark rings. Figure 2.7 shows diffraction patterns for three situations in which light from two point sources passes through a circular aperture. When the sources are far apart, their images are well resolved (Fig. 2.7a). When the angular separation of the sources satisfies Rayleigh's criterion, the images are just resolved (Fig. 2.7b). Finally, when the sources are close together, the images are said to be unresolved (Fig. 2.7c) and the pattern looks like that of a single source. Analysis shows that the limiting angle of resolution of the circular aperture is

$$\theta_{min} = 1.22 \frac{\lambda}{D} \quad (2.6)$$

where D is the diameter of the aperture. This expression is similar to Equation 2.4 except for the factor 1.22, which arises from a mathematical analysis of diffraction from the circular aperture.

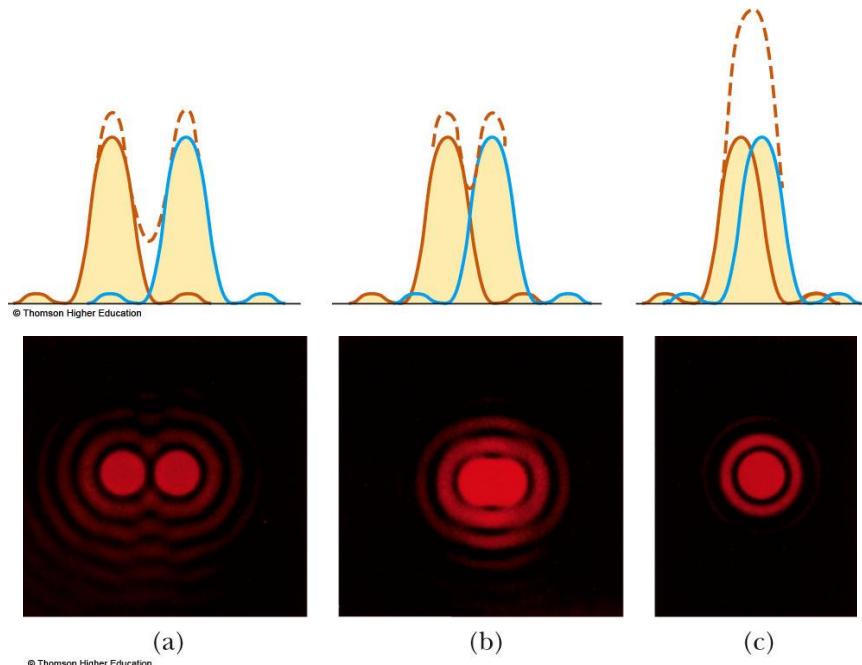


Figure 2.7 Individual diffraction patterns of two-point sources (solid curves) and the resultant patterns (dashed curves) for various angular separations of the sources as the light passes through a circular aperture. In each case, the dashed curve is the sum of the two solid curves.

2.6 DIFFRACTION GRATING

The **diffraction grating**, a useful device for analyzing light sources, consists of many equally spaced parallel slits. A *transmission grating* can be made by cutting parallel grooves on a glass plate with a precision ruling machine. The spaces between the grooves are transparent to the light and hence act as separate slits. A *reflection grating* can be made by cutting parallel grooves on the surface of a reflective material. The reflection of light from the spaces between the grooves is specular, and the reflection from the grooves cut into the material is diffuse. Therefore, the spaces between the grooves act as parallel sources of reflected light like the slits in a transmission grating.

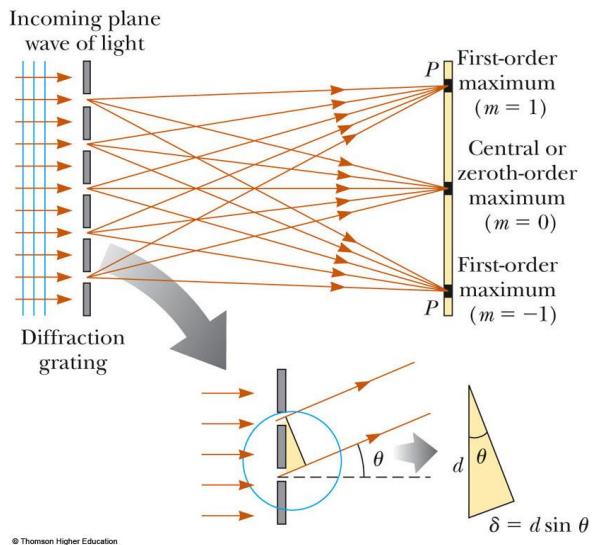


Figure 2.8 Side view of a diffraction grating. The slit separation is d , and the path difference between adjacent slits is $d \sin \theta$.

A plane wave is incident from the left, normal to the plane of the grating. The pattern observed on the screen far to the right of the grating is the result of the combined effects of interference and diffraction. Each slit produces diffraction, and the diffracted beams interfere with one another to produce the final pattern. The waves from all slits are in phase as they leave the slits. For an arbitrary direction θ measured from the horizontal, however, the waves must travel different path lengths before reaching the screen. Notice in Figure 2.8 that the path difference δ between rays from any two adjacent slits is equal to $d \sin \theta$. If this path difference equals one wavelength or any integral multiple of a wavelength, waves from all slits are in phase at the screen and a bright fringe is observed. Therefore, the condition for *maxima* in the interference pattern at the angle θ_{bright} is

$$d \sin \theta_{bright} = m\lambda \quad m = 0, \pm 1, \pm 2, \pm 3, \dots \quad (2.7)$$

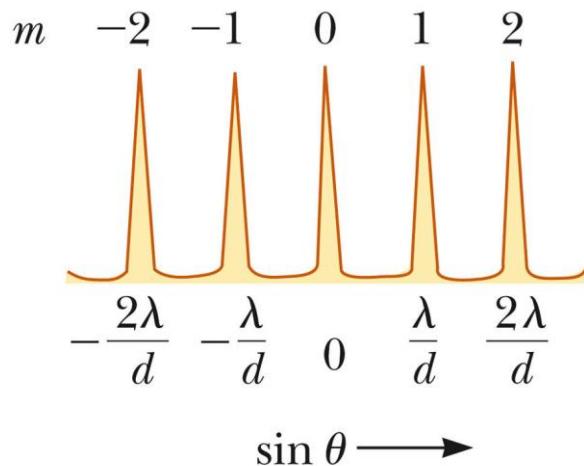


Figure 2.9 Intensity versus $\sin \theta$ for a diffraction grating. The zeroth-, first-, and second-order maxima are shown.

The intensity distribution for a diffraction grating obtained with the use of a monochromatic source is shown in Figure 2.9. Notice the sharpness of the principal maxima and the broadness of the dark areas compared with the broad bright fringes characteristic of the two-slit interference pattern.

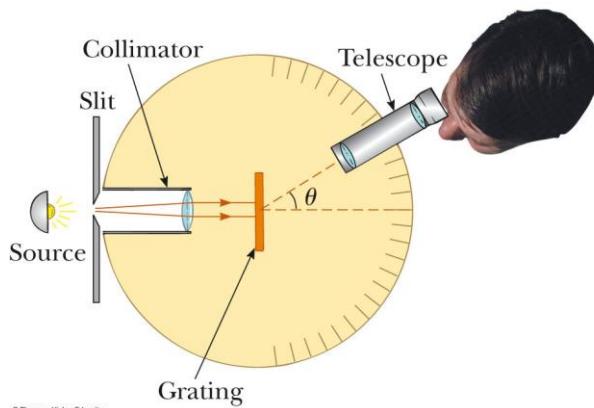


Figure 2.10 Diagram of a diffraction grating spectrometer.

A schematic drawing of a simple apparatus used to measure angles in a diffraction pattern is shown in Figure 2.10. This apparatus is a *diffraction grating spectrometer*. The light to be analyzed passes through a slit, and a collimated beam of light is incident on the grating. The diffracted light leaves the grating at angles that satisfy Equation 2.7, and a telescope is used to view the image of the slit. The wavelength can be determined by measuring the precise angles at which the images of the slit appear for the various orders. The spectrometer is a useful tool in *atomic spectroscopy*, in which the light from an atom is analyzed to find the wavelength components. These wavelength components can be used to identify the atom.

2.7 DIFFRACTION OF X-RAYS BY CRYSTALS

In principle, the wavelength of any electromagnetic wave can be determined if a grating of the proper spacing (on the order of λ) is available. X-rays, discovered by Wilhelm Roentgen (1845–1923) in 1895, are electromagnetic waves of very short wavelength (on the order of 0.1 nm). It would be impossible to construct a grating having such a small spacing by the cutting process. The atomic spacing in a solid is known to be about 0.1 nm, however. In 1913, Max von Laue (1879–1960) suggested that the regular array of atoms in a crystal could act as a three-dimensional diffraction grating for x-rays. Subsequent experiments confirmed this prediction. The diffraction patterns from crystals are complex because of the three-dimensional nature of the crystal structure. Nevertheless, x-ray diffraction has proved to be an invaluable technique for elucidating these structures and for understanding the structure of matter.

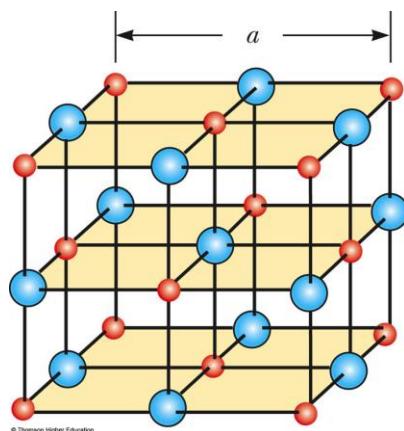


Figure 2.11 Crystalline structure of sodium chloride (NaCl).

The arrangement of atoms in a crystal of sodium chloride (NaCl) is shown in Figure 2.11. Each unit cell (the geometric solid that repeats throughout the crystal) is a cube having an edge length a . A careful examination of the NaCl structure shows that the ions lie in discrete planes (the shaded areas in Fig. 2.11). Now suppose an incident x-ray beam makes an angle θ with one of the planes as in Figure 2.12. The beam can be reflected from both the upper plane and the lower one, but the beam reflected from the lower plane travels farther than the beam reflected from the upper plane. The effective path difference is $2ds\sin\theta$. The two beams reinforce each other (constructive interference) when this path difference equals some integer multiple of λ . The same is true for reflection from the entire family of parallel planes. Hence, the condition for *constructive interference* (maxima in the reflected beam) is

$$2d \sin \theta = m\lambda \quad m = 1, 2, 3, \dots \quad (2.8)$$

This condition is known as **Bragg's law**, after W. L. Bragg, who first derived the relationship. If the wavelength and diffraction angle are measured, Equation 2.8 can be used to calculate the spacing between atomic planes.

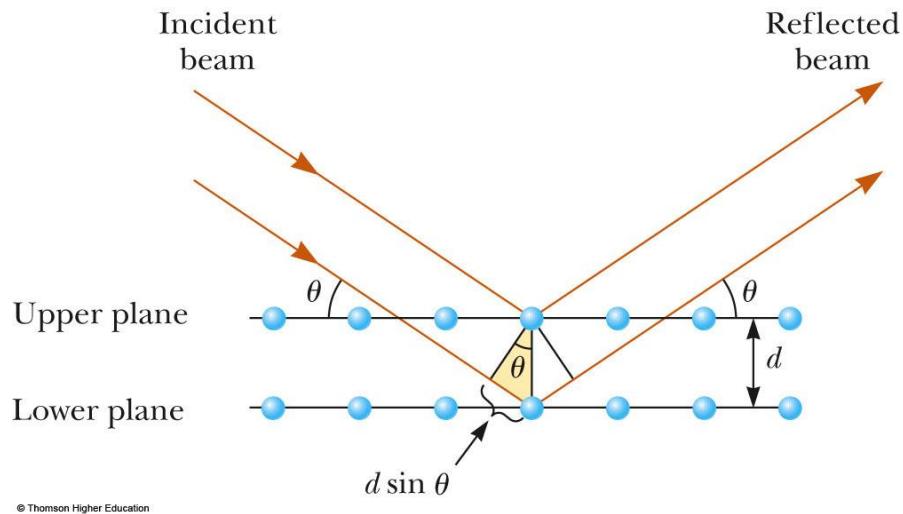


Figure 2.12 A two-dimensional description of the reflection of an x-ray beam from two parallel crystalline planes separated by a distance d .

2.8 POLARIZATION OF LIGHT WAVES

An ordinary beam of light consists of many waves emitted by the atoms of the light source. Each atom produces a wave having some orientation of the electric field vector \vec{E} , corresponding to the direction of atomic vibration. The *direction of polarization* of each individual wave is defined to be the direction in which the electric field is vibrating. In Figure 2.13, this direction happens to lie along the y axis. All individual electromagnetic waves traveling in the x direction have an \vec{E} vector parallel to the yz plane, but this vector could be at any possible angle with respect to the y axis. Because all directions of vibration from a wave source are possible, the resultant electromagnetic wave is a superposition of waves vibrating in many different directions. The result is an **unpolarized** light beam, represented in Figure 2.14a. The direction of wave propagation in this figure is perpendicular to the page. The arrows show a few possible directions of the electric field vectors for the individual waves making up the resultant beam. At any given point and at some instant of time, all these individual electric field vectors add to give one resultant electric field vector.

A wave is said to be **linearly polarized** if the resultant electric field \vec{E} vibrates in the same direction *at all times* at a particular point as shown in Figure 2.14b. (Sometimes, such a wave is described as *plane-polarized*, or simply *polarized*.) The plane formed by \vec{E} and the direction of propagation is called the *plane of polarization* of the wave. If the wave in Figure 2.14b represents the resultant of all individual waves, the plane of polarization is the xy plane. A linearly polarized beam can be obtained from an unpolarized beam by removing all waves from the beam except those whose electric field vectors oscillate in a single plane.

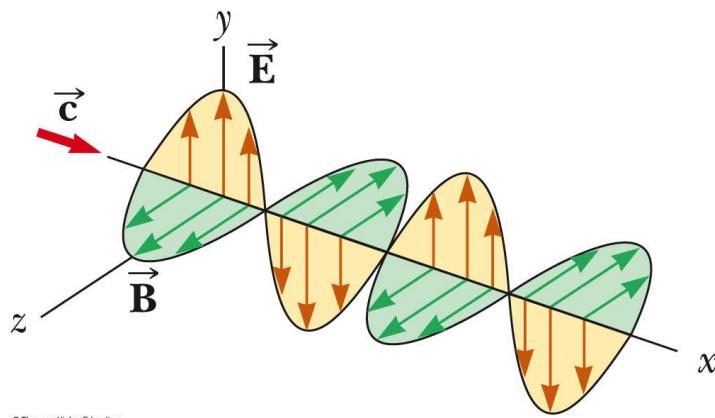


Figure 2.13 Schematic diagram of an electromagnetic wave propagating at velocity c in the x direction. The electric field vibrates in the xy plane, and the magnetic field vibrates in the xz plane.

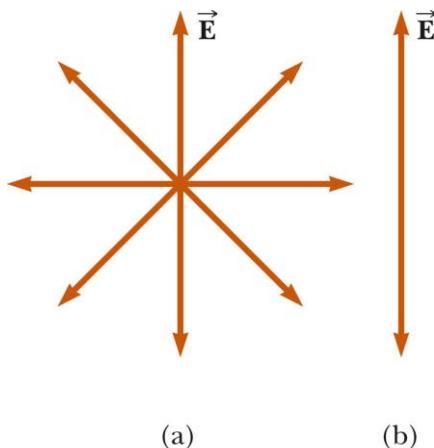


Figure 2.14 (a) A representation of an unpolarized light beam viewed along the direction of propagation. The transverse electric field can vibrate in any direction in the plane of the page with equal probability. (b) A linearly polarized light beam with the electric field vibrating in the vertical direction.

2.9 POLARIZATION BY SELECTIVE ABSORPTION

The most common technique for producing polarized light is to use a material that transmits waves whose electric fields vibrate in a plane parallel to a certain direction and that absorbs waves whose electric fields vibrate in all other directions. *Polaroid*, that polarizes light through selective absorption. This material is fabricated in thin sheets of long-chain hydrocarbons. The sheets are stretched during manufacture so that the long-chain molecules align. After a sheet is dipped into a solution containing iodine, the molecules become good electrical conductors. Conduction takes place primarily along the hydrocarbon chains because electrons can move easily only along the chains.

If light whose electric field vector is parallel to the chains is incident on the material, the electric field accelerates electrons along the chains and energy is absorbed from

the radiation. Therefore, the light does not pass through the material. Light whose electric field vector is perpendicular to the chains passes through the material because electrons cannot move from one molecule to the next. As a result, when unpolarized light is incident on the material, the exiting light is polarized perpendicular to the molecular chains. It is common to refer to the direction perpendicular to the molecular chains as the *transmission axis*. In an ideal polarizer, all light with \vec{E} parallel to the transmission axis is transmitted and all light with \vec{E} perpendicular to the transmission axis is absorbed.

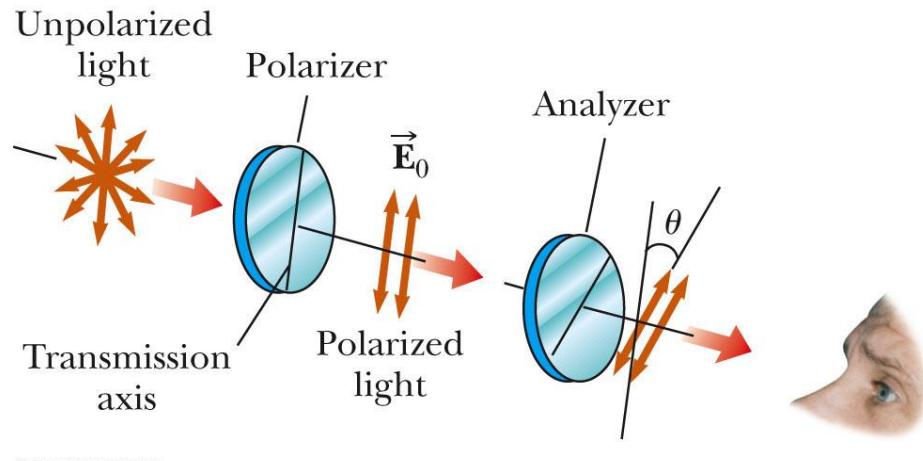


Figure 2.15 Two polarizing sheets whose transmission axes make an angle θ with each other. Only a fraction of the polarized light incident on the analyzer is transmitted through it.

Figure 2.15 represents an unpolarized light beam incident on a first polarizing sheet, called the *polarizer*. Because the transmission axis is oriented vertically in the figure, the light transmitted through this sheet is polarized vertically. A second polarizing sheet, called the *analyzer*, intercepts the beam. In figure, the analyzer transmission axis is set at an angle θ to the polarizer axis. We call the electric field vector of the first transmitted beam \vec{E}_0 . The component of \vec{E}_0 perpendicular to the analyzer axis is completely absorbed. The component of \vec{E}_0 parallel to the analyzer axis, which is transmitted through the analyzer, is $E_0 \cos \theta$. Because the intensity of the transmitted beam varies as the square of its magnitude, we conclude that the intensity I of the (polarized) beam transmitted through the analyzer varies as

$$I = I_{\max} \cos^2 \theta \quad (2.9)$$

where I_{\max} is the intensity of the polarized beam incident on the analyzer. This expression, known as **Malus's law**.

2.10 POLARIZATION BY REFLECTION

When an unpolarized light beam is reflected from a surface, the polarization of the reflected light depends on the angle of incidence. If the angle of incidence is 0° , the

reflected beam is unpolarized. For other angles of incidence, the reflected light is polarized to some extent, and for a particular angle of incidence, the reflected light is completely polarized.

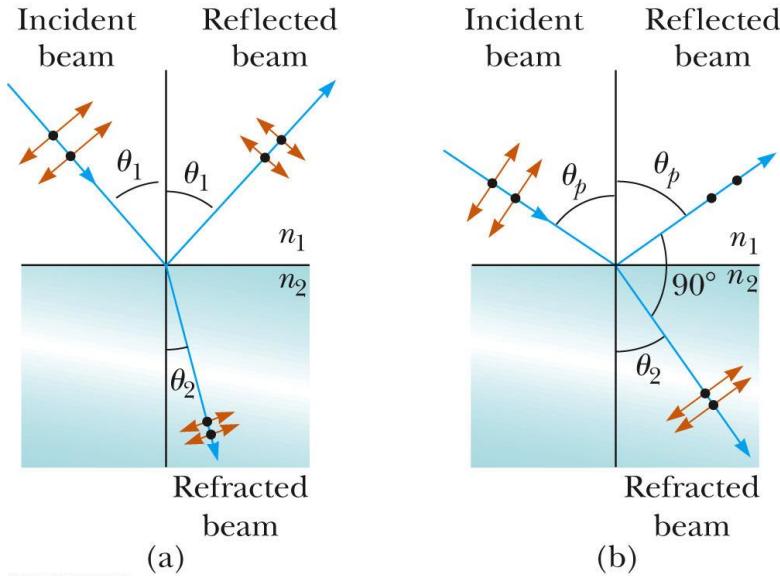


Figure 2.16 (a) When unpolarized light is incident on a reflecting surface, the reflected and refracted beams are partially polarized. (b) The reflected beam is completely polarized when the angle of incidence equals the polarizing angle θ_p , which satisfies the equation $n_2/n_1 = \tan \theta_p$. At this incident angle, the reflected and refracted rays are perpendicular to each other.

Now suppose the angle of incidence θ_i is varied until the angle between the reflected and refracted beams is 90° as in Figure 2.16b. At this angle of incidence, the reflected beam is completely polarized (with its electric field vector parallel to the surface) and the refracted beam is still only partially polarized. The angle of incidence at which this polarization occurs is called the **polarizing angle** θ_p . Using Snell's law of refraction

$$\frac{n_2}{n_1} = \frac{\sin \theta_p}{\sin \theta_2} \quad 2.10$$

But, $\theta_2 = 90 - \theta_p$. So, we can write,

$$\tan \theta_p = \frac{n_2}{n_1} \quad 2.11$$

This expression is called **Brewster's law**, and the polarizing angle θ_p is sometimes called **Brewster's angle**, after its discoverer, David Brewster. Because n varies with wavelength for a given substance, Brewster's angle is also a function of wavelength.

2.11 POLARIZATION BY DOUBLE REFRACTION

In certain class of crystals like calcite and quartz, the speed of light depends on the direction of propagation and on the plane of polarization of the light. Such materials are characterized by two indices of refraction. Hence, they are often referred to as double-refracting or birefringent materials. When unpolarized light enters a birefringent material, it may split into an **ordinary (O) ray** and an **extraordinary (E) ray**. These two rays have mutually perpendicular polarizations and travel at different speeds through the material. There is one direction, called the **optic axis**, along which the ordinary and extraordinary rays have the same speed.

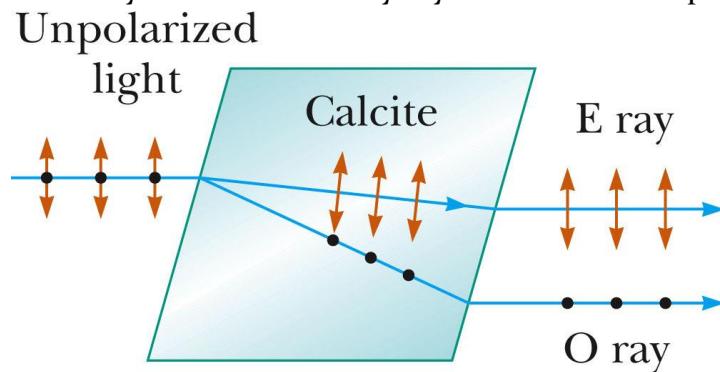


Figure 2.17 Unpolarized light incident at an angle to the optic axis in a calcite crystal splits into an ordinary (O) ray and an extraordinary (E) ray

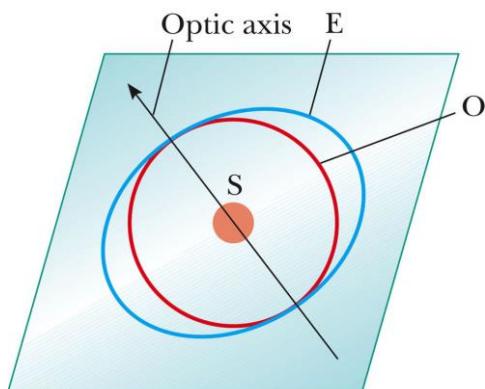


Figure 2.18 Point source S inside a double-refracting crystal (calcite) produces a spherical wave front corresponding to the ordinary (O) ray and an elliptical wave front corresponding to the extraordinary (E) ray.

Some materials such as glass and plastic become birefringent when stressed. Suppose an unstressed piece of plastic is placed between a polarizer and an analyzer so that light passes from polarizer to plastic to analyzer. When the plastic is unstressed, and the analyzer axis is perpendicular to the polarizer axis, none of the polarized light passes through the analyzer. In other words, the unstressed plastic has no effect on the light passing through it. If the plastic is stressed, however,

regions of greatest stress become birefringent and the polarization of the light passing through the plastic changes. Hence, a series of bright and dark bands is observed in the transmitted light, with the bright bands corresponding to regions of greatest stress. Engineers often use this technique, called optical stress analysis, in designing structures ranging from bridges to small tools. They build a plastic model and analyze it under different load conditions to determine regions of potential weakness and failure under stress.

