Bohr’s Model, Energy Bands, Electrons and Holes

Dual Character of Material Particles

Experimental physics before 1900 demonstrated that most of the physical phenomena can be explained by Newton's equation of motion of material particles or bodies and Maxwell's equation of electromagnetic waves and light. These are known as ‘classical physics’.

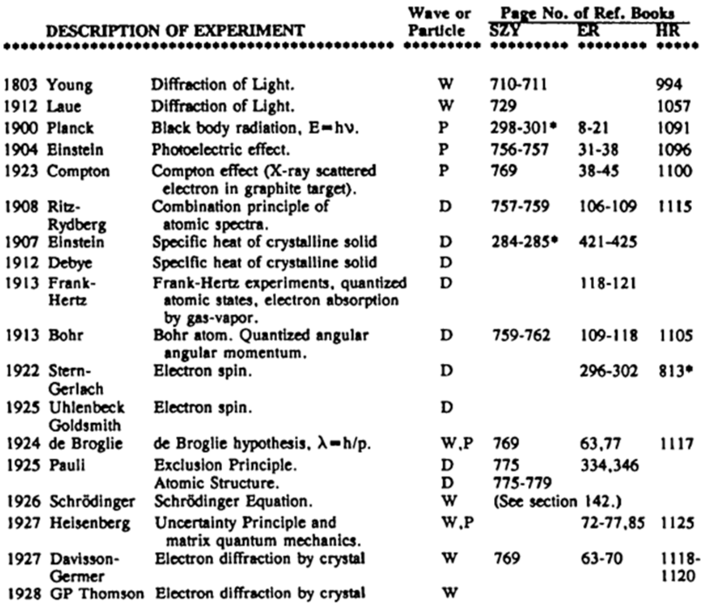
For example, the motion of mechanical objects on earth, celestial bodies, and gas molecules could all be predicted by Newton's equation of motion and classical statistical mechanics (the kinetic theory of gases).

For another example, the wave nature of light, suggested by Young's diffraction experiments in 1803, could be explained by Maxwell's electromagnetic wave equations which connected the optical phenomena with electrical phenomena.

A list of key advances is given in the next slide.

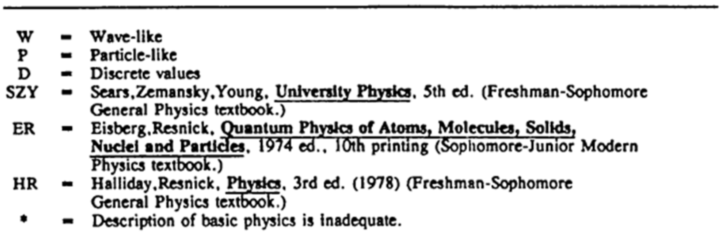
We will discuss the basic physics and the consequences of the Bohr atom model in more details. We will give an experimental and physics based derivation of the Schrodinger wave equation and several solutions that are useful in semiconductor device analyses.

Experiments on the Dual Properties of Material Particles and Light



DESCRIPTION OF EXPERIMENT			Wave or Particle	Page No. of Ref. Books		
				SZY	ER	HR
1803	Young	Diffraction of Light.	W	710-711		994
1912	Laue	Diffraction of Light.	W	729		1057
1900	Planck	Black body radiation, $E=h\nu$.	P	298-301*	8-21	1091
1904	Einstein	Photoelectric effect.	P	756-757	31-38	1096
1923	Compton	Compton effect (X-ray scattered electron in graphite target).	P	769	38-45	1100
1908	Ritz-Rydberg	Combination principle of atomic spectra.	D	757-759	106-109	1115
1907	Einstein	Specific heat of crystalline solid	D	284-285*	421-425	
1912	Debye	Specific heat of crystalline solid	D			
1913	Frank-Hertz	Frank-Hertz experiments, quantized atomic states, electron absorption by gas-vapor.	D		118-121	
1913	Bohr	Bohr atom. Quantized angular angular momentum.	D	759-762	109-118	1105
1922	Stern-Gerlach	Electron spin.	D		296-302	813*
1925	Uhlenbeck Goldsmith	Electron spin.	D			
1924	de Broglie	de Broglie hypothesis, $\lambda=h/p$.	W,P	769	63,77	1117
1925	Pauli	Exclusion Principle.	D	775	334,346	
		Atomic Structure.	D	775-779		
1926	Schrödinger	Schrödinger Equation.	W	(See section 142.)		
1927	Heisenberg	Uncertainty Principle and matrix quantum mechanics.	W,P		72-77,85	1125
1927	Davisson-Germer	Electron diffraction by crystal	W	769	63-70	1118-1120
1928	GP Thomson	Electron diffraction by crystal	W			