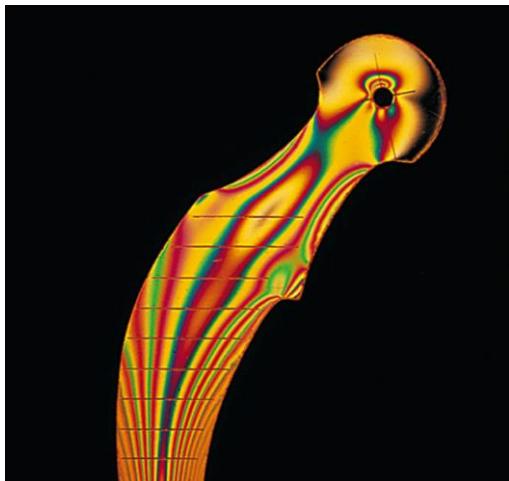


Figure 2.19 The pattern is produced when the plastic model is viewed between a polarizer and analyzer oriented perpendicular to each other. Such patterns are useful in the optimal design of architectural components

2.12 POLARIZATION BY SCATTERING

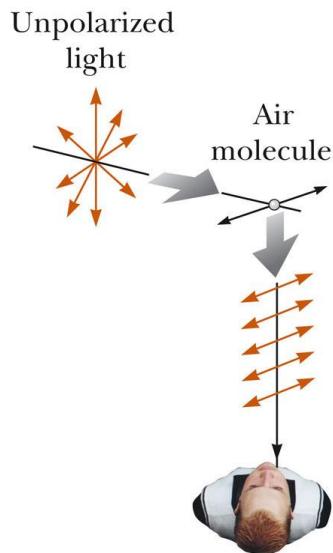


Figure 2.20 The scattering of unpolarized sunlight by air molecules.

When light is incident on any material, the electrons in the material can absorb and reradiate part of the light. Such absorption and reradiation of light by electrons in the gas molecules that make up air is what causes sunlight reaching an observer on the Earth to be partially polarized. An unpolarized beam of sunlight traveling in the horizontal direction (parallel to the ground) strikes a molecule of one of the gases that make up air, setting the electrons of the molecule into vibration. These vibrating charges act like the vibrating charges in an antenna. The horizontal component of the electric field vector in the incident wave results in a horizontal component of the vibration of the charges, and the vertical component of the vector results in a vertical component of vibration. If the observer in Figure 2.20 is looking straight up (perpendicular to the original direction of propagation of the light), the vertical oscillations of the charges send no radiation toward the observer. Therefore, the observer sees light that is completely polarized in the horizontal direction as indicated by the orange arrows. If the observer looks in other directions, the light is partially polarized in the horizontal direction.

2.13 OPTICAL ACTIVITY

Many important applications of polarized light involve materials that display optical activity. A material is said to be optically active if it rotates the plane of polarization of any light transmitted through the material. The angle through which the light is rotated by a specific material depends on the length of the path through the material and on concentration if the material is in solution. One optically active material is a solution of the common sugar dextrose. A standard method for determining the concentration of sugar solutions is to measure the rotation produced by a fixed length of the solution.

2.14 QUESTIONS

1. Explain the term diffraction of light.
2. Discuss qualitatively, the Fraunhofer diffraction at a single-slit.
3. Draw a schematic plot of the intensity of light in single slit diffraction against phase difference.
4. Explain briefly diffraction at a circular aperture.
5. State and explain Rayleigh's criterion for optical resolution.
6. Effect of diffraction is ignored in the case of Young's double slit interference. Give reason.
7. Discuss qualitatively, the diffraction due to multiple slits.
8. What is diffraction grating? Write the grating equation.
9. Briefly explain x-ray diffraction and Bragg's law.
10. Distinguish between unpolarized and linearly polarized light.
11. Explain Malus's law.
12. How to produce linearly polarized light by (a) selective absorption, (b) reflection, (c) double refraction, (d) scattering ? Explain.

2.15 PROBLEMS

1. Light of wavelength 540 nm passes through a slit of width 0.200 mm. (a) The width of the central maximum on a screen is 8.10 mm. How far is the screen from the slit? (b) Determine the width of the first bright fringe to the side of the central maximum. Ans: (a) 1.5 m (b) 4.05 mm
2. Helium-neon laser light ($\lambda = 632.8$ nm) is sent through a 0.300-mm-wide single slit. What is the width of the central maximum on a screen 1.00 m from the slit? Ans: 4.22 mm
3. A screen is placed 50.0 cm from a single slit, which is illuminated with light of wavelength 690 nm. If the distance between the first and third minima in the diffraction pattern is 3.00 mm, what is the width of the slit?
Ans: 2.3×10^{-4} m
4. A beam of monochromatic light is incident on a single slit of width 0.600 mm. A diffraction pattern forms on a wall 1.30 m beyond the slit. The distance between the positions of zero intensity on both sides of the central maximum is 2.00 mm. Calculate the wavelength of the light. Ans: 462 nm
5. A diffraction pattern is formed on a screen 120 cm away from a 0.400-mm-wide slit. Monochromatic 546.1-nm light is used. Calculate the fractional intensity I/I_{\max} at a point on the screen 4.10 mm from the center of the principal maximum. Ans: 0.0162
6. Yellow light of wavelength 589 nm is used to view an object under a microscope. The objective lens diameter is 9.00 mm. (a) What is the limiting angle of resolution? (b) Suppose it is possible to use visible light of any wavelength. What color should you choose to give the smallest possible angle of resolution, and what is this angle? (c) Suppose water fills the space between the object and the objective. What effect does this change have on the resolving power when 589-nm light is used? Ans: (a) 79.8×10^{-6} rad (b) 400 nm, 54.2×10^{-6} rad (c) Resolving power will improve with minimum resolvable angle 60×10^{-6} rad
7. The angular resolution of a radio telescope is to be 0.100° when the incident waves have a wavelength of 3.00 mm. What minimum diameter is required for the telescope's receiving dish? Ans: 2.1 mm
8. White light is spread out into its spectral components by a diffraction grating. If the grating has 2000 grooves per centimeter, at what angle does red light of wavelength 640 nm appear in first order? Ans: $\theta = 7.35^\circ$
9. Light of wavelength 500 nm is incident normally on a diffraction grating. If the third-order maximum of the diffraction pattern is observed at 32.0° , (a) what is the number of rulings per centimeter for the grating? (b) Determine the total number of primary maxima that can be observed in this situation.
Ans: 3530 rulings/cm (b) 11

10. If the spacing between planes of atoms in a NaCl crystal is 0.281 nm, what is the predicted angle at which 0.140-nm x-rays are diffracted in a first-order maximum? Ans: $\theta = 14.4^\circ$
11. The first-order diffraction maximum is observed at 12.6° for a crystal having a spacing between planes of atoms of 0.250 nm. (a) What wavelength x-ray is used to observe this first-order pattern? (b) How many orders can be observed for this crystal at this wavelength? Ans: (a) 0.109 nm (b) 4
12. Plane-polarized light is incident on a single polarizing disk with the direction of E parallel to the direction of the transmission axis. Through what angle should the disk be rotated so that the intensity in the transmitted beam is reduced by a factor of (a) 3.00, (b) 5.00, and (c) 10.0? Ans: (a) 54.7° (b) 63.4° (c) 71.6°
13. Unpolarized light passes through two ideal Polaroid sheets. The axis of the first is vertical, and the axis of the second is at 30.0° to the vertical. What fraction of the incident light is transmitted? Ans: 0.375
14. The angle of incidence of a light beam onto a reflecting surface is continuously variable. The reflected ray in air is completely polarized when the angle of incidence is 48.0° . What is the index of refraction of the reflecting material? Ans: 1.1
15. The critical angle for total internal reflection for sapphire surrounded by air is 34.4° . Calculate the polarizing angle for sapphire. Ans: 60.5°

3 QUANTUM PHYSICS

OBJECTIVES:

- To learn certain experimental results that can be understood only by particle theory of electromagnetic waves.
- To learn the particle properties of waves and the wave properties of the particles.
- To understand the uncertainty principle.

3.1 BLACKBODY RADIATION AND PLANCK'S HYPOTHESIS

A black body is an object that absorbs all incident radiation. A small hole cut into a cavity is the most popular and realistic example. None of the incident radiation escapes. The radiation is absorbed in the walls of the cavity. This causes a heating of the cavity walls. The oscillators in the cavity walls vibrate and re-radiate at wavelengths corresponding to the temperature of the cavity, thereby producing standing waves. Some of the energy from these standing waves can leave through the opening. The electromagnetic radiation emitted by the black body is called **black-body radiation**.

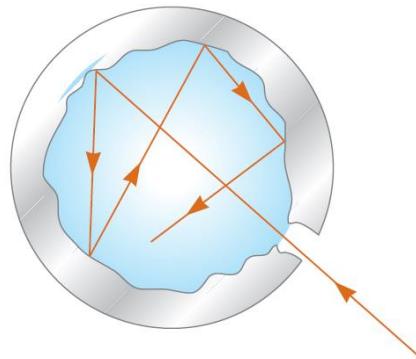


Figure 3.1 A physical model of a blackbody

- The black body is an ideal absorber of incident radiation.
- A black-body reaches thermal equilibrium with the surroundings when the incident radiation power is balanced by the power re-radiated.
- The emitted "thermal" radiation from a black body characterizes the equilibrium temperature of the black-body.

- The nature of radiation from a blackbody does not depend on the material of which the walls are made.

Basic laws of radiation

(1) All objects emit radiant energy.

(2) Hotter objects emit more energy (per unit area) than colder objects. The total power of the emitted radiation is proportional to the fourth power of temperature. This is called **Stefan's Law** and is given by

$$P = \sigma A e T^4 \quad (3.1)$$

where P is power radiated from the surface of the object (W), T is equilibrium surface temperature (K), σ is Stefan-Boltzmann constant ($= 5.670 \times 10^{-8} \text{ W/m}^2\text{K}^4$), A is surface area of

the object (m^2) and e is emissivity of the surface ($e = 1$ for a perfect blackbody).

(3) The peak of the wavelength distribution shifts to shorter wavelengths as the black body temperature increases. This is **Wien's Displacement Law** and is given by

$$\lambda_m T = \text{constant} = 2.898 \times 10^{-3} \text{ m.K}, \text{ or } \lambda_m \propto T^{-1} \quad (3.2)$$

where λ_m is the wavelength corresponding to peak intensity and T is equilibrium temperature of the blackbody.

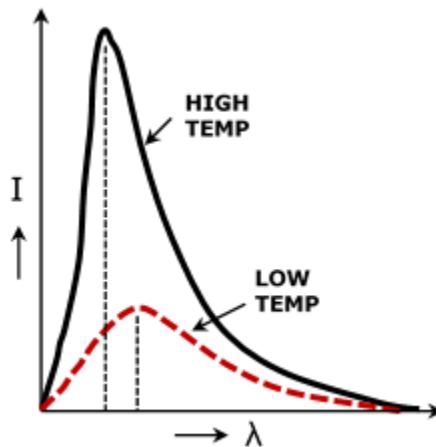


Figure 3.2 Intensity of blackbody radiation versus wavelength at two temperatures

(4) **Rayleigh-Jeans Law:** This law tries to explain the distribution of energy from a black body. The intensity or power per unit area $I(\lambda, T)d\lambda$, emitted in the wavelength interval λ to $\lambda+d\lambda$ from a blackbody is given by

$$I(\lambda, T) = \frac{2\pi c k_B T}{\lambda^4} \quad (3.3)$$

k_B is Boltzmann's constant, c is speed of light in vacuum, T is equilibrium blackbody temperature. It agrees with experimental measurements only for long wavelengths. It predicts an energy output that diverges towards infinity as wavelengths become smaller and is known as the **ultraviolet catastrophe**.

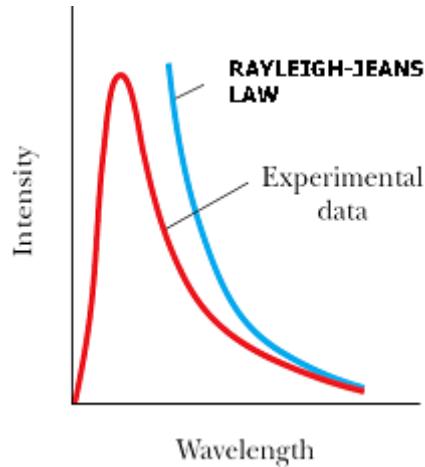


Figure 3.3 Comparison of experimental results and the curve predicted by the Rayleigh-Jeans law for the distribution of blackbody radiation

(5) Planck's Law:

Max Planck developed a theory of blackbody radiation that leads to an equation for $I(\lambda, T)$ that is in complete agreement with experimental results. To derive the law, Planck made two assumptions concerning the nature of the oscillators in the cavity walls:

- (i) The energy of an oscillator is quantized hence it can have only certain discrete values:

$$E_n = n \hbar f \quad (3.4)$$

where n is a positive integer called a **quantum number**, f is the **frequency** of cavity oscillators, and \hbar is a constant called **Planck's constant**. Each discrete energy value corresponds to a different quantum state, represented by the quantum number n .

- (ii) The oscillators emit or absorb energy only when making a transition from one quantum state to another. Difference in energy will be integral multiples of hf .

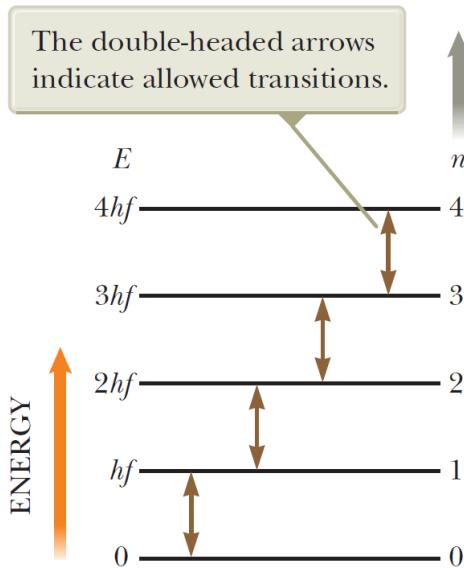


Figure 3.4 Allowed energy levels for an oscillator with frequency f

Planck's law explains the distribution of energy from a black body which is given by,

$$I(\lambda, T) = \frac{2\pi hc^2}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1} \quad (3.5)$$

where $I(\lambda, T) d\lambda$ is the intensity or power per unit area emitted in the wavelength interval $d\lambda$ from a blackbody, h is Planck's constant, k_B is Boltzmann's constant, c is speed of light in vacuum and T is equilibrium temperature of blackbody .

The Planck's Law gives a distribution that peaks at a certain wavelength, the peak shifts to shorter wavelengths for higher temperatures, and the area under the curve grows rapidly with increasing temperature. This law is in agreement with the experimental data.

The results of Planck's law:

- The denominator [$\exp(hc/\lambda kT)$] tends to infinity faster than the numerator (λ^{-5}), thus resolving the ultraviolet catastrophe and hence arriving at experimental observation:

$$I(\lambda, T) \rightarrow 0 \text{ as } \lambda \rightarrow 0.$$

- For very large λ , $\exp\left(\frac{hc}{\lambda kT}\right) - 1 \approx \frac{hc}{\lambda kT} \Rightarrow I(\lambda, T) \rightarrow 2\pi c \lambda^{-4} kT$
i.e. $I(\lambda, T) \rightarrow 0$ as $\lambda \rightarrow \infty$.

From a fit between Planck's law and experimental data, Planck's constant was derived to be $h = 6.626 \times 10^{-34} \text{ J-s}$.

3.2 PHOTOELECTRIC EFFECT

Ejection of electrons from the surface of certain metals when it is irradiated by an electromagnetic radiation of suitable frequency is known as photoelectric effect.

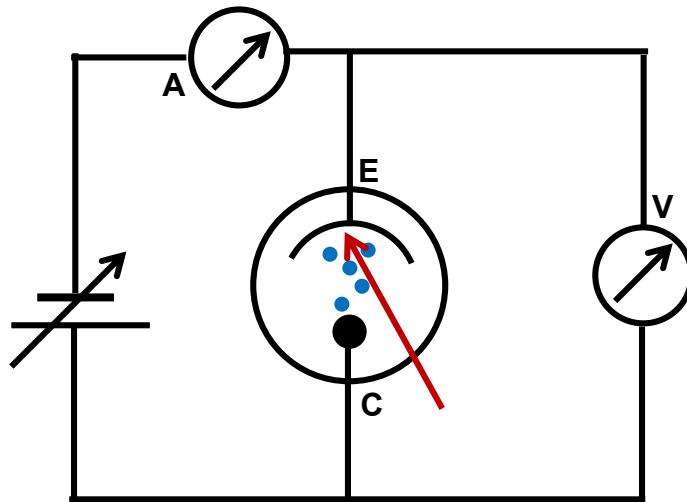


Figure 3.5(a) Apparatus (b) circuit for studying Photoelectric Effect (T – Evacuated glass/ quartz tube, E – Emitter Plate / Photosensitive material / Cathode, C – Collector Plate / Anode, V – Voltmeter, A - Ammeter)

Experimental Observations:

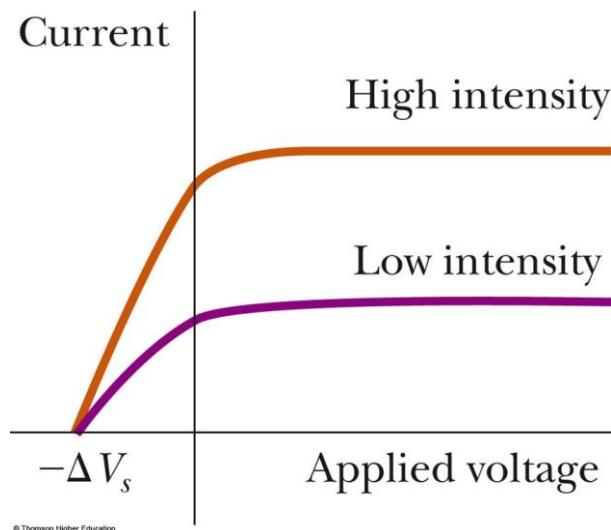


Figure 3.6 Photoelectric current versus applied potential difference for two light intensities

- When plate E is illuminated by light of suitable frequency, electrons are emitted from E and a current is detected in A (Figure 3.5).

2. Photocurrent produced vs potential difference graph shows that kinetic energy of the most energetic photoelectrons is,

$$K_{max} = e \Delta V_s \quad (3.6)$$

where ΔV_s is stopping potential

- 3. Kinetic energy of the most energetic photoelectrons is independent of light intensity.
- 4. Electrons are emitted from the surface of the emitter almost instantaneously
- 5. No electrons are emitted if the incident light frequency falls below a cutoff frequency.
- 6. Kinetic energy of the most energetic photoelectrons increases with increasing light frequency.

Classical Predictions:

- 1. If light is really a wave, it was thought that if one shine of light of any fixed wavelength, at sufficient intensity on the emitter surface, electrons should absorb energy continuously from the **em** waves and electrons should be ejected.
- 2. As the intensity of light is increased (made it brighter and hence classically, a more energetic wave), kinetic energy of the emitted electrons should increase.
- 3. Measurable / larger time interval between incidence of light and ejection of photoelectrons.
- 4. Ejection of photoelectron should not depend on light frequency
- 5. In short experimental results contradict classical predictions.
- 6. Photoelectron kinetic energy should not depend upon the frequency of the incident light.

Einstein's Interpretation of electromagnetic radiation:

- 1. Electromagnetic waves carry discrete energy packets (light quanta called photons now).
- 2. The energy E , per packet depends on frequency f : $E = hf$.
- 3. More intense light corresponds to more photons, not higher energy photons.
- 4. Each photon of energy E moves in vacuum at the speed of light: $c = 3 \times 10^8$ m/s and each photon carries a momentum, $p = E/c$.

Einstein's theory of photoelectric effect:

A photon of the incident light gives all its energy hf to a single electron (absorption of energy by the electrons is not a continuous process as envisioned in the wave model) and the kinetic energy of the most energetic photoelectron

$$K_{max} = hf - \phi \quad (\text{Einstein's photoelectric equation}) \quad (3.7)$$

ϕ is called the work function of the metal. It is the minimum energy with which an electron is bound in the metal.

All the observed features of photoelectric effect could be explained by Einstein's photoelectric equation:

1. Equation shows that K_{max} depends only on frequency of the incident light.
2. Almost instantaneous emission of photoelectrons due to one -to -one interaction between photons and electrons.
3. Ejection of electrons depends on light frequency since photons should have energy greater than the work function ϕ in order to eject an electron.
4. The cutoff frequency f_c is related to ϕ by $f_c = \phi/h$. If the incident frequency f is less than f_c , there is no emission of photoelectrons.

The graph of kinetic energy of the most energetic photoelectron K_{max} vs frequency f is a straight line, according to Einstein's equation.

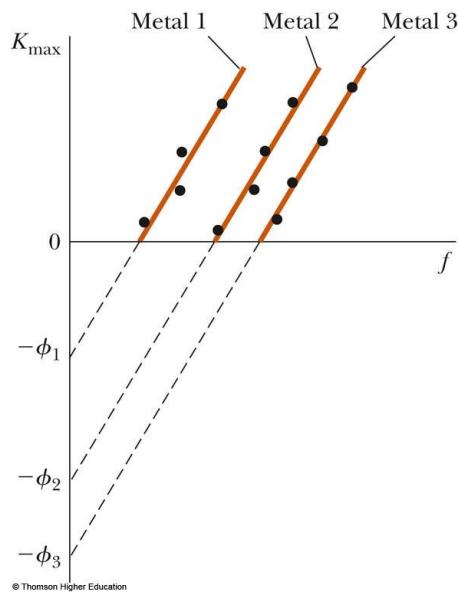


Figure 3.7 A representative plot of K_{max} versus frequency of incident light for three different metals

3.3 COMPTON EFFECT

When X-rays are scattered by free/nearly free electrons, they suffer a change in their wavelength which depends on the scattering angle. This scattering phenomenon is known as Compton Effect.

Classical Predictions: Oscillating **electromagnetic waves** (classically, X-rays are em waves) incident on electrons should have two effects: i) oscillating electromagnetic field causes oscillations in electrons. Each electron first absorbs radiation as a moving particle and then re-radiates in all directions as a moving

particle and thereby exhibiting two Doppler shifts in the frequency of radiation. ii) radiation pressure should cause the electrons to accelerate in the direction of propagation of the waves. Because different electrons will move at different speeds after the interaction, depending on the amount of energy absorbed from electromagnetic waves, the scattered waves at a given angle will have all frequencies (Doppler-shifted values).

Compton's experiment and observation: Compton measured the intensity of scattered X-rays from a solid target (graphite) as a function of wavelength for different angles. The experimental setup is shown in Figure 3.8. Contrary to the classical prediction, only one frequency for scattered radiation was seen at a given angle. This is shown in the Figure 3.9.

The graphs for three nonzero angles show two peaks, one at λ_0 and the other at λ' $> \lambda_0$. The shifted peak at λ' is caused by the scattering of X-rays from free electrons. Shift in wavelength was predicted by Compton to depend on scattering angle as

$$\lambda' - \lambda = \frac{h}{mc}(1 - \cos \theta) \quad (3.8)$$

where m is the mass of the electron, c is velocity of light, h is Planck's constant.

This is known as Compton shift equation, and the factor $\frac{h}{mc}$ is called the Compton wavelength and $\frac{h}{mc} = 2.43 \text{ pm}$.

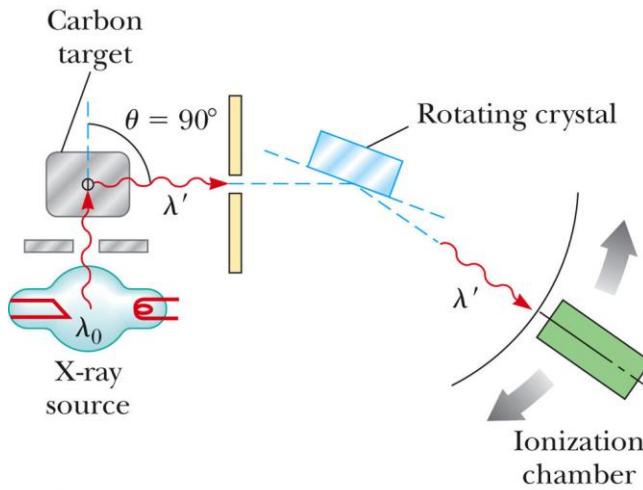


Figure 3.8 Schematic diagram of Compton's apparatus. The wavelength is measured with a rotating crystal spectrometer for various scattering angles θ .

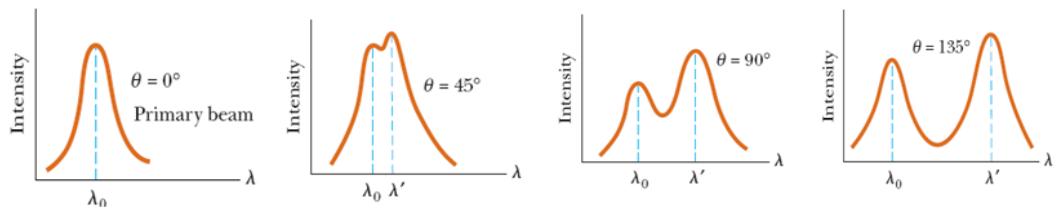


Figure 3.9 Scattered x-ray intensity versus wavelength for Compton scattering at $\theta = 0^\circ, 45^\circ, 90^\circ$, and 135° showing single frequency at a given angle

Derivation of the Compton shift equation:

Compton could explain the experimental result by treating the X-rays not as waves but rather as point like particles (photons) having energy $E = hf_0 = hc/\lambda_0$, momentum $p = hf/c = h/\lambda$ and zero rest energy. Photons collide elastically with free electrons initially at rest and moving relativistically after collision.

Let λ_0 , $p_0 = h/\lambda_0$ and $E_0 = hc/\lambda_0$ be the wavelength, momentum and energy of the incident photon respectively. λ' , $p' = h/\lambda'$ and $E' = hc/\lambda'$ be the corresponding quantities for the scattered photon.

We know that, for the electron, the total **relativistic** energy $E = \sqrt{p^2c^2 + m^2c^4}$

Kinetic energy $K = E - mc^2$

And momentum $p = \gamma mv$. where $\gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}}$

v and m are the speed and mass of the electron respectively.

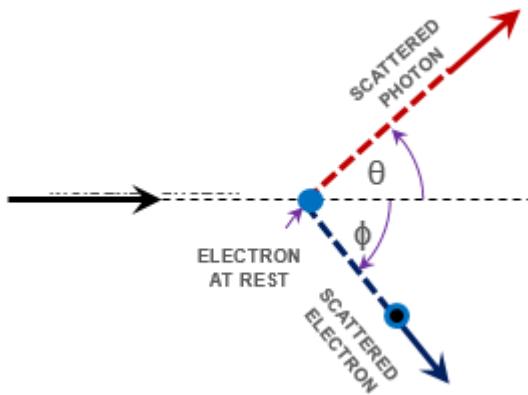


Figure 3.10 Quantum model for X-ray scattering from an electron

In the scattering process, the **total energy and total linear momentum of the system must be conserved**.

For conservation of energy we must have, $E_0 = E' + K$

$$\text{ie, } E_o = E' + (E - m c^2)$$

Or

$$E_o - E' + m c^2 = E = \sqrt{p^2 c^2 + m^2 c^4}$$

$$\text{Squaring both the sides, } (E_o - E')^2 + 2(E_o - E') mc^2 + m^2 c^4 = p^2 c^2 + m^2 c^4$$

For conservation of momentum, x -component: $p_o = p' \cos \theta + p \cos \phi$

y -component: $0 = p' \sin \theta - p \sin \phi$

Rewriting these two equations

$$p_o - p' \cos \theta = p \cos \phi$$

$$p' \sin \theta = p \sin \phi$$

Squaring both the sides and adding,

$$p_o^2 - 2p_o p' \cos \theta + p'^2 = p^2$$

Substituting this p^2 in the equation :

$$(E_o - E')^2 + 2(E_o - E') mc^2 = p^2 c^2, \text{ one gets}$$

$$(E_o - E')^2 + 2(E_o - E') mc^2 = (p_o^2 - 2p_o p' \cos \theta + p'^2) c^2$$

Substituting photon energies and photon momenta one gets

$$\left(\frac{hc}{\lambda_o} - \frac{hc}{\lambda'}\right)^2 + 2 \left(\frac{hc}{\lambda_o} - \frac{hc}{\lambda'}\right) mc^2 = \left(\frac{hc}{\lambda_o}\right)^2 - 2 \left(\frac{hc}{\lambda_o}\right) \left(\frac{hc}{\lambda'}\right) \cos \theta + \left(\frac{hc}{\lambda'}\right)^2$$

Simplifying one gets

$$\left(\frac{hc}{\lambda_o}\right)^2 - 2 \left(\frac{hc}{\lambda_o}\right) \left(\frac{hc}{\lambda'}\right) + \left(\frac{hc}{\lambda'}\right)^2 + 2 hc \left(\frac{1}{\lambda_o} - \frac{1}{\lambda'}\right) mc^2 = \left(\frac{hc}{\lambda_o}\right)^2 - 2 \left(\frac{hc}{\lambda_o}\right) \left(\frac{hc}{\lambda'}\right) \cos \theta + \left(\frac{hc}{\lambda'}\right)^2$$

$$\text{i.e., } -\frac{hc}{\lambda_o \lambda'} + \left(\frac{1}{\lambda_o} - \frac{1}{\lambda'}\right) mc^2 = -\frac{hc}{\lambda_o \lambda'} \cos \theta$$

$$\text{OR, } \left(\frac{\lambda' - \lambda_o}{\lambda_o \lambda'}\right) mc^2 = \frac{hc}{\lambda_o \lambda'} (1 - \cos \theta)$$

Compton shift:

$$\lambda' - \lambda_o = \frac{h}{mc} (1 - \cos \theta)$$

3.4 PHOTONS AND ELECTROMAGNETIC WAVES [DUAL NATURE OF LIGHT]

- Light exhibits diffraction and interference phenomena that are only explicable in terms of wave properties.
- Photoelectric effect and Compton Effect can only be explained taking light as photons / particle.
- This means true nature of light is not describable in terms of any single picture, instead both wave and particle nature have to be considered. In short, the particle model and the wave model of light complement each other.

3.5 de BROGLIE HYPOTHESIS - WAVE PROPERTIES OF PARTICLES

We have seen that light comes in discrete units (photons) with particle properties (energy E and momentum p) that are related to the wave-like properties of frequency and wavelength. Louis de Broglie postulated that because photons have both wave and particle characteristics, perhaps all forms of matter have wave-like properties, with the wavelength λ related to momentum p in the same way as for light.

$$\text{de Broglie wavelength: } \lambda = \frac{h}{p} = \frac{h}{mv} \quad (3.9)$$

where h is Planck's constant and p is momentum of the quantum particle, m is mass of the particle, and v is speed of the particle. The electron accelerated through a potential difference of ΔV , has a non-relativistic kinetic energy

$$\frac{1}{2}mv^2 = e\Delta V \quad \text{where } e \text{ is electron charge.}$$

Hence, the momentum (p) of an electron accelerated through a potential difference of ΔV is

$$p = m v = \sqrt{2m e \Delta V} \quad (3.10)$$

Frequency of the matter wave associated with the particle is $\frac{E}{h}$, where E is total relativistic energy of the particle

Davisson-Germer experiment and G P Thomson's electron diffraction experiment confirmed de Broglie relationship $p = h/\lambda$. Subsequently it was found that atomic beams, and beams of neutrons, also exhibit diffraction when reflected from regular crystals. Thus de Broglie's formula seems to apply to any kind of matter. Now the dual nature of matter and radiation is an accepted fact and it is stated in the

principle of complementarity. This states that wave and particle models of either matter or radiation complement each other.

3.6 THE QUANTUM PARTICLE

Quantum particle is a model by which particles having dual nature are represented. We must choose one appropriate behavior for the quantum particle (particle or wave) in order to understand a particular behavior.

To represent a quantum wave, we have to combine the essential features of both an ideal particle and an ideal wave. An essential feature of a particle is that it is localized in space. But an ideal wave is infinitely long (non-localized) as shown in Figure 3.11.

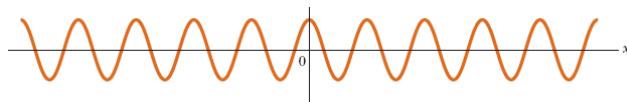


Figure 3.11 Section of an ideal wave of single frequency

Now to build a localized entity from an infinitely long wave, waves of same amplitude, but slightly different frequencies are superposed (Figure 3.12).

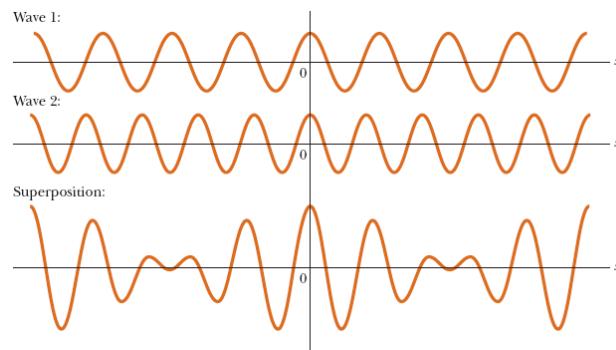


Figure 3.12 Superposition of two waves Wave 1 and Wave 2

If we add up large number of waves in a similar way, the small localized region of space where constructive interference takes place is called a **wave packet**, which represents a quantum particle (Figure 3.13).

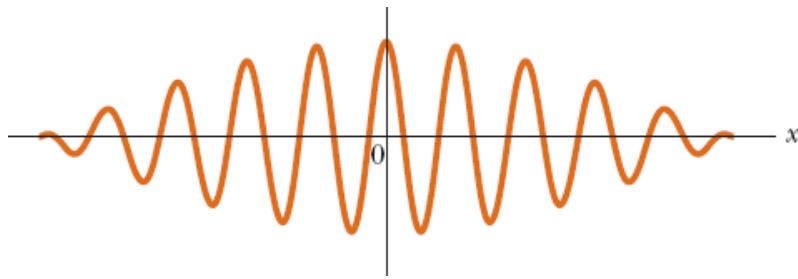


Figure 3.13 Wave packet

Mathematical representation of a wave packet:

Superposition of two waves of equal amplitude, but with slightly different frequencies, f_1 and f_2 , traveling in the same direction are considered. The waves are written as

$$y_1 = A \cos(k_1 x - \omega_1 t) \quad \text{and} \quad y_2 = A \cos(k_2 x - \omega_2 t)$$

where $k = 2\pi/\lambda$, $\omega = 2\pi f$

The resultant wave $y = y_1 + y_2$

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

where $\Delta k = k_1 - k_2$ and $\Delta\omega = \omega_1 - \omega_2$.

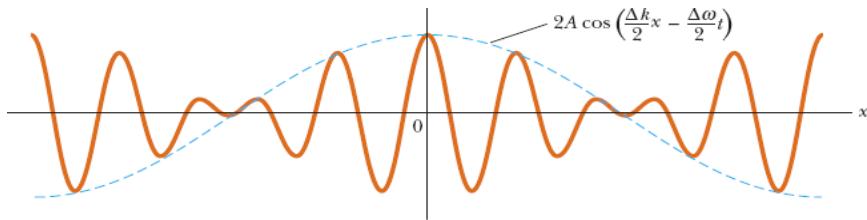


Figure 3.14 Beat pattern due to superposition of wave trains y_1 and y_2

The resulting wave oscillates with the average frequency, and its amplitude envelope (in square brackets, shown by the blue dotted curve in Figure 3.14) varies according to the difference frequency. A realistic wave (one of finite extent in space) is characterized by two different speeds. The **phase speed**, the speed with which wave crest of individual wave moves, is given by

$$v_p = f \lambda \quad \text{or} \quad v_p = \frac{\omega}{k} \quad (3.11)$$

The envelope of group of waves can travel through space with a different speed than the individual waves. This speed is called the **group speed** or the speed of the wave packet which is given by

$$v_g = \frac{\left(\frac{\Delta\omega}{2}\right)}{\left(\frac{\Delta k}{2}\right)} = \frac{\Delta\omega}{\Delta k} \quad (3.12)$$

For a superposition of large number of waves to form a wave packet, this ratio is

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

In general these two speeds are not the same.

Relation between group speed (v_g) and phase speed (v_p):

$$v_p = \frac{\omega}{k} = f \lambda \quad \therefore \quad \omega = k v_p$$

$$\text{But } v_g = \frac{d\omega}{dk} = \frac{d(kv_p)}{dk} = k \frac{dv_p}{dk} + v_p$$

Substituting for k in terms of λ , we get

$$v_g = v_p - \lambda \left(\frac{dv_p}{d\lambda} \right) \quad (3.13)$$

Relation between group speed (v_g) and particle speed (u):

$$\omega = 2\pi f = 2\pi \frac{E}{h} \quad \text{and} \quad k = \frac{2\pi}{\lambda} = \frac{2\pi}{h/p} = \frac{2\pi p}{h}$$

$$v_g = \frac{d\omega}{dk} = \frac{\frac{2\pi}{h} dE}{\frac{2\pi}{h} dp} = \frac{dE}{dp}$$

For a classical particle moving with speed u , the kinetic energy E is given by

$$E = \frac{1}{2} m u^2 = \frac{p^2}{2m} \quad \text{and} \quad dE = \frac{2p dp}{2m} \quad \text{or} \quad \frac{dE}{dp} = \frac{p}{m} = u$$

$$v_g = \frac{d\omega}{dk} = \frac{dE}{dp} = u \quad (3.14)$$

i.e., we should identify the group speed with the particle speed, speed with which the energy moves. To represent a realistic wave packet, confined to a finite region in space, we need the superposition of large number of harmonic waves with a range of k -values.

3.7 DOUBLE-SLIT EXPERIMENT REVISITED

One way to confirm our ideas about the electron's wave-particle duality is through an experiment in which electrons are fired at a double slit. Consider a parallel beam of mono-energetic electrons incident on a double slit as in Figure 3.15. Let's assume the slit widths are small compared with the electron wavelength so that diffraction effects are negligible. An electron detector screen (acts like the "viewing screen" of Young's double-slit experiment) is positioned far from the slits at a distance much greater than d , the separation distance of the slits. If the detector screen collects

electrons for a long enough time, we find a typical wave interference pattern for the counts per minute, or probability of arrival of electrons. Such an interference pattern would not be expected if the electrons behaved as classical particles, giving clear evidence that electrons are interfering, a distinct wave-like behavior.

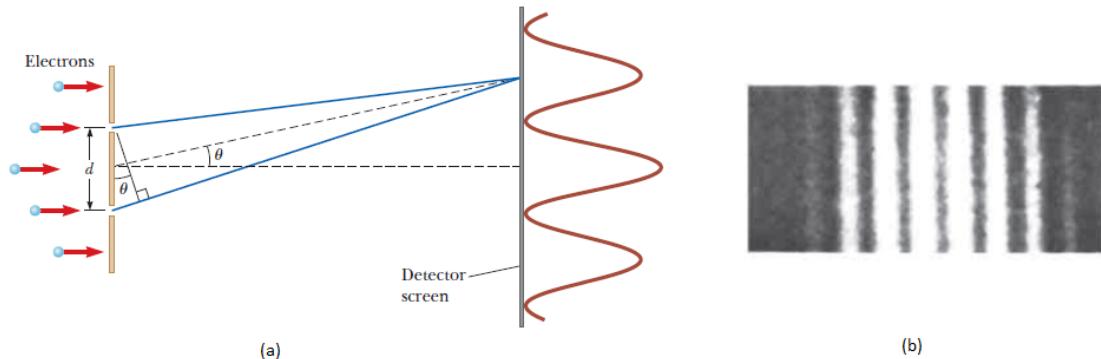


Figure 3.15 (a) Schematic of electron beam interference experiment, (b) Photograph of a double-slit interference pattern produced by electrons

If we measure the angle θ at which the maximum intensity of the electrons arrives at the detector screen, we find they are described by exactly the same equation as that for light: $d \sin \theta = m \lambda$, where m is the order number and λ is the electron wavelength. Therefore, the dual nature of the electron is clearly shown in this experiment: **the electrons are detected as particles at a localized spot on the detector screen at some instant of time, but the probability of arrival at the spot is determined by finding the intensity of two interfering waves.**

3.8 UNCERTAINTY PRINCIPLE

It is fundamentally impossible to make simultaneous measurements of a particle's position and momentum with infinite accuracy. This is known as **Heisenberg uncertainty principle**. The uncertainties arise from the quantum structure of matter.

For a particle represented by a single wavelength wave existing throughout space, λ is precisely known, and according to de Broglie hypothesis, its p is also known accurately. But the position of the particle in this case becomes completely uncertain.

This means $\Delta\lambda = 0$, $\Delta p = 0$; but $\Delta x = \infty$

In contrast, if a particle whose momentum is uncertain (combination of waves / a range of wavelengths are taken to form a wave packet), so that Δx is small, but $\Delta\lambda$ is large. If Δx is made zero, $\Delta\lambda$ and thereby Δp will become ∞ .

$$\text{In short } (\Delta x)(\Delta p_x) \geq h / 4\pi \quad (3.15)$$

where Δx is uncertainty in the measurement of position x of the particle and Δp_x is uncertainty in the measurement of momentum p_x of the particle.

One more relation expressing uncertainty principle is related to energy and time which is given by

$$(\Delta E)(\Delta t) \geq h / 4\pi \quad (3.16)$$

where ΔE is uncertainty in the measurement of energy E of the system when the measurement is done over the time interval Δt .

3.9 QUESTIONS

1. Explain (a) Stefan's law (b) Wien's displacement law (c) Rayleigh-Jeans law.
2. Sketch schematically the graph of wavelength vs intensity of radiation from a blackbody.
3. Explain Planck's radiation law.
4. Write the assumptions made in Planck's hypothesis of blackbody radiation.
5. Explain photoelectric effect.
6. What are the observations in the experiment on photoelectric effect?
7. What are the classical predictions about the photoelectric effect?
8. Explain Einstein's photoelectric equation.
9. Which are the features of photoelectric effect-experiment explained by Einstein's photoelectric equation?
10. Sketch schematically the following graphs with reference to the photoelectric effect: (a) photoelectric current vs applied voltage (b) kinetic energy of most-energetic electron vs frequency of incident light.
11. Explain Compton effect.
12. Explain the experiment on Compton effect.
13. Derive the Compton shift equation.
14. Explain the wave properties of the particles.

15. Explain a wave packet and represent it schematically.
16. Explain (a) group speed (b) phase speed, of a wave packet.
17. Show that the group speed of a wave packet is equal to the particle speed.
18. (a) Name any two phenomena which confirm the particle nature of light.
 (b) Name any two phenomena which confirm the wave nature of light.
19. Explain Heisenberg uncertainty principle.
20. Write the equations for uncertainty in (a) position and momentum (b) energy and time.
21. Mention two situations which can be well explained by the uncertainty relation.

3.10 PROBLEMS

- 1 Find the peak wavelength of the blackbody radiation emitted by each of the following.
 - A. The human body when the skin temperature is 35°C
 - B. The tungsten filament of a light bulb, which operates at 2000 K
 - C. The Sun, which has a surface temperature of about 5800 K .

Ans: $9.4\text{ }\mu\text{m}$, $1.4\text{ }\mu\text{m}$, $0.50\text{ }\mu\text{m}$
- 2 A 2.0- kg block is attached to a spring that has a force constant of $k = 25\text{ N/m}$. The spring is stretched 0.40 m from its equilibrium position and released.
 - A. Find the total energy of the system and the frequency of oscillation according to classical calculations.
 - B. Assuming that the energy is quantized, find the quantum number n for the system oscillating with this amplitude.
 - C. Suppose the oscillator makes a transition from the $n = 5.4 \times 10^{33}$ state to the state corresponding to $n = 5.4 \times 10^{33} - 1$. By how much does the energy of the oscillator change in this one-quantum change?

Ans: 2.0 J , 0.56 Hz , 5.4×10^{33} , $3.7 \times 10^{-34}\text{ J}$
- 3 The human eye is most sensitive to 560 nm light. What is the temperature of a black body that would radiate most intensely at this wavelength?

Ans: 5180 K
- 4 A blackbody at 7500 K consists of an opening of diameter 0.050 mm , looking into an oven. Find the number of photons per second escaping the hole and having wavelengths between 500 nm and 501 nm .

Ans: $1.30 \times 10^{15} \text{ s}$

- 5 The radius of our Sun is $6.96 \times 10^8 \text{ m}$, and its total power output is $3.77 \times 10^{26} \text{ W}$.
(a) Assuming that the Sun's surface emits as a black body, calculate its surface temperature. (b) Using the result, find λ_{\max} for the Sun.

Ans: 5750 K, 504 nm

- 6 Calculate the energy in electron volts, of a photon whose frequency is (a) 620 THz, (b) 3.10 GHz, (c) 46.0 MHz. (d) Determine the corresponding wavelengths for these photons and state the classification of each on the electromagnetic spectrum.

Ans: 2.57 eV, $1.28 \times 10^{-5} \text{ eV}$, $1.91 \times 10^{-7} \text{ eV}$, 484 nm, 9.68 cm, 6.52 m

- 7 An FM radio transmitter has a power output of 150 kW and operates at a frequency of 99.7 MHz. How many photons per second does the transmitter emit?

Ans: 2.27×10^{30} photons/s

- 8 A sodium surface is illuminated with light having a wavelength of 300 nm. The work function for sodium metal is 2.46 eV. Find

- The maximum kinetic energy of the ejected photoelectrons and
- The cutoff wavelength for sodium.

Ans: 1.67 eV, 504 nm

- 9 Molybdenum has a work function of 4.2 eV. (a) Find the cut off wavelength and cut off frequency for the photoelectric effect. (b) What is the stopping potential if the incident light has wavelength of 180 nm?

Ans: 296 nm, $1.01 \times 10^{15} \text{ Hz}$, 2.71 V

- 10 Electrons are ejected from a metallic surface with speeds up to $4.60 \times 10^5 \text{ m/s}$ when light with a wavelength of 625 nm is used. (a) What is the work function of the surface? (b) What is the cut-off frequency for this surface?

Ans: 1.38 eV, $3.34 \times 10^{14} \text{ Hz}$

- 11 The stopping potential for photoelectrons released from a metal is 1.48 V larger compared to that in another metal. If the threshold frequency for the first metal is 40.0 % smaller than for the second metal, determine the work function for each metal.

Ans: 3.70 eV, 2.22 eV

- 12 Two light sources are used in a photoelectric experiment to determine the work function for a metal surface. When green light from a mercury lamp ($\lambda = 546.1 \text{ nm}$) is used, a stopping potential of 0.376 V reduces the photocurrent to zero. (a) Based on this what is the work function of this metal? (b) What stopping potential would be observed when using the yellow light from a helium discharge tube ($\lambda = 587.5 \text{ nm}$)?

Ans: 1.90 eV, 0.215 V

- 13 X-rays of wavelength $\lambda_0 = 0.20 \text{ nm}$ are scattered from a block of material. The scattered X-rays are observed at an angle of 45° to the incident beam. Calculate their wavelength.

What if we move the detector so that scattered X-rays are detected at an angle larger than 45° ? Does the wavelength of the scattered X-rays increase or decrease as the angle θ increase?

Ans: 0.200710 nm, INCREASES

- 14 Calculate the energy and momentum of a photon of wavelength 700 nm.

Ans: 1.78 eV, 9.47×10^{-28} kg.m/s

- 15 A 0.00160 nm photon scatters from a free electron. For what photon scattering angle does the recoiling electron have kinetic energy equal to the energy of the scattered photon?

Ans: 70°

- 16 A 0.880 MeV photon is scattered by a free electron initially at rest such that the scattering angle of the scattered electron is equal to that of the scattered photon ($\theta = \phi$). (a) Determine the angles θ & ϕ . (b) Determine the energy and momentum of the scattered electron and photon.

Ans: 43° , 43° , 0.602 MeV, 3.21×10^{-22} kg.m/s, 0.278 MeV, 3.21×10^{-22} kg.m/s

- 17 Calculate the de-Broglie wavelength for an electron moving at 1.0×10^7 m/s.

Ans: 7.28×10^{-11} m

- 18 A rock of mass 50 g is thrown with a speed of 40 m/s. What is its de Broglie wavelength?

Ans: 3.3×10^{-34} m

- 19 A particle of charge q and mass m has been accelerated from rest to a nonrelativistic speed through a potential difference of ΔV . Find an expression for its de Broglie wavelength.

$$\text{Ans: } \lambda = \frac{h}{\sqrt{2m q \Delta V}}$$

- 20 (a) An electron has a kinetic energy of 3.0 eV. Find its wavelength. (b) Also find the wavelength of a photon having the same energy.

Ans: 7.09×10^{-10} m, 4.14×10^{-7} m

- 21 In the Davisson-Germer experiment, 54.0 eV electrons were diffracted from a nickel lattice. If the first maximum in the diffraction pattern was observed at $\phi = 50.0^\circ$, what was the lattice spacing a between the vertical rows of atoms in the figure?

Ans: 2.18×10^{-10} m

- 22 Consider a freely moving quantum particle with mass m and speed u . Its energy is $E = K = mu^2/2$. Determine the phase speed of the quantum wave representing the particle and show that it is different from the speed at which the particle transports mass and energy.

Ans: $v_{\text{GROUP}} = u \neq v_{\text{PHASE}}$

- 23 Electrons are incident on a pair of narrow slits $0.060 \mu\text{m}$ apart. The ‘bright bands’ in the interference pattern are separated by 0.40 mm on a ‘screen’ 20.0 cm from the slits. Determine the potential difference through which the electrons were accelerated to give this pattern.

Ans: 105 V

- 24 The speed of an electron is measured to be $5.00 \times 10^3 \text{ m/s}$ to an accuracy of 0.0030% . Find the minimum uncertainty in determining the position of this electron.

Ans: 0.383 mm

- 25 The lifetime of an excited atom is given as $1.0 \times 10^{-8} \text{ s}$. Using the uncertainty principle, compute the line width Δf produced by this finite lifetime?