Description of the abbreviations in the previous slide



W = Wave-like
P = Particle-like
D = Discrete values
SZY = Sears,Zemansky,Young, University Physics, 5th ed. (Freshman-Sophomore General Physics textbook.)
ER = Eisberg,Resnick, Quantum Physics of Atoms, Molecules, Solids, Nuclei and Particles, 1974 ed., 10th printing (Sophomore-Junior Modern Physics textbook.)
HR = Halliday,Resnick, Physics, 3rd ed. (1978) (Freshman-Sophomore General Physics textbook.)
* = Description of basic physics is inadequate.

Quantum Concept and Blackbody Radiation

It is a well-known fact that a solid object will glow or give off light if it is heated to a sufficiently high temperature. Actually, solid bodies in equilibrium with their surroundings emit a spectrum of radiation at all times. When the temperature of the body is at or below room temperature, however, the radiation is almost exclusively in the infrared and therefore not detectable by the human eye.

Various attempts to explain the observed blackbody spectrum were made in the latter half of the 19th century. In 1901 Max Planck provided a detailed theoretical fit to the observed blackbody spectrum.

The explanation was based on the then-startling hypothesis that the vibrating atoms in a material could only radiate or absorb energy in discrete packets.

Planck postulated that thermal radiation is emitted from a heated surface in discrete packets of energy called **quanta**. The energy of these quanta is given by

$$\boxed{E = h\nu}$$

where ν is the frequency of the radiation and h is a constant now know known as Plank's constant ($h = 6.625 \times 10^{-34}$ J-s).

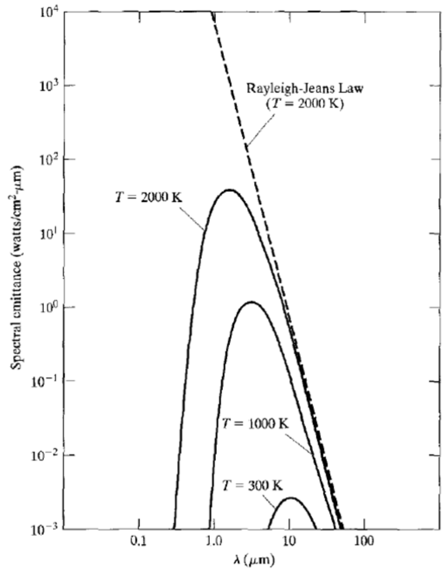


Figure 2.1 Wavelength dependence of the radiation emitted by a blackbody heated to 300 K, 1000 K, and 2000 K. Note that the visible portion of the spectrum is confined to wavelengths $0.4\,\mu\text{m} \lesssim \lambda \lesssim 0.7\,\mu\text{m}$. The dashed line is the predicted dependence for $T = 2000$ K based on classical considerations.