Ans: $8.0 \times 10^6 \text{ Hz}$

- 26 Use the uncertainty principle to show that if an electron were confined inside an atomic nucleus of diameter $2 \times 10^{-15} \text{ m}$, it would have to be moving relativistically, while a proton confined to the same nucleus can be moving nonrelativistically.

Ans: $v_{\text{ELECTRON}} \cong 0.99996 c$, $v_{\text{PROTON}} \cong 1.8 \times 10^7 \text{ m/s}$

- 27 Find the minimum kinetic energy of a proton confined within a nucleus having a diameter of $1.0 \times 10^{-15} \text{ m}$.

Ans: 5.2 MeV

4 QUANTUM MECHANICS

OBJECTIVES:

- To learn the application of Schrödinger equation to a bound particle and to learn the quantized nature of the bound particle, its expectation values and physical significance.
- To understand the tunneling behavior of a particle incident on a potential barrier.
- To understand the behavior of quantum oscillator.

4.1 AN INTERPRETATION OF QUANTUM MECHANICS

Experimental evidences proved that both matter and electromagnetic radiation exhibit wave and particle nature depending on the phenomenon being observed. Making a conceptual connection between particles and waves, for an electromagnetic radiation of amplitude E , the probability per unit volume of finding a photon in a given region of space at an instant of time as

$$\frac{\text{PROBABILITY}}{V} \propto E^2$$

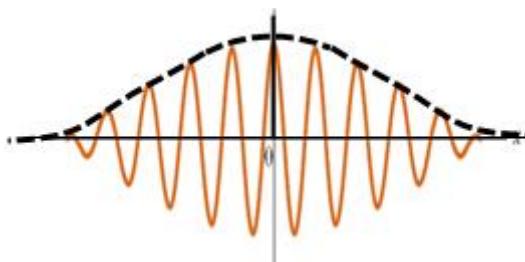


Figure 4.1 Wave packet

Taking the analogy between electromagnetic radiation and matter-the probability per unit volume of finding the particle is proportional to the square of the amplitude of a wave representing the particle, even if the amplitude of the de Broglie wave associated with a particle is generally not a measurable quantity. The amplitude of the de Broglie wave associated with a particle is called probability amplitude, or the wave function, and is denoted by ψ .

In general, the complete wave function Ψ for a system depends on the positions of all the particles in the system and on time. This can be written as

$$\Psi(r_1, r_2, \dots, r_j, \dots, t) = \psi(r_j) e^{-i\omega t}$$

where r_j is the position vector of the j^{th} particle in the system.

For any system in which the potential energy is time-independent and depends only on the position of particles within the system, the important information about the system is contained within the space part of the wave function. The wave function ψ contains within it all the information that can be known about the particle. $|\psi|^2$ is always real and positive, and is proportional to the probability per unit volume, of finding the particle at a given point at some instant. If ψ represents a single particle, then $|\psi|^2$ - called the **probability density** - is the relative probability per unit volume that the particle will be found at any given point in the volume.

One-dimensional wave functions and expectation values: Let ψ be the wave function for a particle moving along the x axis. Then $P(x) dx = |\psi|^2 dx$ is the probability to find the particle in the infinitesimal interval dx around the point x . The probability of finding the particle in the arbitrary interval $a \leq x \leq b$ is

$$P_{ab} = \int_a^b |\psi|^2 dx \quad (4.1)$$

The probability of a particle being in the interval $a \leq x \leq b$ is the area under the probability density curve from a to b . The total probability of finding the particle is one. Forcing this condition on the wave function is called **normalization**.

$$\int_{-\infty}^{+\infty} |\psi|^2 dx = 1 \quad (4.2)$$

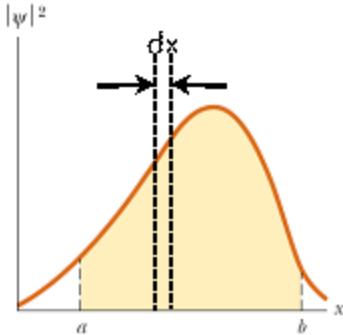


Figure 4.2 An arbitrary probability density curve for a particle

All the measurable quantities of a particle, such as its position, momentum and energy can be derived from the knowledge of ψ . e.g., the average position at which one expects to find the particle after many measurements is called the **expectation value of x** and is defined by the equation

$$\langle x \rangle \equiv \int_{-\infty}^{+\infty} \psi^* x \psi dx \quad (4.3)$$

The important mathematical features of a physically reasonable wave function $\psi(x)$ for a system are

- $\psi(x)$ may be a complex function or a real function, depending on the system.
- $\psi(x)$ must be finite, continuous and single valued everywhere.
- The space derivatives of ψ , must be finite, continuous and single valued everywhere.
- ψ must be normalizable.

4.2 THE SCHRÖDINGER EQUATION

The appropriate wave equation for matter waves was developed by Schrödinger. Schrödinger equation as it applies to a particle of mass m confined to move along x axis and interacting with its environment through a potential energy function $U(x)$ is

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + U\psi = E\psi \quad (4.4)$$

where E is a constant equal to the total energy of the system (the particle and its environment) and $\hbar = h/2\pi$. This equation is referred to as the one dimensional, time-independent Schrödinger equation.

Application of Schrödinger equation:

1. Particle in an infinite potential well (particle in a box)
2. Particle in a finite potential well
3. Tunneling
4. Quantum oscillator

4.3 PARTICLE IN AN INFINITE POTENTIAL WELL (PARTICLE IN A “BOX”)

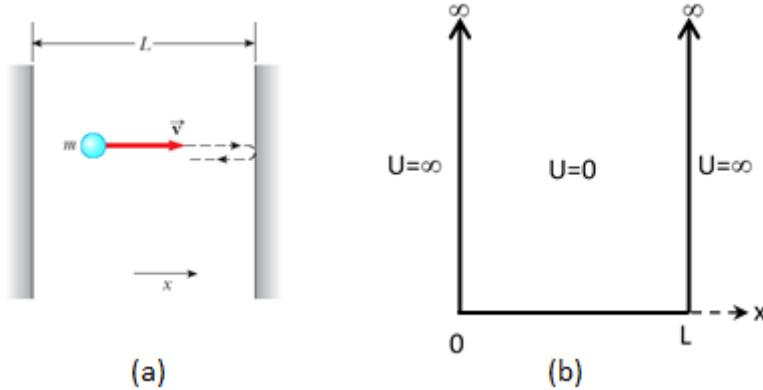


Figure 4.3 (a) Particle in a potential well of infinite height, (b) Sketch of potential well

Consider a particle of mass m and velocity v , confined to bounce between two impenetrable walls separated by a distance L as shown in Figure 4.3(a). Figure 4.3(b) shows the potential energy function for the system.

$$\begin{aligned} U(x) &= 0, && \text{for } 0 < x < L, \\ U(x) &= \infty, && \text{for } x \leq 0, x \geq L \end{aligned}$$

Since $U(x) = \infty$, for $x < 0, x > L$, $\psi(x) = 0$ in these regions. Also $\psi(0) = 0$ and $\psi(L) = 0$. Only those wave functions that satisfy these boundary conditions are allowed. In the region $0 < x < L$, where $U = 0$, the Schrödinger equation takes the form

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E \psi = 0$$

$$\text{Or } \frac{d^2\psi}{dx^2} = -k^2 \psi, \quad \text{where } k^2 = \frac{2mE}{\hbar^2} \quad \text{or} \quad k = \frac{\sqrt{2mE}}{\hbar}$$

The most general form of the solution to the above equation is

$$\psi(x) = A \sin(kx) + B \cos(kx)$$

where A and B are constants determined by the boundary and normalization conditions.

Applying the first boundary condition,

i.e., at $x = 0$, $\psi = 0$ leads to

$$0 = A \sin 0 + B \cos 0 \quad \text{or} \quad B = 0,$$

And at $x = L$, $\psi = 0$,

$$o = A \sin(kL) + B \cos(kL) = A \sin(kL) + o,$$

Since $A \neq o$, $\sin(kL) = o$. $\therefore kL = n\pi$; ($n = 1, 2, 3, \dots$)

Now the wave function reduces to $\psi_n(x) = A \sin\left(\frac{n\pi x}{L}\right)$

To find the constant A, apply normalization condition

$$\int_{-\infty}^{+\infty} |\psi|^2 dx = 1 \quad \text{or} \quad \int_0^L A^2 \left[\sin\left(\frac{n\pi x}{L}\right) \right]^2 dx = 1.$$

$$A^2 \int_0^L \frac{1}{2} [1 - \cos\left(\frac{2n\pi x}{L}\right)] dx = 1$$

$$\text{Solving we get } A = \sqrt{\frac{2}{L}}$$

Thus $\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$ is the wave function for particle in a box.

$$\text{Since } k = \frac{\sqrt{2mE}}{\hbar} \text{ and } kL = n\pi$$

$$\text{We get, } \frac{\sqrt{2mE}}{\hbar} L = n\pi.$$

$$\therefore E_n = \left(\frac{\hbar^2}{8mL^2}\right) n^2, \quad n = 1, 2, 3, \dots \quad (4.5)$$

Each value of the integer n corresponds to a quantized energy value, E_n .

$$\text{The lowest allowed energy } (n = 1), \quad E_1 = \frac{\hbar^2}{8mL^2}.$$

This is the ground state energy for the particle in a box. Excited states correspond to $n = 2, 3, 4, \dots$ which have energies given by $4E_1, 9E_1, 16E_1, \dots$ respectively. Energy level diagram, wave function and probability density sketches are shown in Figure 4.4 and 4.5 respectively. Since ground state energy $E_1 \neq 0$, the particle can never be at rest.

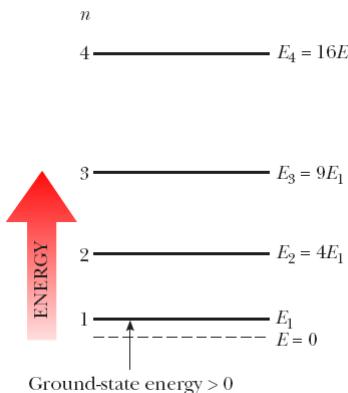


Figure 4.4 Energy level diagram for a particle in potential well of infinite height

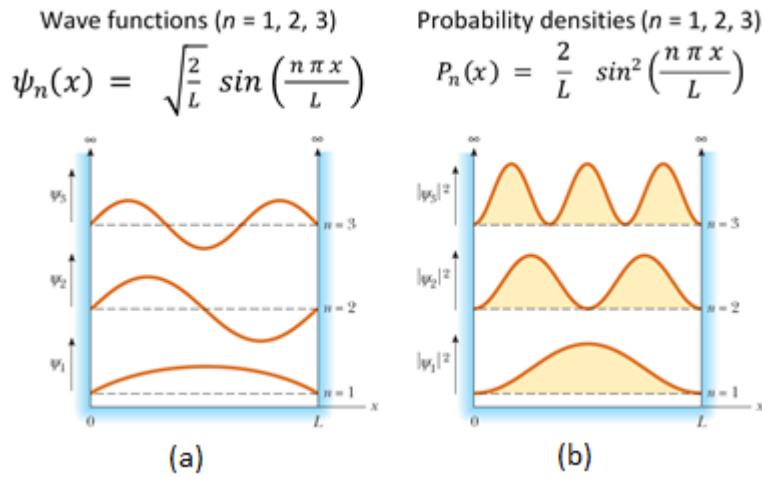


Figure 4.5 Sketch of (a) wave function, (b) Probability density for a particle in potential well of infinite height

4.4 A PARTICLE IN A POTENTIAL WELL OF FINITE HEIGHT

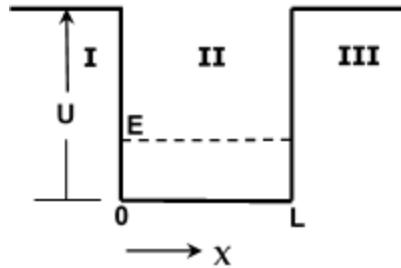


Figure 4.6 Potential well of finite height U and length L

Consider a particle with the total energy E , trapped in a finite potential well of height U such that

$$U(x) = 0, \quad 0 < x < L,$$

$$U(x) = U, \quad x \leq 0, \quad x \geq L$$

Classically, for energy $E < U$, the particle is permanently bound in the potential well. However, according to quantum mechanics, a finite probability exists that the particle can be found outside the well even if $E < U$. That is, the wave function is generally nonzero in the regions I and III. In region II, where $U = 0$, the allowed wave functions are again sinusoidal. But the boundary conditions no longer require that the wave function must be zero at the ends of the well.

Schrödinger equation outside the finite well in regions I & III

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2} (U - E) \psi \quad \text{or} \quad \frac{d^2\psi}{dx^2} = C^2 \psi \quad \text{where} \quad C^2 = \frac{2m}{\hbar^2} (U - E)$$

General solution of the above equation is

$$\psi(x) = Ae^{Cx} + Be^{-Cx}$$

where A and B are constants.

A must be zero in Region III and B must be zero in Region I, otherwise, the probabilities would be infinite in those regions. For solution to be finite,

$$\psi_I = Ae^{Cx} \quad \text{for } x \leq 0$$

$$\psi_{III} = Be^{-Cx} \quad \text{for } x \geq L$$

This shows that the wave function outside the potential well decay exponentially with distance.

Schrodinger equation inside the square well potential in region II, where $U = 0$

$$\frac{d^2\psi_{II}}{dx^2} + \left(\frac{2m}{\hbar^2} E\right)\psi_{II} = 0, \quad \frac{2mE}{\hbar^2} = k^2$$

General solution of the above equation

$$\psi_{II} = F \sin[kx] + G \cos[kx]$$

To determine the constants A, B, F, G and the allowed values of energy E , apply the four boundary conditions and the normalization condition:

$$\text{At } x = 0, \quad \psi_I(0) = \psi_{II}(0) \text{ and } \left[\frac{d\psi_I}{dx}\right]_{x=0} = \left[\frac{d\psi_{II}}{dx}\right]_{x=0}$$

$$\text{At } x = L, \quad \psi_{II}(L) = \psi_{III}(L) \quad \text{and} \quad \left[\frac{d\psi_{II}}{dx}\right]_{x=L} = \left[\frac{d\psi_{III}}{dx}\right]_{x=L}$$

$$\int_{-\infty}^{+\infty} |\psi|^2 dx = 1$$

Figure 4.7 shows the plots of wave functions and their respective probability densities.

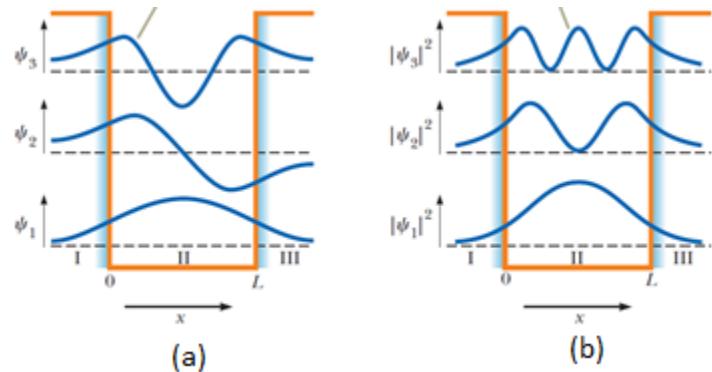


Figure 4.7 Sketch of (a) wave function, (b) Probability density for a particle in potential well of finite height

It is seen that wavelengths of the wave functions are longer than those of wave functions of infinite potential well of same length and hence the quantized energies of the particle in a finite well are lower than those for a particle in an infinite well.

4.5 TUNNELING THROUGH A POTENTIAL ENERGY BARRIER

Consider a particle of energy E approaching a potential barrier of height U , ($E < U$). Potential energy has a constant value of U in the region of width L and is zero in all other regions. This is called a square barrier and U is called the barrier height. Since $E < U$, classically the regions II and III shown in the figure are forbidden to the particle incident from left. But according to quantum mechanics, all regions are accessible to the particle, regardless of its energy.

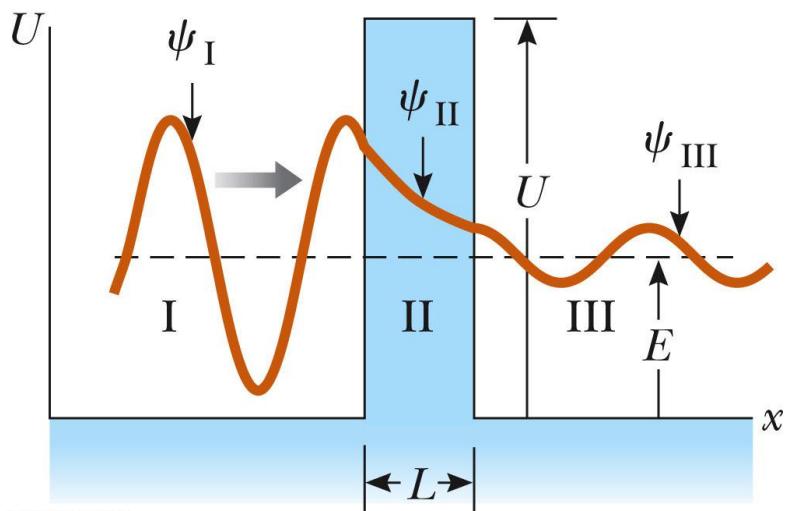


Figure 4.8 Tunneling through a potential barrier of finite height

By applying the boundary conditions, i.e. ψ and its first derivative must be continuous at boundaries (at $x = 0$ and $x = L$), full solution to the Schrödinger equation can be found which is shown in figure. The wave function is sinusoidal in regions I and III but exponentially decaying in region II. The probability of locating the particle beyond the barrier in region III is nonzero. The movement of the particle to the far side of the barrier is called tunneling or barrier penetration. The probability of tunneling can be described with a transmission coefficient T and a reflection coefficient R .

The transmission coefficient represents the probability that the particle penetrates to the other side of the barrier, and reflection coefficient is the probability that the particle is reflected by the barrier. Because the particles must be either reflected or transmitted we have, $R + T = 1$.

An approximate expression for the transmission coefficient, when $T \ll 1$ is

$$T \approx e^{-2CL}, \text{ where } C = \frac{\sqrt{2m(U-E)}}{\hbar}. \quad (4.6)$$

4.6 THE SIMPLE HARMONIC OSCILLATOR

Consider a particle that is subject to a linear restoring force $F = -kx$, where k is a constant and x is the position of the particle relative to equilibrium (at equilibrium position $x=0$).

Classically, the potential energy of the system is,

$$U = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2$$

where the angular frequency of vibration is $\omega = \sqrt{k/m}$.

The total energy E of the system is,

$$E = \text{Kinetic Energy} + \text{Potential Energy} = K + U = \frac{1}{2}kA^2 = \frac{1}{2}m\omega^2A^2$$

where A is the amplitude of motion. In the classical model, any value of E is allowed, including $E=0$, which is the total energy when the particle is at rest at $x=0$.

A quantum mechanical model for simple harmonic oscillator can be obtained by substituting $U = \frac{1}{2}m\omega^2x^2$ in Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi$$

The solution for the above equation is

$$\psi = Be^{-Cx^2}$$

where $C = m\omega/2\hbar$ and $E = \frac{1}{2}\hbar\omega$. The constant B can be determined from normalization condition.

In quantum model, the energy levels of a harmonic oscillator are quantized. The energy of a state having an arbitrary quantum number n is given by

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega; \quad n = 0, 1, 2, \dots \quad (4.7)$$

The state $n = 0$ corresponds to the ground state, whose energy is $E_0 = \frac{1}{2}\hbar\omega$ the state $n = 1$ corresponds to the first excited state, whose energy is $E_1 = \frac{3}{2}\hbar\omega$ and so on. The energy-level diagram for this system is shown in Figure 4.9. The separations between adjacent levels are equal and given by $\Delta E = \hbar\omega$.

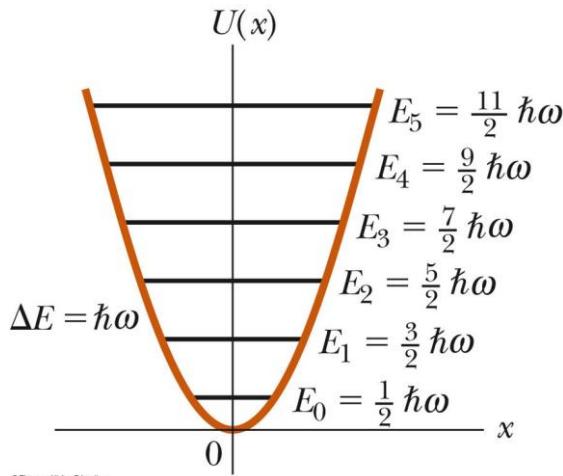


Figure 4.9 Energy-level diagram for a simple harmonic oscillator, superimposed on the potential energy function.

4.7 QUESTIONS

- 1 What is a wave function ? What is its physical interpretation ?
- 2 What are the mathematical features of a wave function?
- 3 By solving the Schrödinger equation, obtain the wave-functions for a particle of mass m in a one-dimensional “box” of length L .
- 4 Apply the Schrödinger equation to a particle in a one-dimensional “box” of length L and obtain the energy values of the particle.
- 5 Sketch the lowest three energy states, wave-functions, probability densities for the particle in a one-dimensional “box”.
- 6 The wave-function for a particle confined to moving in a one-dimensional box is

$\psi(x) = A \sin\left(\frac{n\pi x}{L}\right)$. Use the normalization condition on ψ to show that $A = \sqrt{\frac{2}{L}}$.

- 7 The wave-function of an electron is $\psi(x) = A \sin\left(\frac{n\pi x}{L}\right)$. Obtain an expression for the probability of finding the electron between $x = a$ and $x = b$.
- 8 Sketch the potential-well diagram of finite height U and length L , obtain the general solution of the Schrödinger equation for a particle of mass m in it.
- 9 Sketch the wave-functions and the probability densities for the lowest three energy states of a particle in a potential well of finite height.
- 10 Give a brief account of tunneling of a particle through a potential energy barrier.
- 11 Give a brief account of the quantum mechanical treatment of a simple harmonic oscillator.

4.8 PROBLEMS

1 A particle wave function is given by the equation $\psi(x) = A e^{-ax^2}$

(A) What is the value of A if this wave function is normalized?

(B) What is the expectation value of x for this particle?

Ans: $A = (2a/\pi)^{1/4}$, $\langle x \rangle = 0$

2 A free electron has a wave function $\psi(x) = A \exp[i(5.0 \times 10^{10})x]$

where x is in meters. Find (a) its de Broglie wavelength, (b) its momentum, and (c) its kinetic energy in electron volts.

Ans: $1.26 \times 10^{-10} \text{ m}$, $5.27 \times 10^{-24} \text{ kg.m/s}$, 95.5 eV

3 An electron is confined between two impenetrable walls 0.20 nm apart. Determine the energy levels for the states $n = 1, 2$, and 3 .

Ans: 9.2 eV, 37.7 eV, 84.8 eV

4 A 0.50 kg baseball is confined between two rigid walls of a stadium that can be modeled as a “box” of length 100 m. Calculate the minimum speed of the baseball. If the baseball is moving with a speed of 150 m/s, what is the quantum number of the state in which the baseball will be?

Ans: $6.63 \times 10^{-36} \text{ m/s}$, 2.26×10^{37}

5 A proton is confined to move in a one-dimensional “box” of length 0.20 nm. (a) Find the lowest possible energy of the proton. (b) What is the lowest possible

energy for an electron confined to the same box? (c) Account for the great difference in results for (a) and (b).

Ans: 5.13×10^{-3} eV, 9.41 eV

- 6 (A) Using the simple model of a particle in a box to represent an atom, estimate the energy (in eV) required to raise an atom from the state $n = 1$ to the state $n = 2$. Assume the atom has a radius of 0.10 nm and that the moving electron carries the energy that has been added to the atom.

- (B) Atoms may be excited to higher energy states by absorbing photon energy. Calculate the wavelength of the photon that would cause the transition from the state $n = 1$ to the state $n = 2$.

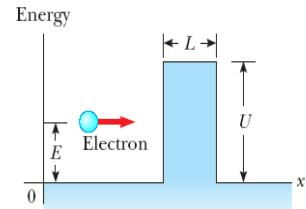
Ans: 28.3 eV, 43.8 nm

- 7 A 30-eV electron is incident on a square barrier of height 40 eV. What is the probability that the electron will tunnel through the barrier if its width is (A) 1.0 nm? (B) 0.10 nm?

Ans: 8.5×10^{-15} , 0.039

- 8 An electron with kinetic energy $E = 5.0$ eV is incident on a barrier with thickness $L = 0.20$ nm and height $U = 10.0$ eV as shown in the figure. What is the probability that the electron (a) will tunnel through the barrier? (b) will be reflected?

Ans: 0.0103, 0.990



- 9 A quantum simple harmonic oscillator consists of an electron bound by a restoring force proportional to its position relative to a certain equilibrium point. The proportionality constant is 8.99 N/m. What is the longest wavelength of light that can excite the oscillator?

Ans: 600nm

- 10 A quantum simple harmonic oscillator consists of a particle of mass m bound by a restoring force proportional to its position relative to a certain equilibrium point. The proportionality constant is k . What is the longest wavelength of light that can excite the oscillator? Ans: $2\pi c \sqrt{\frac{m}{k}}$

5 ATOMIC PHYSICS

OBJECTIVES:

- To know about the quantum model of H-atom and its wave functions.
- To understand more about Visible and X ray spectra
- To explain basic interactions of radiation with matter.
- To understand the basic principles and requirements for working of laser.
- To recognize the various applications of laser.
- To apply and evaluate the above concepts by solving numerical problems

5.1 THE QUANTUM MODEL OF THE HYDROGEN ATOM

The formal procedure for solving the problem of the hydrogen atom is to substitute the appropriate potential energy function into the Schrödinger equation, find solutions to the equation, and apply boundary conditions as we did for the particle in a box.

The potential energy function for the H-atom is

$$U(r) = -\frac{k_e e^2}{r} \quad (5.1)$$

where $k_e = 1/4\pi\epsilon_0 = 8.99 \times 10^9 \text{ N.m}^2/\text{C}^2$ Coulomb constant and r is radial distance of electron from H-nucleus. The mathematics for the hydrogen atom is more complicated than that for the particle in a box because the atom is three-dimensional, and U depends on the radial coordinate r .

The time-independent Schrödinger equation in 3-dimensional space is

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + U \psi = E \psi \quad (5.2)$$

Since U has spherical symmetry, it is easier to solve the Schrödinger equation in spherical polar coordinates (r, θ, ϕ) where $r = \sqrt{x^2 + y^2 + z^2}$,

θ is the angle between z-axis and \vec{r} . ϕ is the angle between the x-axis and the projection of \vec{r} onto the xy-plane.

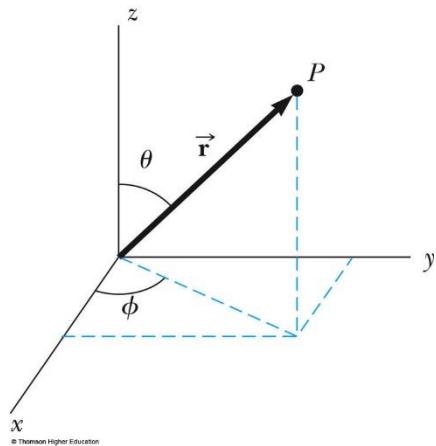


Figure 5.1 Spherical polar coordinate system

It is possible to separate the variables r, θ, ϕ as follows:

$$\psi(r, \theta, \phi) = R(r)f(\theta)g(\phi)$$

By solving the three separate ordinary differential equations for $R(r), f(\theta), g(\phi)$, with conditions that the normalized ψ and its first derivative are continuous and finite everywhere, one gets three different quantum numbers for each allowed state of the H-atom. The quantum numbers are integers and correspond to the three independent degrees of freedom.

The radial function $R(r)$ of ψ is associated with the **principal** quantum number n . Solving $R(r)$, we get an expression for energy as,

$$E_n = -\left(\frac{k_e e^2}{2 a_0}\right) \frac{1}{n^2} = -\frac{13.606 \text{ eV}}{n^2}, \quad n = 1, 2, 3, \dots \quad (5.3)$$

which is in agreement with Bohr theory.

The polar function $f(\theta)$ is associated with the **orbital** quantum number ℓ . The azimuthal function $g(\phi)$ is associated with the **orbital magnetic** quantum number m_ℓ . The application of boundary conditions on the three parts of ψ leads to important relationships among the three quantum numbers:

n can range from 1 to ∞ ,

ℓ can range from 0 to $n-1$; [n allowed values].

m_ℓ can range from $-\ell$ to $+\ell$; [$(2\ell+1)$ allowed values].

All states having the same principal quantum number are said to form a shell. All states having the same values of n and ℓ are said to form a subshell:

$$n = 1 \Rightarrow \text{K shell}$$

$$\ell = 0 \Rightarrow \text{s subshell}$$

$n = 2 \Rightarrow$	L shell	$\ell = 1 \Rightarrow$	p subshell
$n = 3 \Rightarrow$	M shell	$\ell = 2 \Rightarrow$	d subshell
$n = 4 \Rightarrow$	N shell	$\ell = 3 \Rightarrow$	f subshell
$n = 5 \Rightarrow$	O shell	$\ell = 4 \Rightarrow$	g subshell
$n = 6 \Rightarrow$	P shell	$\ell = 5 \Rightarrow$	h subshell
...	

5.2 WAVE FUNCTIONS FOR HYDROGEN

The potential energy for H-atom depends only on the radial distance r between nucleus and electron. Therefore some of the allowed states for the H-atom can be represented by wave functions that depend only on r (spherically symmetric function). The simplest wave function for H-atom is the **1s-state (ground state) wave function** ($n = 1, \ell = 0$):

$$\psi_{1s}(r) = \frac{1}{\sqrt{\pi a_0^3}} \exp\left(-\frac{r}{a_0}\right) \text{ where } a_0 \text{ is Bohr radius (0.0529 nm).} \quad (5.4)$$

$|\psi_{1s}|^2$ is the probability density for H-atom in 1s-state:

$$|\psi_{1s}|^2 = \frac{1}{\pi a_0^3} \exp\left(-\frac{2r}{a_0}\right) \quad (5.5)$$

The **radial probability density $P(r)$** is the probability per unit radial length of finding the electron in a spherical shell of radius r and thickness dr .

$P(r)dr$ is the probability of finding the electron in this shell.

$$\begin{aligned} P(r) dr &= |\psi|^2 dv = |\psi|^2 4\pi r^2 dr \\ \therefore P(r) &= 4\pi r^2 |\psi|^2 \end{aligned}$$

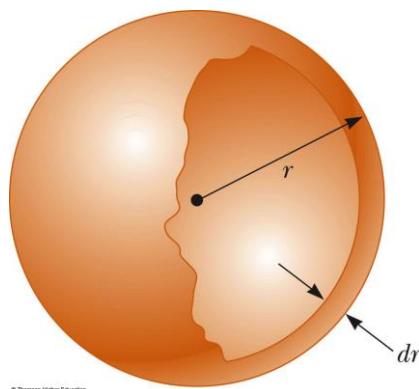


Figure 5.2 A spherical shell of radius r and thickness dr has a volume equal to $4\pi r^2 dr$

Radial probability density for H-atom in its ground state:

$$P_{1s} = \left(\frac{4r^2}{a_0^3}\right) \exp\left(-\frac{2r}{a_0}\right)$$

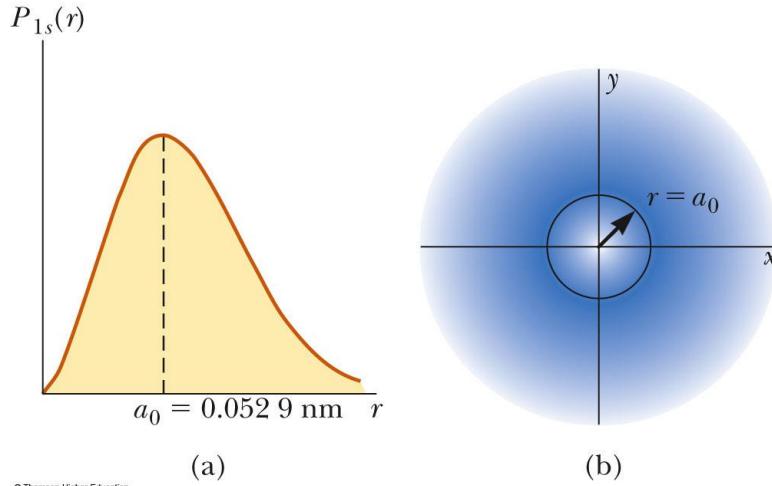


Figure 5.3 (a) The probability of finding the electron as a function of distance from the nucleus for the hydrogen atom in the 1s (ground) state. (b) The cross section in the xy plane of the spherical electronic charge distribution for the hydrogen atom in its 1s state

The next simplest wave function for the H-atom is the **2s-state wave function** ($n = 2$, $\ell = 0$):

$$\psi_{2s}(r) = \frac{1}{\sqrt{32\pi a_0^3}} \left(2 - \frac{r}{a_0}\right) \exp\left(-\frac{r}{a_0}\right) \quad (5.6)$$

ψ_{2s} is spherically symmetric (depends only on r). Energy corresponding to $n = 2$ (first excited state) is $E_2 = E_1/4 = -3.401$ eV.

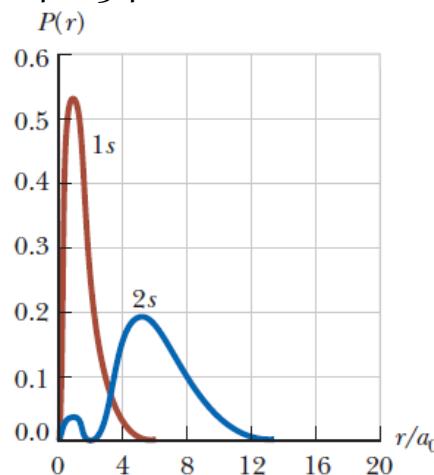


Figure 5.4 Plot of radial probability density versus r/a_0 (normalized radius) for 1s and 2s states of hydrogen atom

5.3 MORE ON ATOMIC SPECTRA: VISIBLE AND X-RAY

These spectral lines have their origin in transitions between quantized atomic states. A modified energy-level diagram for hydrogen is shown in the Figure 5.5.

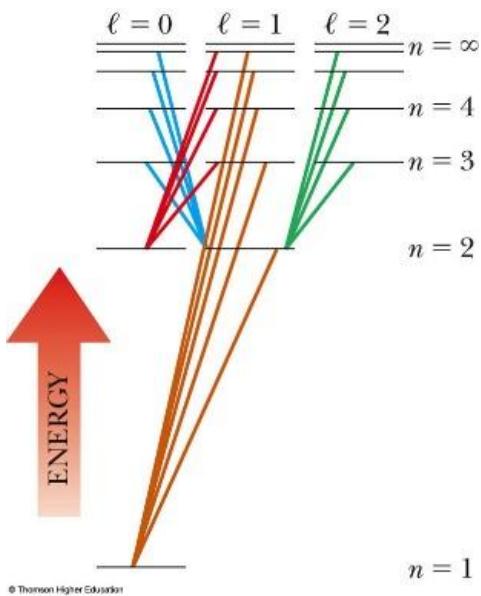


Figure 5.5 Some allowed electronic transitions for hydrogen, represented by the colored lines

In this diagram, the allowed values of ℓ , for each shell are separated horizontally. Figure shows only those states up to $\ell = 2$, the shells from $n = 4$, upward would have more sets of states to the right, which are not shown. Transitions for which ℓ does not change are very unlikely to occur and are called *forbidden transitions*. (Such transitions actually can occur, but their probability is very low relative to the probability of “allowed” transitions.) The various diagonal lines represent allowed transitions between stationary states. Whenever an atom makes a transition from a higher energy state to a lower one, a photon of light is emitted.

The frequency of this photon is $f = \Delta E/h$, where ΔE is the energy difference between the two states and h is Planck’s constant. The **selection rules** for the *allowed transitions* are

$$\Delta\ell = \pm 1 \quad \text{and} \quad \Delta m_\ell = 0, \pm 1$$

The allowed energies for one-electron atoms and ions, such as hydrogen (H) and helium ion (He^+), are

$$E_n = -\frac{k_e e^2}{2a_0} \left(\frac{Z^2}{n^2} \right) = -\frac{(13.6 \text{ eV}) Z^2}{n^2} \quad (5.7)$$

This equation was developed from the Bohr theory, but it serves as a good first approximation in quantum theory as well. For multi-electron atoms, the positive nuclear charge Ze is largely shielded by the negative charge of the inner-shell electrons. Therefore, the outer electrons interact with a net charge that is smaller than the nuclear charge.

Hence, we can write

$$E_n = -\frac{(13.6 \text{ eV}) Z_{\text{eff}}^2}{n^2} \quad (5.8)$$

where Z_{eff} depends on n and ℓ

5.4 X-RAY SPECTRA

X-rays are emitted when high-energy electrons or any other charged particles bombard a metal target. The x-ray spectrum typically consists of a broad continuous band containing a series of sharp lines as shown in Figure 5.6. So, the x-ray spectrum has two parts: **continuous spectrum** and **characteristic spectrum**.

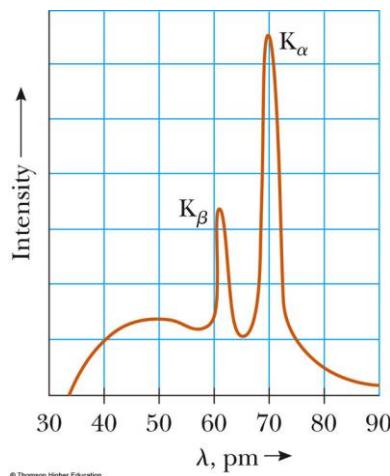


Figure 5.6 The x-ray spectrum of a metal target. The data shown were obtained when 37-keV electrons bombarded a molybdenum target.

An accelerated electric charge emits electromagnetic radiation. The x-rays in figure are the result of the slowing down of high-energy electrons as they strike the target. It may take several interactions with the atoms of the target before the electron loses all its kinetic energy. The amount of kinetic energy lost in any given interaction can vary from zero up to the entire kinetic energy of the electron. Therefore, the wavelength of radiation from these interactions lies in a **continuous** range from some minimum value up to infinity. It is this general slowing down of the electrons

that provides the continuous curve, which shows the cutoff of x-rays below a minimum wavelength value that depends on the kinetic energy of the incoming electrons. X-ray radiation with its origin in the slowing down of electrons is called **bremsstrahlung**, the German word for “braking radiation”.

Thus the emitted x-rays can have any value for the wavelength above λ_{MIN} in the continuous x-ray spectrum. Thus

$$e\Delta V = hf_{MAX} = \frac{hc}{\lambda_{MIN}}$$

$$\lambda_{MIN} = \frac{hc}{e\Delta V} \quad (5.9)$$

λ_{MIN} depends only on ΔV

The peaks in the x-ray spectrum is the **characteristic of the target element** in the x-ray tube and hence they form the characteristic x-ray spectrum. When a high energy ($K = e\Delta V$, ΔV = x-ray tube voltage) electron strikes a target atom and knocks out one of its electrons from the inner shells with energy E_{nf} ($|E_{nf}| \leq K$, n_f = integer), the vacancy in the inner shell is filled up by an electron from the outer shell (energy = E_{ni} , n_i = integer). The characteristic x-ray photon emitted has the energy:

$$hf = \frac{hc}{\lambda} = E_{ni} - E_{nf}$$

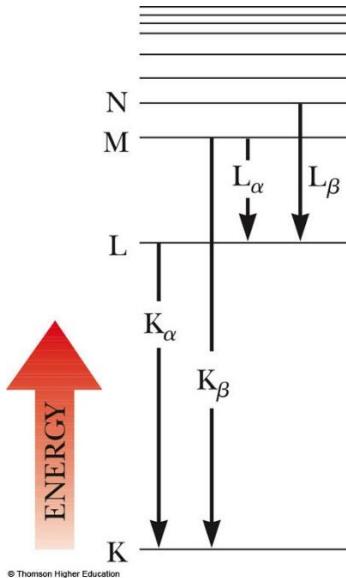


Figure 5.7 Transitions between higher and lower atomic energy levels that give rise to x-ray photons from heavy atoms when they are bombarded with high-energy electrons.

A K_{α} x-ray results due to the transition of the electron from L-shell to K-shell. A K_{β} x-ray results due to the transition of the electron from M-shell to K-shell. When the vacancy arises in the L-shell, an L-series ($L_{\alpha}, L_{\beta}, L_{\gamma}$) of x-rays results. Similarly, the origin of M-series of x-rays can be explained. **Moseley's observation** on the characteristic K_{α} x-rays shows a relation between the frequency (f) of the K_{α} x-rays and the atomic number (Z) of the target element in the x-ray tube:

$$\sqrt{f} = C(Z - 1) \quad (5.10)$$

where C is a constant.

Note: Based on this observation, the elements are arranged according to their atomic numbers in the periodic table

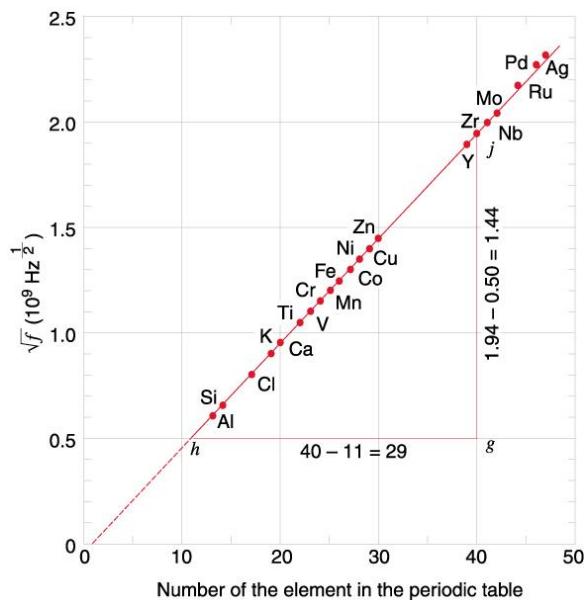


Figure 5.8 Moseley plot

5.5 SPONTANEOUS AND STIMULATED TRANSITIONS

There are three possible processes that involve interaction between matter and radiation.

Stimulated Absorption: Absorption of a photon of frequency f takes place when the energy difference $E_2 - E_1$ of the allowed energy states of the atomic/molecular system equals the energy hf of the photon. Then the photon disappears and the atomic system moves to upper energy state E_2 .

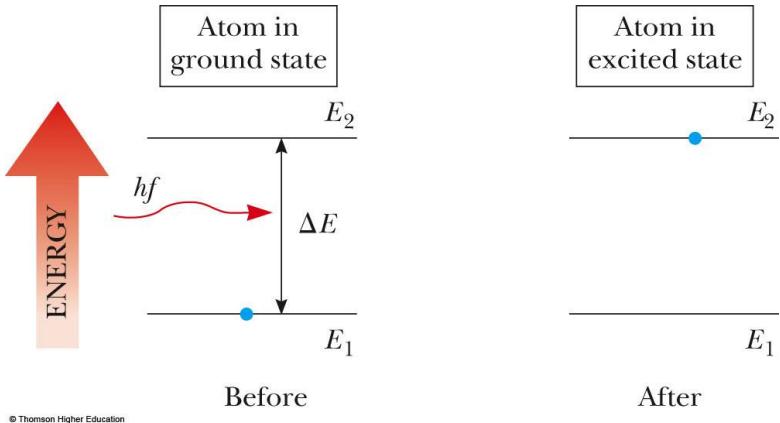


Figure 5.9 Stimulated absorption of a photon

Spontaneous Emission: The average life time of the atomic system in the excited state is of the order of 10^{-8} s. After the life time of the atomic system in the excited state, it comes back to the state of lower energy on its own accord by emitting a photon of energy $hf = E_2 - E_1$.

This is the case with ordinary light sources. The radiations are emitted in different directions in random manner. Such type of emission of radiation is called spontaneous emission and the emitted light is not coherent.

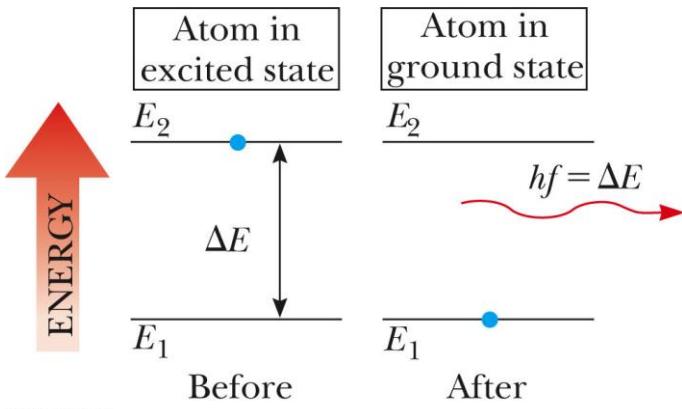


Figure 5.10 Spontaneous Emission of a photon

Stimulated Emission: When a photon (called stimulating photon) of suitable frequency interacts with an excited atomic system, the latter comes down to ground state by emitting a photon of same energy. Such an emission of radiation is called stimulated emission. In stimulated emission, both the stimulating photon and the emitted photon (due to stimulation) are of same frequency, same phase, same state of polarization and in the same direction. In other words, these two photons are coherent.

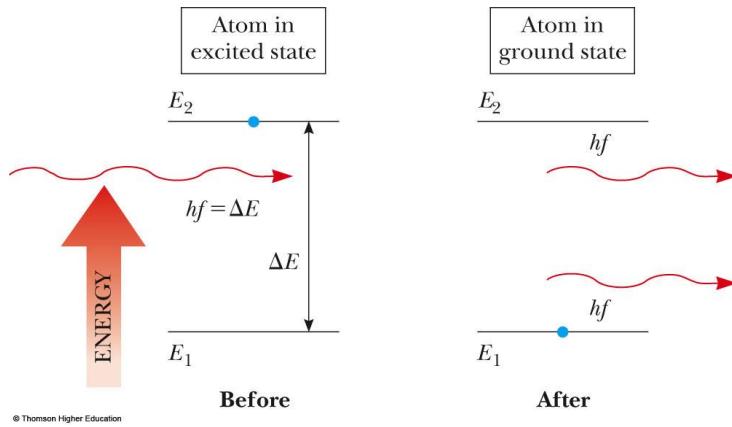


Figure 5.11 Stimulated Emission

All the three processes are taking place simultaneously to varying degrees, in the matter when it is irradiated by radiation of suitable frequency.

Population inversion: From Boltzmann statistics, the ratio of population of atoms in two energy states E_1 and E_2 at equilibrium temperature T is,

$$\frac{n(E_2)}{n(E_1)} = \exp\left(-\frac{E_2 - E_1}{kT}\right) \quad (5.11)$$

where k is Boltzmann constant, $n(E_1)$ is the number density of atoms with energy E_1 , $n(E_2)$ is the number density of atoms with energy E_2 . Under normal condition, where populations are determined only by the action of thermal agitation, population of the atoms in upper energy state is less than that in lower energy state (i.e. $n(E_2) < n(E_1)$, Figure 5.12a).

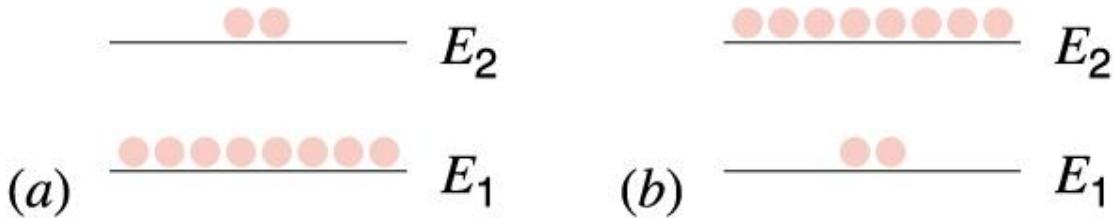


Figure 5.12 (a) Normal thermal equilibrium distribution of atomic systems (b) An inverted population, obtained using special techniques

We have described how an incident photon can cause atomic energy transitions either upward (stimulated absorption) or downward (stimulated emission). The two processes are equally probable. When light is incident on a collection of atoms, a net absorption of energy usually occurs because when the system is in thermal equilibrium, many more atoms are in the ground state than in excited states. If the situation can be inverted so that more atoms are in an excited state than in the

ground state, however, a net emission of photons can result. Such a condition is called **population inversion**.

5.6 LASER (LIGHT AMPLIFICATION BY STIMULATED EMISSION OF RADIATION)

Laser light is highly monochromatic, intense, coherent, directional and can be sharply focused. Each of these characteristics that are not normally found in ordinary light makes laser a unique and the most powerful tool. Population inversion is, in fact, the fundamental principle involved in the operation of a **laser**. The full name indicates one of the requirements for laser light: to achieve laser action, the process of stimulated emission must occur.

For the stimulated emission rate to exceed the absorption rate it is necessary to have higher population of upper energy state than that of lower energy state. This condition is called population inversion [$n(E_2) > n(E_1)$]. This is a non-equilibrium condition and is facilitated by the presence of energy states called '**metastable states**' where the average life time of the atom is 10^{-3} s which is much longer than that of the ordinary excited state ($\approx 10^{-8}$ s).

Suppose an atom is in the excited state E_2 as in the below figure and a photon with energy $hf = E_2 - E_1$ is incident on it. The incoming photon can stimulate the excited atom to return to the ground state and thereby emit a second photon having the same energy hf and traveling in the same direction. The incident photon is not absorbed, so after the stimulated emission, there are two identical photons: the incident photon and the emitted photon. The emitted photon is in phase with the incident photon. These photons can stimulate other atoms to emit photons in a chain of similar processes. The many photons produced in this fashion are the source of the intense, coherent light in a laser.

For the stimulated emission to result in laser light, there must be a buildup of photons in the system. The following three conditions must be satisfied to achieve this buildup:

- The system must be in a state of **population inversion**: there must be more atoms in an excited state than in the ground state. That must be true because the number of photons emitted must be greater than the number absorbed.
- The excited state of the system must be a **metastable state**, meaning that its lifetime must be long compared with the usually short lifetimes of excited states, which are typically 10^{-8} s. In this case, the population inversion can be established and stimulated emission is likely to occur before spontaneous emission.
- The **emitted photons must be confined** in the system long enough to enable them to stimulate further emission from other excited atoms. That is achieved by using reflecting mirrors at the ends of the system. One end is made totally reflecting,

and the other is partially reflecting. A fraction of the light intensity passes through the partially reflecting end, forming the beam of laser light.