Photoelectric Effect

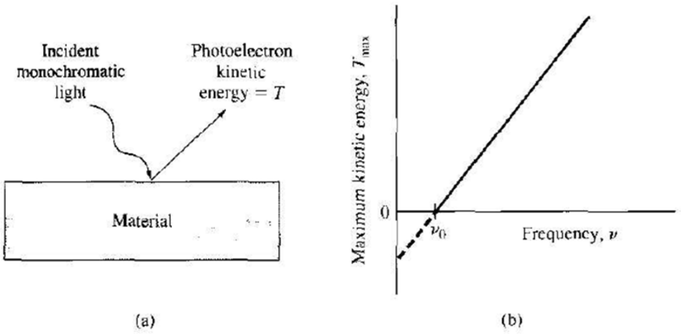


Figure 2.1 | *(a) The photoelectric effect and (b) the maximum kinetic energy of the photoelectron as a function of incident frequency.*

In 1905, Einstein interpreted the photoelectric results by suggesting that the energy in a light wave is also contained in discrete packets or bundles. The particle-like packet of energy is called a **photon**, whose energy is also given by

$$\boxed{E = h\nu}$$

A photon with sufficient energy, then, can knock an electron from the surface of the material. The minimum energy required to remove an electron is called the work function of the material and any excess photon energy goes into the kinetic energy of the photoelectron. This result was confirmed experimentally as demonstrated in the figure above.

The photoelectric effect shows the discrete nature of the photon and demonstrates the particle-like behaviour of the photon. The maximum kinetic energy of the photoelectron can be written as

$$T_{\max} = \frac{1}{2}mv^2 = h\nu - h\nu_0$$

where $h\nu$ is the incident photon energy and $h\nu_0$ is the minimum energy, of work function, required to remove an electron from the surface.

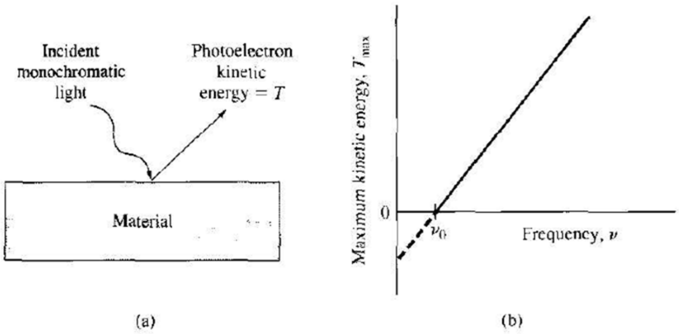


Figure 2.1 | *(a) The photoelectric effect and (b) the maximum kinetic energy of the photoelectron as a function of incident frequency.*

EXAMPLE 2.1

Objective

To calculate the photon energy corresponding to a particular wavelength.

Consider an x-ray with a wavelength of $\lambda = 0.708 \times 10^{-8}$ cm.

■ Solution

The energy is

$$E = h\nu = \frac{hc}{\lambda} = \frac{(6.625 \times 10^{-34})(3 \times 10^{10})}{0.708 \times 10^{-8}} = 2.81 \times 10^{-15} \text{ J}$$

This value of energy may be given in the more common unit of electron-volt (see Appendix F). We have

$$E = \frac{2.81 \times 10^{-15}}{1.6 \times 10^{-19}} = 1.75 \times 10^{4} \text{ eV}$$

■ Comment

The reciprocal relation between photon energy and wavelength is demonstrated: A large energy corresponds to a short wavelength.

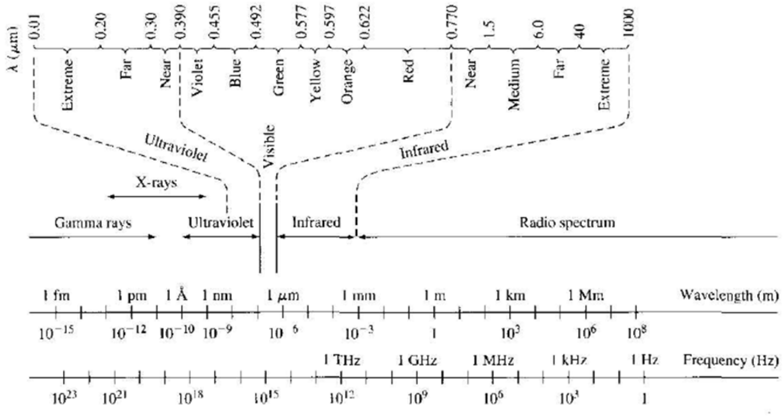


Figure 2.4 | The electromagnetic frequency spectrum.