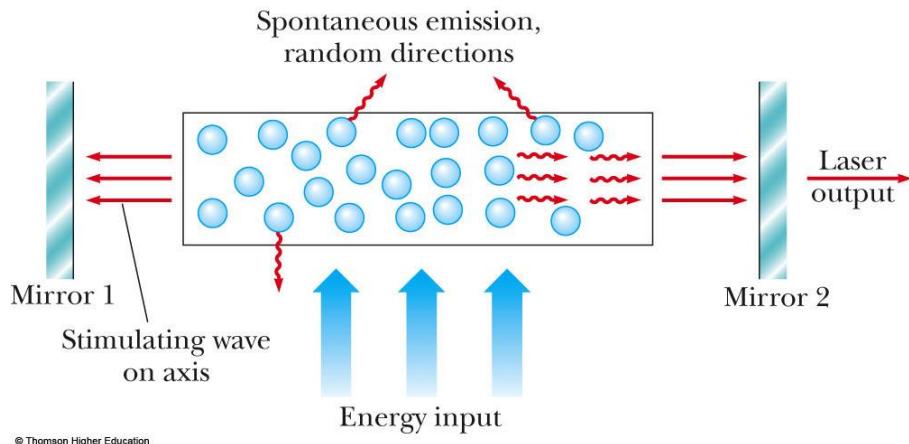


Figure 5.13 Schematic diagram of a laser design.

Lasing medium (active medium), resonant cavity and pumping system are the essential parts of any lasing system. Lasing medium has atomic systems (active centers), with special energy levels which are suitable for laser action. This medium may be a gas, or a liquid, or a crystal or a semiconductor. The atomic systems in this may have energy levels including a ground state (E_1), an excited state (E_3^*) and a metastable state (E_2). The resonant cavity is a pair of parallel mirrors to reflect the radiation back into the lasing medium. Pumping is a process of exciting more number of atoms in the ground state to higher energy states, which is required for attaining the population inversion.

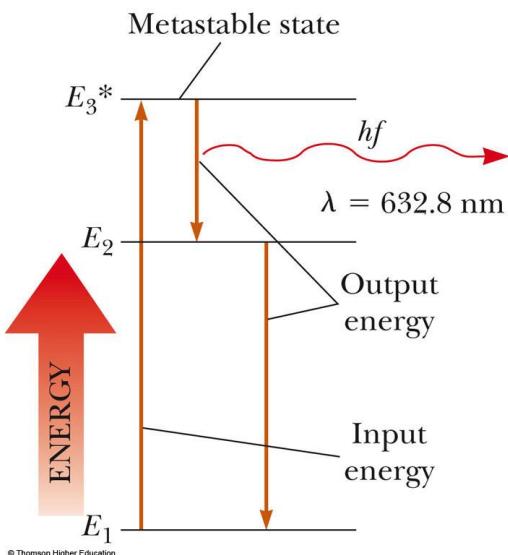


Figure 5.14 Energy-level diagram for a neon atom in a helium–neon laser.

In He-Ne laser, the mixture of helium and neon is confined to a glass tube that is sealed at the ends by mirrors. A voltage applied across the tube causes electrons to sweep through the tube, colliding with the atoms of the gases and raising them into excited states. Neon atoms are excited to state E_3^* through this process (the asterisk indicates a metastable state) and also as a result of collisions with excited helium atoms. Stimulated emission occurs, causing neon atoms to make transitions to state E_2 . Neighboring excited atoms are also stimulated. The result is the production of coherent light at a wavelength of 632.8 nm.

5.7 APPLICATIONS OF LASER

Laser is used in various scientific, engineering and medical applications. It is used in investigating the basic laws of interaction of atoms and molecules with electromagnetic wave of high intensity. Laser is widely used in engineering applications like optical communication, micro-welding and sealing etc. In medical field, laser is used in bloodless and painless surgery especially in treating the retinal detachment. Also used as a tool in treating dental decay, tooth extraction, cosmetic surgery.

5.8 QUESTIONS

- 1 Give a brief account of quantum model of H-atom.
Explain the origin of (i) orbital quantum number (ii) magnetic orbital quantum number and write the relation between them
- 2 The wave function for H-atom in ground state is $\psi_{1s}(r) = \frac{1}{\sqrt{\pi a_0^3}} \exp\left(-\frac{r}{a_0}\right)$. Obtain an expression for the radial probability density of H-atom in ground state.
Sketch schematically the plot of this vs. radial distance.
- 3 The wave function for H-atom in $2s$ state is $\psi_{2s}(r) = \frac{1}{\sqrt{32\pi a_0^3}} \left(2 - \frac{r}{a_0}\right) \exp\left(-\frac{r}{a_0}\right)$. Write the expression for the radial probability density of H-atom in $2s$ state. Sketch schematically the plot of this vs. radial distance.
- 4 Sketch schematically the plot of the radial probability density vs. radial distance for H-atom in $1s$ -state and $2s$ -state.
- 5 Explain the continuous x-ray spectrum with a schematic plot of the spectrum.
- 6 Explain the origin of characteristic x-ray spectrum with a sketch of x-ray energy level diagram.

- 7 Write Moseley's relation for the frequency of characteristic x-rays. sketch schematically the Moseley's plot of characteristic x-rays.
- 8 Explain three types of transitions between two energy levels, when radiation interacts with matter
- 9 Explain the characteristics of a laser beam
- 10 Explain metastable state
- 11 What is population inversion? explain
- 12 Describe the principle of a laser using necessary schematic design and energy level diagram
- 13 Mention any four applications of laser.
- 14 Describe the three important conditions need to be satisfied to achieve laser action

5.9 PROBLEMS

- 1 For a H-atom, determine the number of allowed states corresponding to the principal quantum number $n = 2$, and calculate the energies of these states.

Ans: 4 states (one $2s$ -state + three $2p$ -states), -3.401 eV

- 2 A general expression for the energy levels of one-electron atoms and ions is $E_n = -\frac{\mu k_e^2 q_1^2 q_2^2}{2 \hbar^2 n^2}$, where k_e is the Coulomb constant, q_1 and q_2 are the charges of the electron and the nucleus, and μ is the reduced mass, given by $\mu = \frac{m_1 m_2}{m_1 + m_2}$. The wavelength for $n = 3$ to $n = 2$ transition of the hydrogen atom is 656.3 nm (visible red light). What are the wavelengths for this same transition (a) positronium, which consists of an electron and a positron, and (b) singly ionized helium ?

Ans: 1310 nm , 164 nm

- 3 Calculate the most probable value of r (= distance from nucleus) for an electron in the ground state of the H-atom. Also calculate the average value r for the electron in the ground state.

Ans: a_0 , $3 a_0/2$

- 4 Calculate the probability that the electron in the ground state of H-atom will be found outside the Bohr radius.

Ans: 0.677

- 5 For a spherically symmetric state of a H-atom the Schrodinger equation in spherical coordinates is $-\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial r^2} + \frac{2}{r} \frac{\partial \psi}{\partial r} \right) - \frac{k_e e^2}{r} \psi = E \psi$. Show

that the $1s$ wave function for an electron in H-atom $\psi_{1s}(r) = \frac{1}{\sqrt{\pi a_0^3}} \exp\left(-\frac{r}{a_0}\right)$ satisfies the Schrodinger equation.

- 6** The ground-state wave function for the electron in a hydrogen atom is

$$\psi_{1s}(r) = \frac{1}{\sqrt{\pi a_0^3}} \exp\left(-\frac{r}{a_0}\right)$$

where r is the radial coordinate of the electron and a_0 is the Bohr radius.

- (a) Show that the wave function as given is normalized. (b) Find the probability of locating the electron between $r_1 = a_0/2$ and $r_2 = 3a_0/2$.
- 7 What minimum accelerating voltage would be required to produce an x-ray with a wavelength of 70.0 pm? Ans: 17.7 kV
- 8 A tungsten target is struck by electrons that have been accelerated from rest through a 40.0-keV potential difference. Find the shortest wavelength of the radiation emitted. Ans: 0.031 nm
- 9** A bismuth target is struck by electrons, and x-rays are emitted. Estimate (a) the M- to L-shell transitional energy for bismuth and (b) the wavelength of the x-ray emitted when an electron falls from the M shell to the L shell.
Ans: (a) 14 keV (b) 0.885 Å
- 10 The $3p$ level of sodium has an energy of -3.0 eV, and the $3d$ level has an energy of -1.5 eV. (a) Determine Z_{eff} for each of these states. (b) Explain the difference. Ans: (a) 1.4 and 1.0
- 11 The K series of the discrete x-ray spectrum of tungsten contains wavelengths of 0.0185 nm, 0.0209 nm, and 0.0215 nm. The K-shell ionization energy is 69.5 keV.
(a) Determine the ionization energies of the L, M, and N shells.
(b) Draw a diagram of the transitions.
Ans: (a) L shell = 11.8 keV ; M shell = 10.2 keV ; N shell = 2.47 keV

- [12]** When an electron drops from the M shell ($n = 3$) to a vacancy in the K shell ($n = 1$), the measured wavelength of the emitted x-ray is found to be 0.101 nm. Identify the element. Ans: Gallium ($Z=31$)
- [13]** A ruby laser delivers a 10.0-ns pulse of 1.00-MW average power. If the photons have a wavelength of 694.3 nm, how many are contained in the pulse? Ans: 3.49×10^{16} photons
- 14** A pulsed laser emits light of wavelength λ . For a pulse of duration Δt having energy T_{ER} , find (a) the physical length of the pulse as it travels through space and (b) the number of photons in it. (c) The beam has a circular cross section having diameter d . Find the number of photons per unit volume. (a) $c\Delta t$ (b) $\frac{\lambda T_{ER}}{hc}$ (c) $n = \frac{4\lambda T_{ER}}{\pi h c^2 d^2 \Delta t}$

6 MOLECULES AND SOLIDS

OBJECTIVES:

- To understand the bonding mechanism, energy states and spectra of molecules
- To understand the cohesion of solid metals using bonding in solids
- To comprehend the electrical properties of metals, semiconductors and insulators
- To understand the effect of doping on electrical properties of semiconductors
- To understand superconductivity and its engineering applications

6.1 MOLECULAR BONDS

The bonding mechanisms in a molecule are fundamentally due to electric forces between atoms (or ions). The forces between atoms in the system of a molecule are related to a potential energy function. A *stable molecule is expected at a configuration for which the potential energy function for the molecule has its minimum value*. A potential energy function that can be used to model a molecule should account for two known features of molecular bonding:

1. The force between atoms is repulsive at very small separation distances. This repulsion is partly electrostatic in origin and partly the result of the exclusion principle.
2. At relatively larger separations, the force between atoms is attractive. Considering these two features, the potential energy for a system of two atoms can be represented by an expression of the form (Lennard-Jones potential)

$$U(r) = -\frac{A}{r^n} + \frac{B}{r^m} \quad (6.1)$$

where r is the internuclear separation distance between the two atoms and n and m are small integers. The parameter A is associated with the attractive force and B with the repulsive force. Potential energy versus internuclear separation distance for a two-atom system is graphed in Figure 6.1.

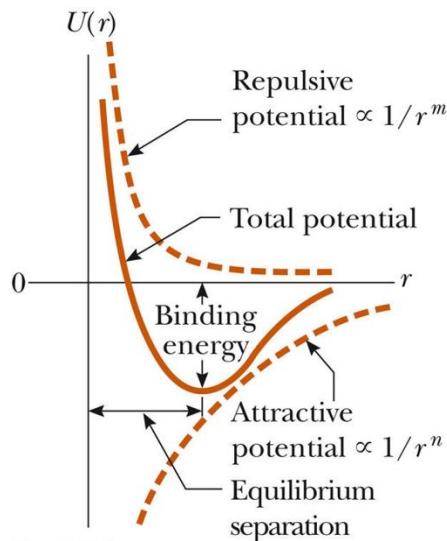


Figure 6.1 Total potential energy as a function of internuclear separation distance for a system of two atoms.

Ionic Bonding: When two atoms combine in such a way that one or more outer electrons are transferred from one atom to the other, the bond formed is called an ionic bond. Ionic bonds are fundamentally caused by the Coulomb attraction between oppositely charged ions.

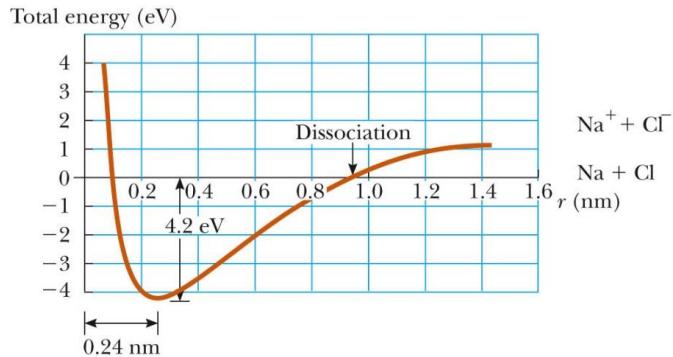


Figure 6.2 Total energy versus internuclear separation distance for Na^+ and Cl^- ions.

A familiar example of an ionically bonded solid is sodium chloride, NaCl , which is common table salt. Sodium, which has the electronic configuration $1s^2 2s^2 2p^6 3s^1$, is ionized relatively easily, giving up its $3s$ electron to form a Na^+ ion. The energy required to ionize the atom to form Na^+ is 5.1 eV. Chlorine, which has the electronic configuration $1s^2 2s^2 2p^5$ is one electron short of the filled-shell structure of argon. The amount of energy released when an electron joins Cl atom to make the Cl^- ion, called the **electron affinity** of the atom, is 3.6 eV. Therefore, the energy required to form Na^+ and Cl^- from isolated atoms is $5.1 - 3.6 = 1.5$ eV. The total energy of the NaCl molecule versus internuclear separation distance is graphed in Figure 6.2. At very large separation distances, the energy of the system of ions is 1.5 eV as calculated above. The total energy has a minimum value of - 4.2 eV at the equilibrium

separation distance, which is approximately 0.24 nm. Hence, the energy required to break the $\text{Na}^+ - \text{Cl}^-$ bond and form neutral sodium and chlorine atoms, called the **dissociation energy**, is 4.2 eV. The energy of the molecule is lower than that of the system of two neutral atoms. Consequently, it is **energetically favorable** for the molecule to form.

Covalent Bonding: A covalent bond between two atoms is one in which electrons supplied by either one or both atoms are shared by the two atoms. Many diatomic molecules such as H_2 , F_2 , and CO —owe their stability to covalent bonds. The bond between two hydrogen atoms can be described by using atomic wave functions for two atoms. There is very little overlap of the wave functions $\psi_1(r)$ for atom 1, located at $r = 0$, and $\psi_2(r)$ for atom 2, located some distance away (Figure 6.3a). Suppose now the two atoms are brought close together, their wave functions overlap and form the compound wave function $\psi_1(r) + \psi_2(r)$ shown in Figure 6.3b. Notice that the probability amplitude is larger between the atoms than it is on either side of the combination of atoms. As a result, the probability is higher that the electrons associated with the atoms will be located between the atoms than on the outer regions of the system. Consequently, the average position of negative charge in the system is halfway between the atoms.

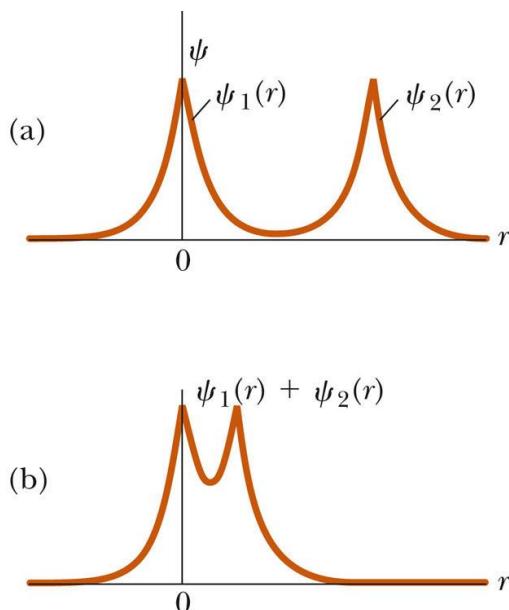


Figure 6.3 Ground-state wave functions $\psi_1(r)$ and $\psi_2(r)$ for two atoms making a covalent bond. (a) The atoms are far apart, and their wave functions overlap minimally. (b) The atoms are close together, forming a composite wave function $\psi_1(r) + \psi_2(r)$ for the system.

Van der Waals Bonding: Ionic and covalent bonds occur between atoms to form molecules or ionic solids, so they can be described as bonds *within* molecules. The

van der Waals force results from the following situation. While being electrically neutral, a molecule has a charge distribution with positive and negative centers at different positions in the molecule. As a result, the molecule may act as an electric dipole. Because of the dipole electric fields, two molecules can interact such that there is an attractive force between them. There are three types of van der Waals forces.

The first type, called the **dipole-dipole force**, is an interaction between two molecules each having a permanent electric dipole moment. For example, polar molecules such as HCl have permanent electric dipole moments and attract other polar molecules.

The second type, the **dipole-induced dipole force**, results when a polar molecule having a permanent electric dipole moment induces a dipole moment in a nonpolar molecule. In this case, the electric field of the polar molecule creates the dipole moment in the nonpolar molecule, which then results in an attractive force between the molecules.

The third type is called the **dispersion force**, an attractive force that occurs between two nonpolar molecules. Two nonpolar molecules near each other tend to have dipole moments that are correlated in time so as to produce an attractive van der Waals force.

Hydrogen Bonding: Because hydrogen has only one electron, it is expected to form a covalent bond with only one other atom within a molecule. A hydrogen atom in a given molecule can also form a second type of bond between molecules called a **hydrogen bond**. Let's use the water molecule H_2O as an example. In the two covalent bonds in this molecule, the electrons from the hydrogen atoms are more likely to be found near the oxygen atom than near the hydrogen atoms, leaving essentially bare protons at the positions of the hydrogen atoms. This unshielded positive charge can be attracted to the negative end of another polar molecule. Because the proton is unshielded by electrons, the negative end of the other molecule can come very close to the proton to form a bond strong enough to form a solid crystalline structure, such as that of ordinary ice. The bonds within a water molecule are covalent, but the bonds between water molecules in ice are hydrogen bonds. The hydrogen bond is relatively weak compared with other chemical bonds and can be broken with an input energy of approximately 0.1 eV. Because of this weakness, ice melts at the low temperature of 0°C.

6.2 ENERGY STATES AND SPECTRA OF MOLECULES

Consider an individual molecule in the gaseous phase of a substance. The energy E of the molecule can be divided into four categories: (1) electronic energy, due to the interactions between the molecule's electrons and nuclei; (2) translational energy, due to the motion of the molecule's center of mass through space; (3) rotational energy, due to the rotation of the molecule about its center of mass; and (4) vibrational energy, due to the vibration of the molecule's constituent atoms:

$$E = E_{\text{el}} + E_{\text{trans}} + E_{\text{rot}} + E_{\text{vib}}$$

Because the translational energy is unrelated to internal structure, this molecular energy is unimportant in interpreting molecular spectra. Although the electronic energies can be studied, significant information about a molecule can be determined by analyzing its quantized rotational and vibrational energy states. Transitions between these states give spectral lines in the microwave and infrared regions of the electromagnetic spectrum, respectively.

6.3 ROTATIONAL MOTION OF MOLECULES

Let's consider the rotation of a diatomic molecule around its center of mass (Figure 6.4a). A diatomic molecule aligned along a y axis has only two rotational degrees of freedom, corresponding to rotations about the x and z axes passing through the molecule's center of mass. If ω is the angular frequency of rotation about one of these axes, the rotational kinetic energy of the molecule about that axis can be expressed as

$$E_{\text{rot}} = \frac{1}{2} I \omega^2 \quad (6.2)$$

In this equation, I is the moment of inertia of the molecule about its center of mass, given by

$$I = \left(\frac{m_1 m_2}{m_1 + m_2} \right) r^2 = \mu r^2 \quad (6.3)$$

where m_1 and m_2 are the masses of the atoms that form the molecule, r is the atomic separation, and μ is the **reduced mass** of the molecule

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \quad (6.4)$$

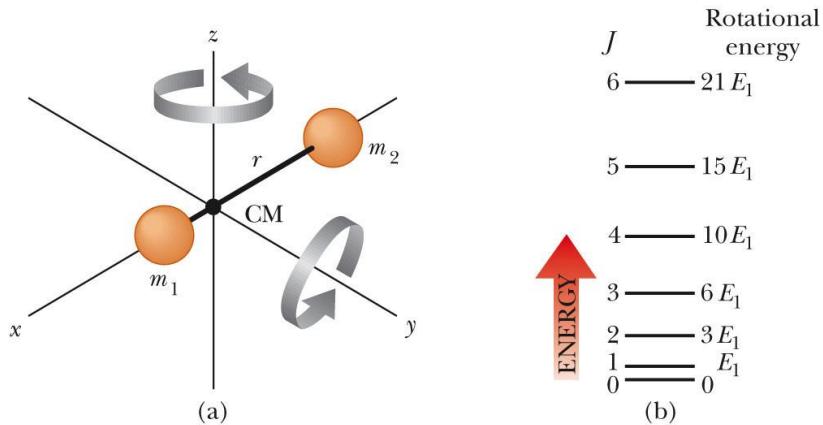


Figure 6.4 Rotation of a diatomic molecule around its center of mass. (a) A diatomic molecule oriented along the y axis. (b) Allowed rotational energies of a diatomic molecule expressed as multiples of $E_l = \hbar^2/I$.

The magnitude of the molecule's angular momentum about its center of mass is $L=I\omega$, which can attain quantized values given by,

$$L = \sqrt{J(J+1)} \hbar \quad J = 0, 1, 2, \dots \quad (6.5)$$

where J is an integer called the **rotational quantum number**. Combining Equations 6.5 and 6.2, we obtain an expression for the allowed values of the rotational kinetic energy of the molecule:

$$E_{\text{rot}} = E_J = \frac{\hbar^2}{2I} J(J+1) \quad J = 0, 1, 2, \dots \quad (6.6)$$

The allowed rotational energies of a diatomic molecule are plotted in Figure 6.4b. The allowed rotational transitions of linear molecules are regulated by the selection rule $\Delta J = \pm 1$. From Equation 6.6, the energies of the absorbed photons are given by,

$$E_{\text{photon}} = \frac{\hbar^2}{I} J = \frac{\hbar^2}{4\pi^2 I} J \quad J = 1, 2, 3, \dots \quad (6.7)$$

where J is the rotational quantum number of the higher energy state.

6.4 VIBRATIONAL MOTION OF MOLECULES

If we consider a molecule to be a flexible structure in which the atoms are bonded together by “effective springs” as shown in Figure 6.5a, we can model the molecule as a simple harmonic oscillator as long as the atoms in the molecule are not too far from their equilibrium positions. Figure 6.5b shows a plot of potential energy versus

atomic separation for a diatomic molecule, where r_0 is the equilibrium atomic separation. For separations close to r_0 , the shape of the potential energy curve closely resembles a parabola. According to classical mechanics, the frequency of vibration for the system is given by

$$f = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}} \quad (6.8)$$

where k is the effective spring constant and μ is the reduced mass given by Equation 6.4. The vibrational motion and quantized vibrational energy can be altered if the molecule acquires energy of the proper value to cause a transition between quantized vibrational states. The allowed vibrational energies are

$$E_{\text{vib}} = \left(v + \frac{1}{2} \right) hf \quad v = 0, 1, 2, \dots \quad (6.9)$$

where v is an integer called the **vibrational quantum number**.

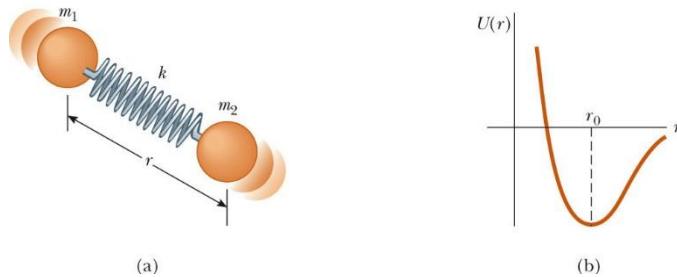


Figure 6.5 (a) Effective-spring model of a diatomic molecule. (b) Plot of the potential energy of a diatomic molecule versus atomic separation distance.