Wave-Particle Duality

We have seen that light waves, in the photoelectric effect, behave as if they are particles. The particle-like behavior of electromagnetic waves was also instrumental in the explanation of the Compton effect. In this experiment, an x-ray beam was incident on a solid. A portion of the x-ray beam was deflected and the frequency of the deflected wave had shifted compared to the incident wave. The observed change in frequency and the deflected angle corresponded exactly to the expected results of a "billiard ball" collision between an x-ray quanta, or photon, and an electron in which both energy and momentum are conserved.

In 1924, De Broglie postulated the existence of matter waves. He suggested that since waves exhibit particle-like behavior, then particles should be expected to show wave-like properties. The hypothesis of De Broglie was the existence of a **wave-particle duality** principle. The momentum of a photon is given by

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

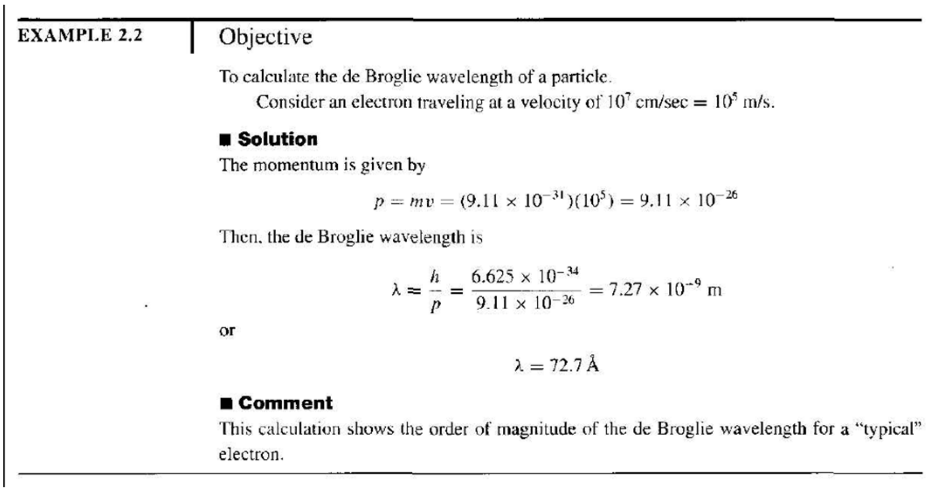
where λ is the wavelength of the light wave.

Then, De Broglie hypothesized that the wavelength of a particle can be expressed as

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

where p is the momentum of the particle and λ is known as the **De Broglie** wavelength of the matter wave.

The Planck and De Broglie relationships are fundamental in quantum physics and are valid for all situations and objects, including photons and electrons. They connect the wave description of phenomena (frequency and wavelength) to a particle description (energy and momentum). The relation between frequency and wavelength, known as the *dispersion relationship*, however, is not the same for different objects. For example, for photons, the wavelength (λ) is related to frequency by $\lambda = c/\nu$, where c is the speed of light. For electrons, it is a different relationship, known as the band structure, which will be discussed later.



EXAMPLE 2.2

Objective

To calculate the de Broglie wavelength of a particle.

Consider an electron traveling at a velocity of 10^7 cm/sec = 10^5 m/s.

■ Solution

The momentum is given by

$$p = mv = (9.11 \times 10^{-31})(10^5) = 9.11 \times 10^{-26}$$

Then, the de Broglie wavelength is

$$\lambda = \frac{h}{p} = \frac{6.625 \times 10^{-34}}{9.11 \times 10^{-26}} = 7.27 \times 10^{-9} \text{ m}$$

or

$$\lambda = 72.7 \text{ Å}$$

■ Comment

This calculation shows the order of magnitude of the de Broglie wavelength for a "typical" electron.

The Uncertainty Principle

The Heisenberg uncertainty principle, given in 1927, applies primarily to very small particles, and states that we cannot describe with absolute accuracy the behaviour of these subatomic particles. The uncertainty principle describes a fundamental relationship between conjugate variables, including position and momentum and also energy and time.

The first statement of the uncertainty principle is that it is impossible to simultaneously describe with absolute accuracy the position and momentum of a particle. If the uncertainty in the momentum is Δp and the uncertainty in the position is Δx, then the uncertainty principle is stated as

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

where $\hbar$ is defined as $\hbar = h/2\pi = 1.054 \times l0^{-34}$ J-s and is called a modified Planck's constant. The second statement of the uncertainty principle is that it is impossible to simultaneously describe with absolute accuracy the energy of a particle and the instant of time the particle has this energy:

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

One way to visualize the uncertainty principle is to consider the simultaneous measurement of position and momentum, and the simultaneous measurement of energy and time. The uncertainty principle implies that these simultaneous measurements are in error to a certain extent. However, the modified Planck's constant $\hbar$ is very small; the uncertainty principle is only significant for subatomic particles. We must keep in mind nevertheless that the uncertainty principle is a fundamental statement and does not deal only with measurements.

One consequence of the uncertainty principle is that we cannot, for example, determine the exact position of an electron. We will, instead, determine the probability of finding an electron at a particular position.

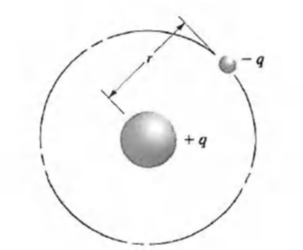
The Bohr Model

The results of emission spectra experiments led Niels Bohr to construct a model for the hydrogen atom, based on the mathematics of planetary systems. If the electron in the hydrogen atom has a series of planetary-type orbits available to it, it can be excited to an outer orbit and then can fall to any one of the inner orbits, giving off energy. To develop the model, Bohr made several postulates

1. Electrons exist in certain stable, circular orbits about the nucleus.
2. The electron may shift to an orbit of higher or lower energy, thereby gaining or losing energy equal to the difference in the energy levels (by absorption or emission of a photon of energy $h\nu$).
3. The angular momentum p_θ of the electron in an orbit is always an integral multiple of the modified Planck's constant $\hbar$,

   $$p_\theta = mvr = n\hbar \qquad n = 1, 2, \ldots$$

   The geometrical interpretation is that the electron wave is a standing wave around the nucleus. Thus, the circumference of the orbit must be an integer number of wave length, $2\pi r = n\lambda$.



If we visualize the electron in a stable orbit of radius r about the proton of the hydrogen atom, we can equate the electrostatic force between the charges to the centripetal force:

$$-\frac{q^2}{4\pi\epsilon_0 r^2} = -\frac{mv^2}{r}$$

Using the angular momentum equation, we arrive at

$$r_n = \frac{4\pi\epsilon_0 n^2\hbar^2}{mq^2} \qquad \text{and}$$

$$v = \frac{q^2}{4\pi\epsilon_0 n\hbar}$$

Therefore, the kinetic energy of the electron is

$$E_K = \frac{1}{2}mv^2 = \frac{mq^4}{2K^2n^2\hbar^2} \qquad \ldots K = 4\pi\epsilon_0$$

The potential energy is the product of the electrostatic force and the distance between the charges

$$E_P = -\frac{q^2}{Kr_n} = -\frac{mq^4}{K^2n^2\hbar^2}$$

Thus, the total energy of the electron in the n-th orbit is

$$E_n = E_K + E_P = -\frac{mq^4}{2K^2n^2\hbar^2}$$

The critical test of the model is whether energy differences between orbits correspond to the observed photon energies of the hydrogen spectrum. The energy difference between orbits n_1 and n_2 is given by

$$E_{n_2} - E_{n_1} = \frac{mq^4}{2K^2\hbar^2}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

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n_i are the major quantum numbers.