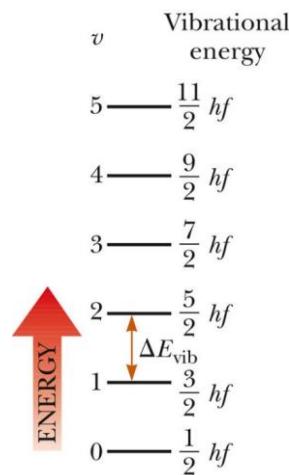


Figure 6.6 Allowed vibrational energies of a diatomic molecule, where f is the frequency of vibration of the molecule

Substituting Equation 6.8 into Equation 6.9 gives the following expression for the allowed vibrational energies:

$$E_{\text{vib}} = \left(v + \frac{1}{2}\right) \frac{h}{2\pi} \sqrt{\frac{k}{\mu}} \quad v = 0, 1, 2, \dots \quad (6.10)$$

The selection rule for the allowed vibrational transitions is $\Delta v = \pm 1$. The photon energy for transition is given by,

$$E_{\text{photon}} = \Delta E_{\text{vib}} = \frac{h}{2\pi} \sqrt{\frac{k}{\mu}} \quad (6.11)$$

The vibrational energies of a diatomic molecule are plotted in Figure 6.6. At ordinary temperatures, most molecules have vibrational energies corresponding to the $v = 0$ state because the spacing between vibrational states is much greater than $k_B T$, where k_B is Boltzmann's constant and T is the temperature.

6.5 MOLECULAR SPECTRA

In general, a molecule vibrates and rotates simultaneously. To a first approximation, these motions are independent of each other, so the total energy of the molecule is the sum of Equations 6.6 and 6.9:

$$E = \left(v + \frac{1}{2}\right) hf + \frac{\hbar^2}{2I} J(J+1) \quad (6.12)$$

The energy levels of any molecule can be calculated from this expression, and each level is indexed by the two quantum numbers v and J . From these calculations, an energy-level diagram like the one shown in Figure 6.7a can be constructed. For each allowed value of the vibrational quantum number v , there is a complete set of rotational levels corresponding to $J = 0, 1, 2, \dots$. The energy separation between successive rotational levels is much smaller than the separation between successive vibrational levels. The molecular absorption spectrum in Figure 6.7b consists of two groups of lines: one group to the right of center and satisfying the selection rules $\Delta J = +1$ and $\Delta v = +1$, and the other group to the left of center and satisfying the selection rules $\Delta J = -1$ and $\Delta v = +1$. The energies of the absorbed photons can be calculated from Equation 6.12:

$$E_{\text{photon}} = \Delta E = hf + \frac{\hbar^2}{I}(J+1) \quad J = 0, 1, 2, \dots \quad (\Delta J = +1) \quad (6.13)$$

$$E_{\text{photon}} = \Delta E = hf - \frac{\hbar^2}{I}J \quad J = 1, 2, 3, \dots \quad (\Delta J = -1) \quad (6.14)$$

where J is the rotational quantum number of the *initial* state.

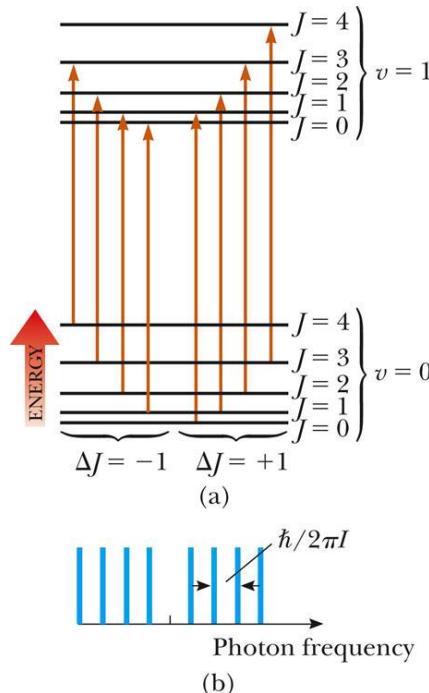


Figure 6.7 (a) Absorptive transitions between the $v = 0$ and $v = 1$ vibrational states of a diatomic molecule. (b) Expected lines in the absorption spectrum of a molecule.

The experimental absorption spectrum of the HCl molecule shown in Figure 6.8. One peculiarity is apparent, however: each line is split into a doublet. This doubling occurs because two chlorine isotopes were present in the sample used to obtain this spectrum. Because the isotopes have different masses, the two HCl molecules have different values of I .

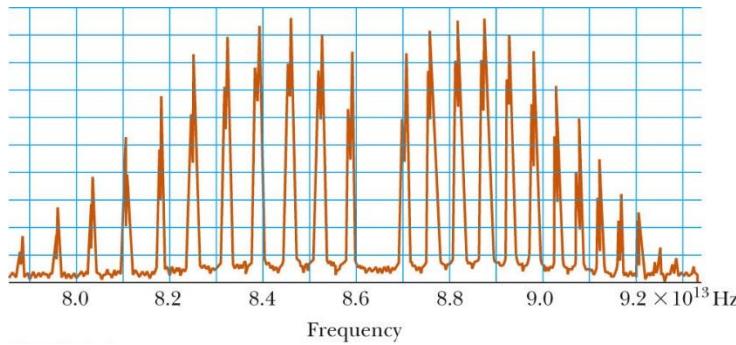


Figure 6.8 Experimental absorption spectrum of the HCl molecule

The second function determining the envelope of the intensity of the spectral lines is the Boltzmann factor. The number of molecules in an excited rotational state is given by

$$n = n_0 e^{\frac{-\hbar^2 J(J+1)}{2Ik_B T}}$$

where n_0 is the number of molecules in the $J = 0$ state.

Multiplying these factors together indicates that the intensity of spectral lines should be described by a function of J as follows:

$$\text{Intensity} \propto (2J + 1) e^{\frac{-\hbar^2 J(J+1)}{2Ik_B T}} \quad (6.15)$$

6.6 BONDING IN SOLIDS

A crystalline solid consists of a large number of atoms arranged in a regular array, forming a periodic structure.

Ionic Solids: Many crystals are formed by ionic bonding, in which the dominant interaction between ions is the Coulomb force. Consider a portion of the NaCl crystal shown in Figure 6.9a. The red spheres are sodium ions, and the blue spheres are chlorine ions. As shown in Figure 6.9b, each Na^+ ion has six nearest-neighbor Cl^- ions. Similarly, in Figure 6.9c, each Cl^- ion has six nearest-neighbor Na^+ ions. Each Na^+ ion is attracted to its six Cl^- neighbors. The corresponding potential energy is $-6k_e e^2/r$, where k_e is the Coulomb constant and r is the separation distance between each Na^+ and Cl^- . In addition, there are 12 next-nearest-neighbor Na^+ ions at a distance of $\sqrt{2}r$ from the Na^+ ion, and these 12 positive ions exert weaker repulsive forces on the central Na^+ . Furthermore, beyond these 12 Na^+ ions are more Cl_2 ions that exert an attractive force, and so on. The net effect of all these interactions is a resultant negative electric potential energy

$$U_{\text{attractive}} = -\alpha k_e \frac{e^2}{r} \quad (6.16)$$

where α is a dimensionless number known as the **Madelung constant**. The value of α depends only on the particular crystalline structure of the solid ($\alpha = 1.747$ for the NaCl structure). When the constituent ions of a crystal are brought close together, a repulsive force exists because of electrostatic forces and the exclusion principle. The potential energy term B/r_m in Equation 6.1 accounts for this repulsive force. The repulsive forces occur only for ions that are very close together.

Therefore, we can express the total potential energy of the crystal as

$$U_{\text{total}} = -\alpha k_e \frac{e^2}{r} + \frac{B}{r^m} \quad (6.17)$$

where m in this expression is some small integer.

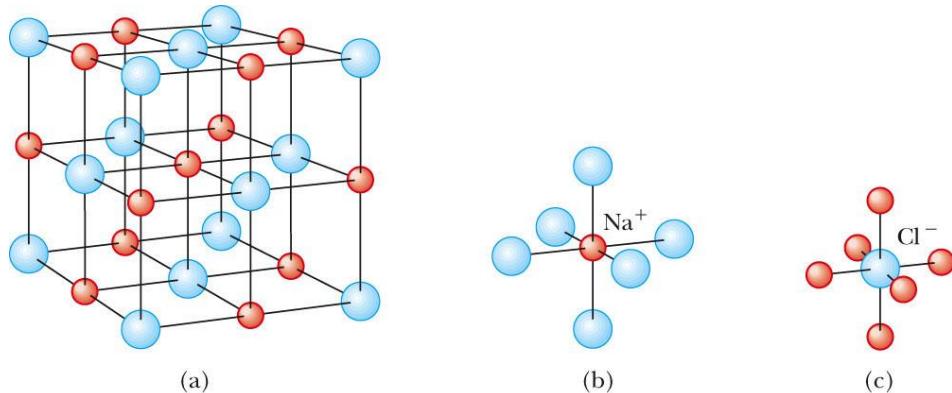


Figure 6.9 (a) Crystalline structure of NaCl. (b) Each positive sodium ion is surrounded by six negative chlorine ions. (c) Each chlorine ion is surrounded by six sodium ions

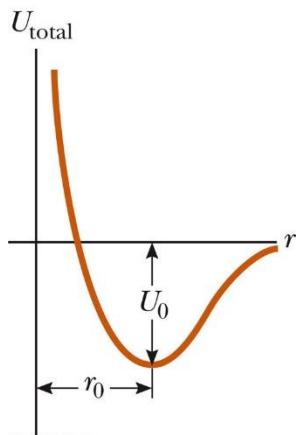


Figure 6.10 Total potential energy versus ion separation distance for an ionic solid, where U_0 is the ionic cohesive energy and r_0 is the equilibrium separation distance between ions

A plot of total potential energy versus ion separation distance is shown in Figure 6.10. The potential energy has its minimum value U_0 at the equilibrium separation, when $r = r_o$.

$$U_0 = -\alpha k_e \frac{e^2}{r_0} \left(1 - \frac{1}{m}\right) \quad (6.18)$$

This minimum energy U_0 is called the **ionic cohesive energy** of the solid, and its absolute value represents the energy required to separate the solid into a collection of isolated positive and negative ions.

Covalent Solids: Solid carbon, in the form of diamond, is a crystal whose atoms are covalently bonded. In the diamond structure, each carbon atom is covalently bonded to four other carbon atoms located at four corners of a cube as shown in Figure 6.11a. The crystalline structure of diamond is shown in Figure 6.11b. The basic structure of diamond is called tetrahedral (each carbon atom is at the center of a regular tetrahedron), and the angle between the bonds is 109.5° . Other crystals such as silicon and germanium have the same structure. Covalently bonded solids are usually very hard, have high bond energies and high melting points, and are good electrical insulators.

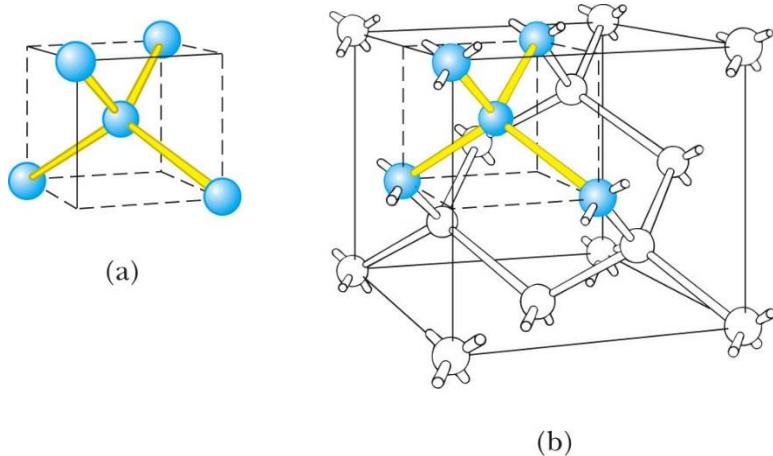


Figure 6.11 (a) Each carbon atom in a diamond crystal is covalently bonded to four other carbon atoms so that a tetrahedral structure is formed. (b) The crystal structure of diamond, showing the tetrahedral bond arrangement

Metallic Solids: Metallic bonds are generally weaker than ionic or covalent bonds. The outer electrons in the atoms of a metal are relatively free to move throughout the material, and the number of such mobile electrons in a metal is large. The metallic structure can be viewed as a “sea” or a “gas” of nearly free electrons surrounding a lattice of positive ions (Fig. 6.14). The bonding mechanism in a metal

is the attractive force between the entire collection of positive ions and the electron gas.

Light interacts strongly with the free electrons in metals. Hence, visible light is absorbed and re-emitted quite close to the surface of a metal, which accounts for the shiny nature of metal surfaces. Because the bonding in metals is between all the electrons and all the positive ions, metals tend to bend when stressed.

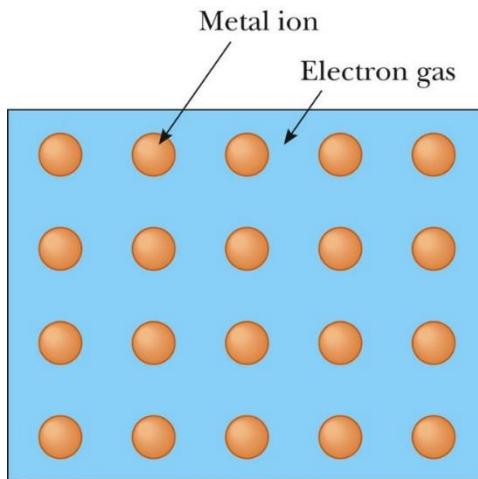


Figure 6.12 Highly schematic diagram of a metal

6.7 FREE-ELECTRON THEORY OF METALS

Quantum based free electron theory of metals is centered on wave nature of electrons. In this model, one imagines that the outer-shell electrons are free to move through the metal but are trapped within a three-dimensional box formed by the metal surfaces. Therefore, each electron is represented as a particle in a box and is restricted to quantized energy levels. Each energy state can be occupied by only two electrons (one with spin up & the other with spin down) as a consequence of exclusion principle. In quantum statistics, it is shown that the probability of a particular energy state E being occupied by an electrons is given by

$$f(E) = \frac{1}{\exp\left(\frac{E - E_F}{kT}\right) + 1} \quad (6.19)$$

where $f(E)$ is called the **Fermi-Dirac distribution function** and E_F is called the **Fermi energy**. Plot of $f(E)$ versus E is shown in figure 6.13.

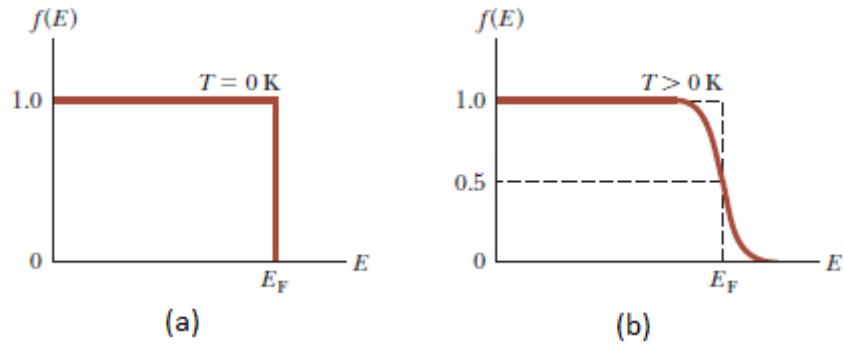


Figure. 6.13 Plot of Fermi-Dirac distribution function $f(E)$ Vs energy E at (a) $T = 0\text{K}$ and (b) $T > 0\text{K}$

At zero kelvin (0 K), all states having energies less than the Fermi energy are occupied, and all states having energies greater than the Fermi energy are vacant. i.e. Fermi energy is the highest energy possessed by an electron at 0 K (Figure 6.13a). As temperature increases ($T > 0\text{K}$), the distribution rounds off slightly due to thermal excitation and probability of Fermi level being occupied by an electron becomes half (Figure 6.13b). In other words, Fermi energy is that energy state at which probability of electron occupation is half. The Fermi energy E_F also depends on temperature, but the dependence is weak in metals.

Density of states: From particle in a box problem, for a particle of mass m is confined to move in a one-dimensional box of length L , the allowed states have quantized energy levels given by,

$$E_n = \frac{\hbar^2}{8mL^2} n^2 = \frac{\hbar^2\pi^2}{2mL^2} n^2 \quad n = 1, 2, 3 \dots \quad (6.20)$$

An electron moving freely in a metal cube of side L , can be modeled as particle in a three-dimensional box. It can be shown that the energy for such an electron is

$$E = \frac{\hbar^2\pi^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2) \quad (6.21)$$

where m is mass of the electron and n_x, n_y, n_z are quantum numbers(positive integers). Each allowed energy value is characterized by a set of three quantum numbers (n_x, n_y, n_z - one for each degree of freedom). Imagine a three-dimensional **quantum number space** whose axes represent n_x, n_y, n_z . The allowed energy states in this space can be represented as dots located at positive integral values of the three quantum numbers as shown in the Figure 6.14.

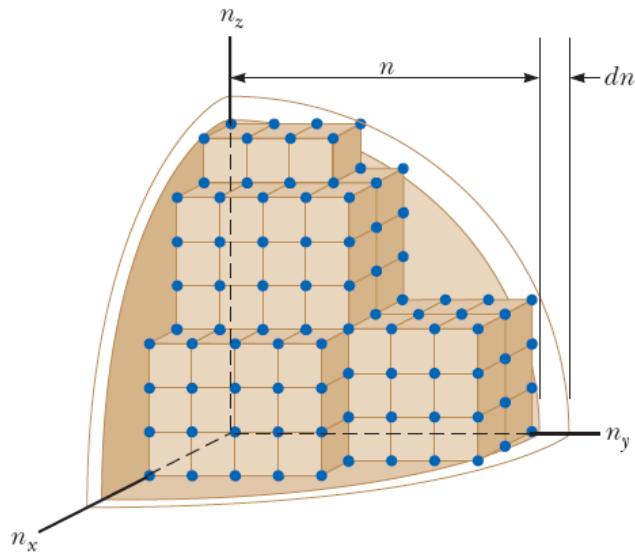


Figure 6.14 Representation of the allowed energy states in a quantum number space (dots represent the allowed states)

Eq. 6.21 can be written as

$$n_x^2 + n_y^2 + n_z^2 = \frac{E}{E_o} = n^2 \quad (6.22)$$

$$\text{where } E_o = \frac{\hbar^2 \pi^2}{2 m L^2} \text{ and } n = \sqrt{\frac{E}{E_o}}$$

Eq. 6.22 represents a sphere of radius n . Thus, the number of allowed energy states having energies between E and $E+dE$ is equal to the number of points in a spherical shell of radius n and thickness dn . In this quantum number space each point is at the corners of a **unit cube** and each corner point is shared by eight unit cubes and as such the contribution of each point to the cube is $1/8^{\text{th}}$. Because a cube has eight corners, the effective point per unit cube and hence unit volume is one. In other words, **number of points is equal to the volume of the shell**. The “volume” of this shell, denoted by $G(E)dE$.

$$G(E) dE = \left(\frac{1}{8}\right)(4\pi n^2 dn) = \left(\frac{1}{2}\right)\pi n^2 dn$$

$$G(E) dE = \frac{1}{2} \pi \left(\frac{E}{E_o} \right) d \left[\left(\frac{E}{E_o} \right)^{\frac{1}{2}} \right] \quad \text{using the relation } n = \sqrt{\frac{E}{E_o}}$$

$$G(E) dE = \frac{1}{2} \pi \left(\frac{E}{E_o} \right) E_o^{-\frac{1}{2}} \frac{1}{2} E^{-\frac{1}{2}} dE = \frac{1}{4} \pi E_o^{-\frac{3}{2}} E^{\frac{1}{2}} dE$$

$$G(E) dE = \frac{1}{4} \pi \left(\frac{\hbar^2 \pi^2}{2mL^2} \right)^{-\frac{3}{2}} E^{\frac{1}{2}} dE$$

$$G(E) dE = \frac{\sqrt{2}}{2} \frac{m^{\frac{3}{2}} L^3}{\pi^2 \hbar^3} E^{\frac{1}{2}} dE , \quad L^3 = V$$

Number of states per unit volume per unit energy range, called **density of states**, $g(E)$ is given by

$$g(E) = G(E)/V$$

$$g(E) dE = \frac{G(E)}{V} dE = \frac{\sqrt{2}}{2} \frac{m^{\frac{3}{2}}}{\pi^2 \hbar^3} E^{\frac{1}{2}} dE$$

$$g(E) dE = \frac{4\sqrt{2} \pi m^{\frac{3}{2}}}{h^3} E^{\frac{1}{2}} dE \quad \because \hbar = \frac{h}{2\pi}$$

Finally, we multiply by 2 for the two possible spin states of each particle.

$$g(E) dE = \frac{8\sqrt{2} \pi m^{\frac{3}{2}}}{h^3} E^{\frac{1}{2}} dE \quad (6.23)$$

$g(E)$ is called the **density-of-states function**.

Electron density: For a metal in thermal equilibrium, the number of electrons $N(E) dE$, per unit volume, that have energy between E and $E+dE$ is equal to the product of the density of states and the probability that a state is occupied. that is,

$$N(E)dE = [g(E)dE] f(E)$$

$$N(E) dE = \frac{8\sqrt{2} \pi m^{3/2}}{h^3} \frac{E^{1/2} dE}{\exp\left(\frac{E-E_F}{kT}\right) + 1} \quad (6.24)$$

Plots of $N(E)$ versus E for two temperatures are given in figure 6.15.

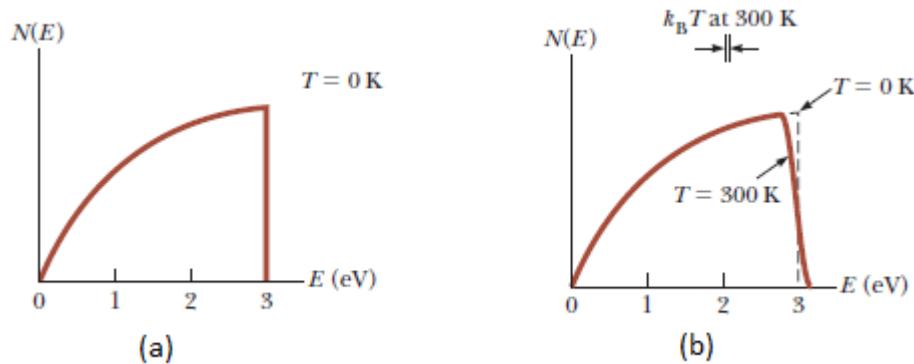


Figure 6.15 Plots of $N(E)$ versus E for (a) $T = 0K$ (b) $T = 300K$

If n_e is the total number of electrons per unit volume, we require that

$$n_e = \int_0^\infty N(E) dE = \frac{8\sqrt{2} \pi m^{3/2}}{h^3} \int_0^\infty \frac{E^{1/2} dE}{\exp\left(\frac{E-E_F}{kT}\right) + 1} \quad (6.25)$$

At $T = 0K$, the Fermi-Dirac distribution function $f(E) = 1$ for $E < E_F$ and $f(E) = 0$ for $E > E_F$. Therefore, at $T = 0K$, Equation 5.7 becomes

$$n_e = \frac{8\sqrt{2} \pi m^{3/2}}{h^3} \int_0^{E_F} E^{1/2} dE = \frac{8\sqrt{2} \pi m^{3/2}}{h^3} \left(\frac{2}{3}\right) E_F^{3/2} = \frac{16\sqrt{2} \pi m^{3/2}}{3h^3} E_F^{3/2} \quad (6.26)$$

Solving for Fermi energy at $0K$, we obtain

$$E_F(0) = \frac{\hbar^2}{2m} \left(\frac{3n_e}{8\pi} \right)^{2/3} \quad (6.27)$$

The average energy of a free electron in a metal at $0K$ is $E_{av} = (3/5)E_F$.

6.8 BAND THEORY OF SOLIDS

When a quantum system is represented by wave function, probability density $|\Psi|^2$ for that system is physically significant while the probability amplitude Ψ not. Consider an atom such as sodium that has a single s electron outside of a closed shell. Both the wave functions $\psi_s^+(r)$ and $\psi_s^-(r)$ are valid for such an atom [$\psi_s^+(r)$ and $\psi_s^-(r)$ are symmetric and anti symmetric wave functions]. As the two sodium atoms are brought closer together, their wave functions begin to overlap. Figure 6.16 represents two possible combinations : i) symmetric - symmetric and ii) symmetric - antisymmetric . **These two possible combinations of wave functions represent two possible states of the two-atom system.** Thus, the states are split into two energy levels. The energy difference between these states is relatively small, so the two states are close together on an energy scale.

When two atoms are brought together, each energy level will split into 2 energy levels. (In general, when N atoms are brought together N split levels will occur which can hold $2N$ electrons). The split levels are so close that they may be regarded as a continuous **band** of energy levels. Figure 6.17 shows the splitting of $1s$ and $2s$ levels of sodium atom when : (a) two sodium atoms are brought together (b) five sodium atoms are brought together (c) a large number of sodium atoms are assembled to form a solid. The close energy levels forming a band are seen clearly in (c).

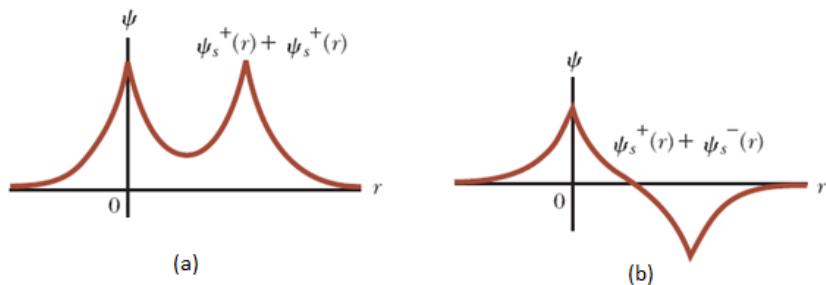


Figure. 6.16 The wave functions of two atoms combine to form a composite wave function : a) symmetric-symmetric b) symmetric-antisymmetric

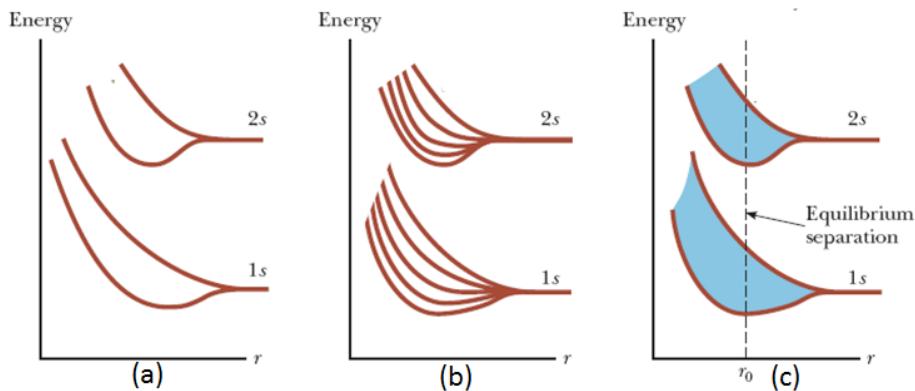


Figure 6.17 Splitting of 1s and 2s levels of sodium atoms due to interaction between them

Some bands may be wide enough in energy so that there is an overlap between the adjacent bands. Some other bands are narrow so that a gap may occur between the allowed bands, and is known as **forbidden energy gap**. The 1s, 2s, and 2p bands of solid sodium are filled completely with electrons. The 3s band ($2N$ states) of solid sodium has only N electrons and is partially full; The 3p band, which is the higher region of the overlapping bands, is completely empty as shown in Figure 6.18

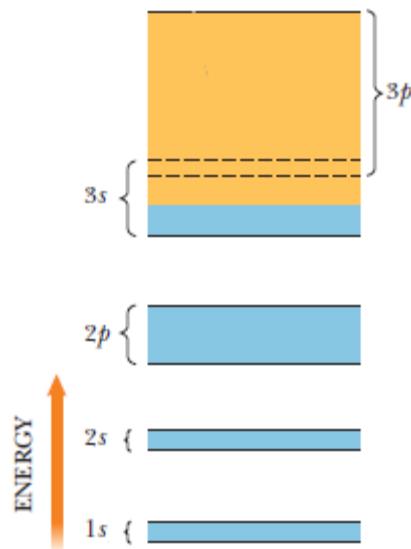


Figure 6.18 Energy bands of a sodium crystal

6.9 ELECTRICAL CONDUCTION IN METALS, INSULATORS AND SEMICONDUCTORS

Good electrical conductors contain high density of free charge carriers, and the density of free charge carriers in insulators is nearly zero. In semiconductors free-charge-carrier densities are intermediate between those of insulators and those of conductors.

Metals: Metal has a partially filled energy band (Figure 6.19a). At 0K Fermi level is the highest electron-occupied energy level. If a potential difference is applied to the metal, electrons having energies near the Fermi energy require only a small amount of additional energy to reach nearby empty energy states above the Fermi-level. Therefore, electrons in a metal experiencing a small force (from a weak applied electric field) are free to move because many empty levels are available close to the occupied energy levels. The model of metals based on band theory demonstrates that metals are excellent electrical conductors.

Insulators: Consider the two outermost energy bands of a material in which the lower band is filled with electrons and the higher band is empty at 0 K (Figure 6.19b). The lower, filled band is called the valence band, and the upper, empty band is the conduction band. The energy separation between the valence and conduction band, called energy gap E_g , is large for insulating materials. The Fermi level lies somewhere in the energy gap. Due to larger energy gap compare to thermal energy kT (26meV) at room temperature, excitation of electrons from valence band to conduction band is hardly possible. Since the free-electron density is nearly zero, these materials are bad conductors of electricity.

Semiconductors: Semiconductors have the same type of band structure as an insulator, but the energy gap is much smaller, of the order of 1 eV. The band structure of a semiconductor is shown in Figure 6.19c. Because the Fermi level is located near the middle of the gap for a semiconductor and E_g is small, appreciable numbers of electrons are thermally excited from the valence band to the conduction band. Because of the many empty levels above the thermally filled levels in the conduction band, a small applied potential difference can easily raise the energy of the electrons in the conduction band, resulting in a moderate conduction. At T = 0 K, all electrons in these materials are in the valence band and no energy is available to excite them across the energy gap. Therefore, semiconductors are poor conductors at very low temperatures. Because the thermal excitation of electrons across the narrow gap is more probable at higher temperatures, the conductivity of

semiconductors increases rapidly with temperature. This is in sharp contrast with the conductivity of metals, where it decreases with increasing temperature. Charge carriers in a semiconductor can be negative, positive, or both. When an electron moves from the valence band into the conduction band, it leaves behind a vacant site, called a hole, in the otherwise filled valence band.

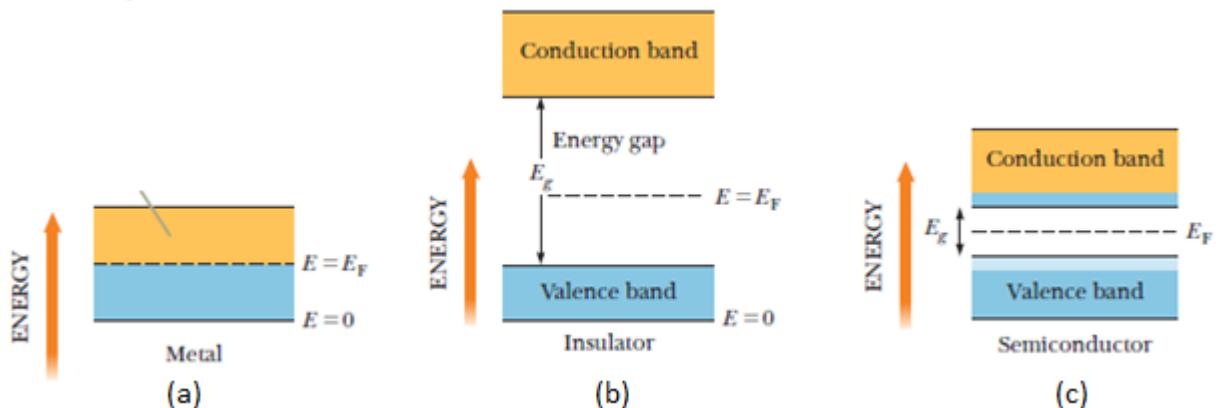


Figure 6.19 Band structure of (a) Metals (b) Insulators (c) Semiconductors

In an intrinsic semiconductor (pure semiconductor) there are equal number of conduction electrons and holes. In the presence of an external electric field, the holes move in the direction of field and the conduction electrons move opposite to the direction of the field. Both these motions correspond to the current in the same direction (Figure 6.20).

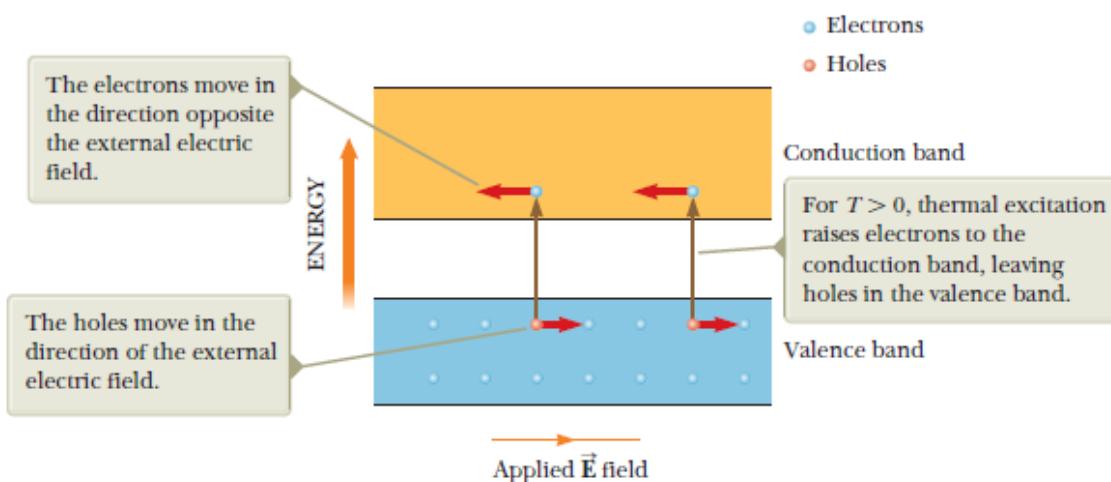


Figure 6.20 Movement of electrons and holes in an intrinsic semiconductor

Doped Semiconductors (Extrinsic semiconductors): Semiconductors in their pure form are called intrinsic semiconductors while doped semiconductors are called extrinsic semiconductors. Doping is the process of adding impurities to a semiconductor. By doping both the band structure of the semiconductor and its resistivity are modified. If a tetravalent semiconductor (Si or Ge) is doped with a pentavalent impurity atom (donor atom), four of the electrons form covalent bonds with atoms of the semiconductor and one is left over (Figure 6.21). At zero K, this extra electron resides in the donor-levels, that lie in the energy gap, just below the conduction band. Since the energy E_d between the donor levels and the bottom of the conduction band is small, at room temperature, the extra electron is thermally excited to the conduction band. This type of semiconductors are called n-type semiconductors because the majority of charge carriers are electrons (negatively charged).

If a tetravalent semiconductor is doped with a trivalent impurity atom (acceptor atom), the three electrons form covalent bonds with neighboring semiconductor atoms, leaving an electron deficiency (a hole) at the site of fourth bond (Figure 6.22). At zero K, this hole resides in the acceptor levels that lie in the energy gap just above the valence band. Since the energy E_a between the acceptor levels and the top of the valence band is small, at room temperature, an electron from the valence band is thermally excited to the acceptor levels leaving behind a hole in the valence band. This type of semiconductors are called p-type semiconductors because the majority of charge carriers are holes (positively charged).

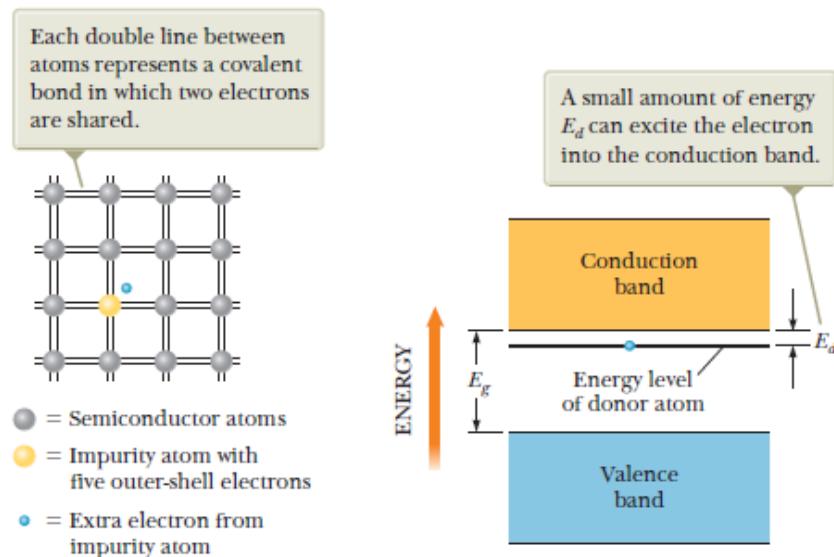


Figure 6.21 n-type semiconductor – two dimensional representation and band structure

When conduction in a semiconductor is the result of acceptor or donor impurities, the material is called an extrinsic semiconductor. The typical range of doping densities for extrinsic semiconductors is 10^{13} to 10^{19} cm $^{-3}$, whereas the electron density in a typical semiconductor is roughly 10^{21} cm $^{-3}$.

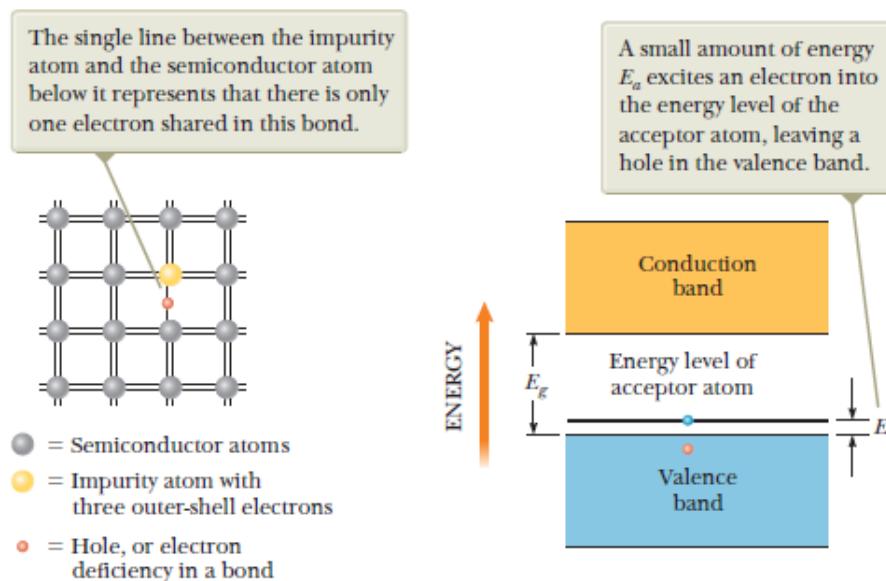


Figure 6.22 p-type semiconductor: two-dimensional representation and band structure

6.10 SUPERCONDUCTIVITY-PROPERTIES AND APPLICATIONS

Superconductor is a class of metals and compounds whose electrical resistance decreases to virtually zero below a certain temperature T_c called the critical temperature. The critical temperature is different for different superconductors. Mercury loses its resistance completely and turns into a superconductor at 4.2K. Critical temperatures for some important elements/compounds are listed below.

Element/Compound	T_c (K)
La	6.0
NbNi	10.0
Nb ₃ Ga	23.8

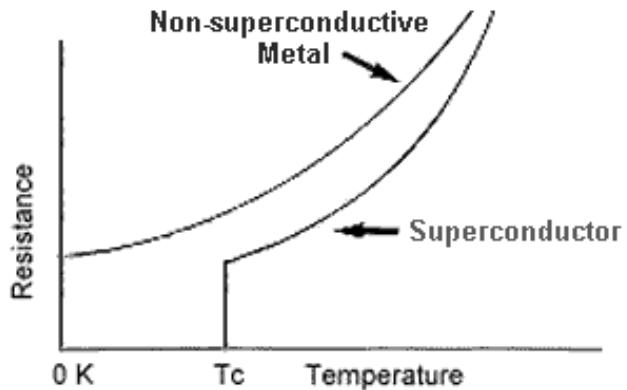


Figure 6.23 Plot of Resistance Vs Temperature for normal metal and a superconductor

Meissner Effect: In the presence of magnetic field, as the temperature of superconducting material is lowered below T_c , the field lines are spontaneously expelled from the interior of the superconductor ($B = 0$, Figure 6.24). Therefore, a superconductor is more than a perfect conductor; it is also a perfect diamagnet. The property that $B = 0$ in the interior of a superconductor is as fundamental as the property of zero resistance. If the magnitude of the applied magnetic field exceeds a critical value B_c , defined as the value of B that destroys a material's superconducting properties, the field again penetrates the sample. Meissner effect can be explained in the following way.

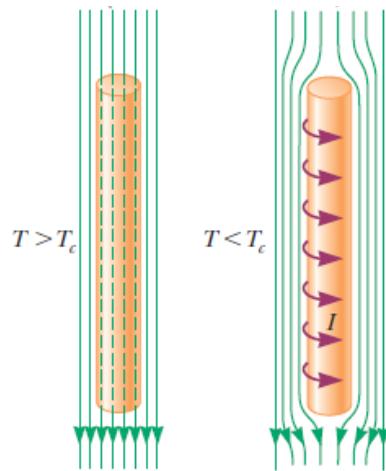


Figure 6.24 A superconductor in the form of a long cylinder in the presence of an external magnetic field.

A good conductor expels static electric fields by moving charges to its surface. In effect, the surface charges produce an electric field that exactly cancels the externally applied field inside the conductor. In a similar manner, a superconductor expels magnetic fields by forming surface currents. Consider the superconductor

shown in Figure 6.24. Let's assume the sample is initially at a temperature $T > T_c$ so that the magnetic field penetrates the cylinder. As the cylinder is cooled to a temperature $T < T_c$, the field is expelled. Surface currents induced on the superconductor's surface produce a magnetic field that exactly cancels the externally applied field inside the superconductor. As expected, the surface currents disappear when the external magnetic field is removed.

BCS Theory: In 1957, Bardeen, Cooper and Schrieffer gave a successful theory to explain the phenomenon of superconductivity, which is known as BCS theory. According to this theory, two electrons can interact via distortions in the array of lattice ions so that there is a net attractive force between the electrons. As a result, the two electrons are bound into an entity called a **Cooper pair**, which behaves like a single particle with integral spin. Particles with integral spin are called bosons. An important feature of bosons is that they do not obey the Pauli exclusion principle. Consequently, at very low temperatures, it is possible for all bosons in a collection of such particles to be in the lowest quantum state and as such the entire collection of Cooper pairs in the metal is described by a single wave function. There is an energy gap equal to the binding energy of a Cooper pair between this lowest state and the next higher state.. Under the action of an applied electric field, the Cooper pairs experience an electric force and move through the metal. A random scattering event of a Cooper pair from a lattice ion would represent resistance to the electric current. Such a collision would change the energy of the Cooper pair because some energy would be transferred to the lattice ion. There are no available energy levels below that of the Cooper pair (it is already in the lowest state), however, and none available above because of the energy gap. As a result, collisions do not occur and there is no resistance to the movement of Cooper pairs.

Applications: Most important and basic application of superconductors is in high field solenoids which can be used to produce intense magnetic field. Superconducting magnets are used in magnetic resonance imaging (MRI) technique. Magnetic levitation, based on Meissner effect, is another important application of superconductors. This principle is used in maglev vehicles. Detection of a weak magnetic field and lossless power transmission are some other important applications of superconductors.

6.11 QUESTIONS

1. Sketch schematically the plot of potential energy and its components as a function of inter-nuclear separation distance for a system of two atoms.

2. Explain briefly (a) ionic bonding, (b) covalent bonding, (c) van der Walls bonding, (d) hydrogen bonding.
3. Obtain an expression for rotational energy of a diatomic molecule. Sketch schematically these rotational energy levels.
4. Obtain expressions for rotational transition photon energies and frequencies.
5. Obtain an expression for vibrational energy of a diatomic molecule. Sketch schematically these vibrational energy levels. Obtain expression for vibrational transition photon energies.
6. Write expression for total energy (vibrational and rotational) of a molecule. Sketch schematically these energy levels of a diatomic molecule for the lowest two vibrational energy values, indicating the possible transitions. Write the expressions for the energy of the photon in the molecular energy transitions. Write the expression for the frequency separation of adjacent spectral lines.
7. Explain the expression for the total potential energy of a crystal. Sketch schematically the plot of the same.
8. Define (a) ionic cohesive energy (b) atomic cohesive energy, of a solid.
9. Write the expression for Fermi-Dirac distribution function. Sketch schematically the plots of this function for zero kelvin and for temperature above zero kelvin.
10. Derive an expression for density-of-states.
11. Assuming the Fermi-Dirac distribution function , obtain an expression for the density of free-electrons in a metal with Fermi energy E_F , at zero K and, hence obtain expression for Fermi energy E_F in a metal at zero K. [

Given: density-of-states function $g(E) dE = \frac{8\sqrt{2} \pi m^{3/2}}{h^3} E^{1/2} dE$]

12. Explain the formation of energy bands in solids with necessary diagrams.
13. Distinguish between conductors, insulators and semiconductors on the basis of band theory
14. Indicate the position of (a) donor levels (b) acceptor levels, in the energy band diagram of a semiconductor.
15. What is the difference between p-type and n-type semiconductors? Explain with band diagram.
16. With necessary diagrams, explain doping in semiconductors.
17. Why the electrical conductivity of an intrinsic semiconductor increases with increasing temperature?

18. What are superconductors? Draw a representative graph of Resistance Vs Temperature for a superconductor.
19. Explain Meissner effect.
20. Explain briefly the BCS theory of superconductivity in metals.

6.12 PROBLEMS

- 1.** A K^+ ion and a Cl^- ion are separated by a distance of 5.00×10^{-10} m. Assuming the two ions act like point charges, determine (a) the force each ion exerts on the other and (b) the potential energy of the two-ion system in electron volts.

Ans: a) 921 pN toward the other ion b) - 2.88 eV

- 2.** The potential energy (U) of a diatomic molecule is given by Lennard-Jones potential:

$$U = \frac{A}{r^{12}} - \frac{B}{r^6}$$

where A and B are constants. Find, in terms of A and B , (a) the value of r_0 at which the energy is minimum and (b) the energy E required to break up a diatomic molecule. (c) Evaluate r_0 in metres and E in electron-volts for the H_2 molecule.

Take $A = 0.124 \times 10^{-120} \text{ eV.m}^{12}$ and $B = 1.488 \times 10^{-60} \text{ eV.m}^6$.

Ans: a) $(2A/B)^{1/6}$ b) $B^2/4A$ c) 74.2 pm , 4.46 eV

- 3.** An HCl molecule is excited to its first rotational energy level, corresponding to $J = 1$. If the distance between its nuclei is $r_0 = 0.1275 \text{ nm}$, what is the angular speed of the molecule about its center of mass?

Ans: $5.69 \times 10^{12} \text{ rad/s}$

- 4.** The rotational spectrum of the HCl molecule contains lines with wavelengths of 0.0604 , 0.0690 , 0.0804 , 0.0964 , and 0.1204 mm . What is the moment of inertia of the molecule?

Ans: $2.72 \times 10^{-47} \text{ kg.m}^2$

- 5.** The frequency of photon that causes $v=0$ to $v=1$ transition in the CO molecule is $6.42 \times 10^{13} \text{ Hz}$. Ignore any changes in the rotational energy. (A) Calculate the force constant k for this molecule. (B) What is the maximum classical amplitude of vibration for this molecule in the $v=0$ vibrational state?

Ans: A) $1.85 \times 10^3 \text{ N/m}$ B) 0.00479 nm

- 6.** Consider a one-dimensional chain of alternating positive and negative ions. Show that the potential energy associated with one of the ions and its interactions with the rest of this hypothetical crystal is

$$U(r) = -k_e \alpha \frac{e^2}{r}$$

where the Madelung constant is $\alpha = 2 \ln 2$ and r is the inter-ionic spacing. Hint: Use the series expansion

$$\ln(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \dots$$

7. Each atom of gold (Au) contributes one free-electron to the metal. The concentration of free-electron in gold is $5.90 \times 10^{28}/\text{m}^3$. Compute the Fermi Energy of gold.

Ans: 5.53 eV

8. Sodium is a monovalent metal having a density of 971 kg/m^3 and a molar mass of 0.023 kg/mol . Use this information to calculate (a) the density of charge carriers and (b) the Fermi energy.

Ans: $2.54 \times 10^{28}/\text{m}^3$, 3.15 eV

9. Calculate the energy of a conduction electron in silver at 800 K, assuming the probability of finding an electron in that state is 0.950. The Fermi energy is 5.48 eV at this temperature.

Ans: 5.28 eV

10. Show that the average kinetic energy of a conduction electron in a metal at zero K is $(3/5) E_F$

Suggestion: In general, the average kinetic energy is

$$E_{AV} = \frac{1}{n_e} \int E N(E) dE$$

where the density of particles

$$n_e = \int_0^\infty N(E) dE$$

$$N(E) dE = \frac{8\sqrt{2} \pi m^{\frac{3}{2}}}{h^3} \frac{E^{\frac{1}{2}} dE}{\exp\left(\frac{E - E_F}{kT}\right) + 1}$$

- 11.** (a) Consider a system of electrons confined to a three-dimensional box. Calculate the ratio of the number of allowed energy levels at 8.50 eV to the number at 7.00 eV. (b) Copper has a Fermi energy of 7.0 eV at 300 K. Calculate the ratio of the number of occupied levels at an energy of 8.50 eV to the number at Fermi energy. Compare your answer with that obtained in part (a).

Ans: (a) 1.10 (b) 1.46×10^{-25}

- 12.** Most solar radiation has a wavelength of 1 μm or less. What energy gap should the material in solar cell have in order to absorb this radiation? Is silicon ($E_g = 1.14$ eV) appropriate?

Ans: 1.24 eV or less; yes

- 13.** The energy gap for silicon at 300 K is 1.14 eV. (a) Find the lowest-frequency photon that can promote an electron from the valence band to the conduction band. (b) What is the wavelength of this photon?

Ans: 2.7×10^{14} Hz, 1090 nm

- 14.** A light-emitting diode (LED) made of the semiconductor GaAsP emits red light ($\lambda = 650\text{nm}$). Determine the energy-band gap E_g in the semiconductor.

Ans: 1.91 eV