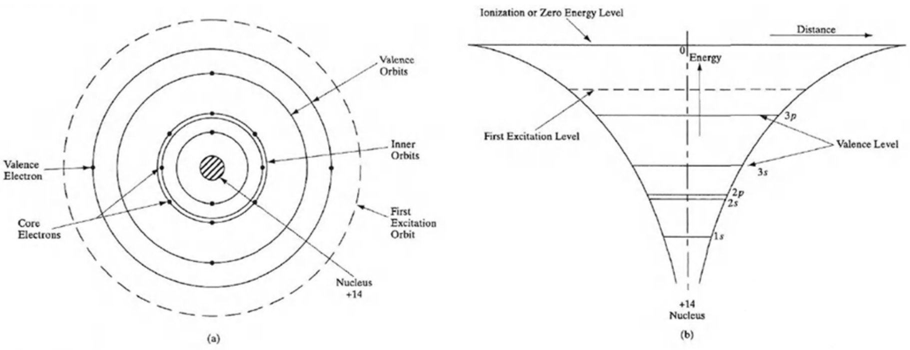
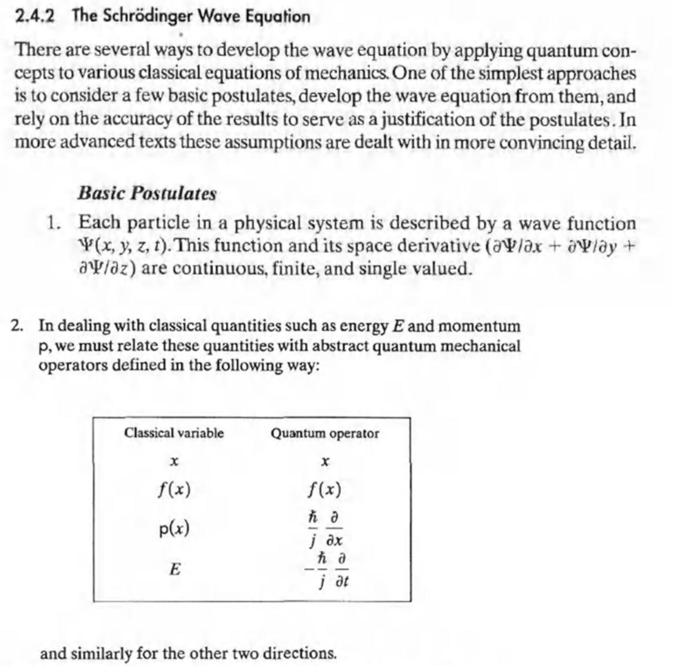


Figure 2–8
Electronic structure and energy levels in a Si atom: (a) The orbital model of a Si atom showing the 10 core electrons (**n** = 1 and 2), and the 4 valence electrons (**n** = 3); (b) energy levels in the coulombic potential of the nucleus are also shown schematically.

Schrodinger's Equation



2.4.2 The Schrödinger Wave Equation

There are several ways to develop the wave equation by applying quantum concepts to various classical equations of mechanics. One of the simplest approaches is to consider a few basic postulates, develop the wave equation from them, and rely on the accuracy of the results to serve as a justification of the postulates. In more advanced texts these assumptions are dealt with in more convincing detail.

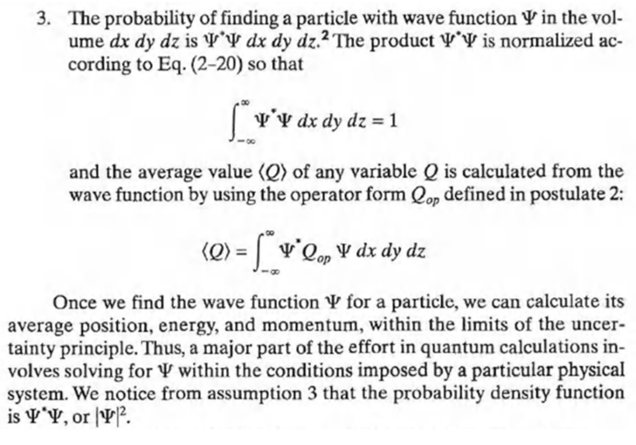
Basic Postulates

1. Each particle in a physical system is described by a wave function $\Psi(x, y, z, t)$. This function and its space derivative ($\partial\Psi/\partial x + \partial\Psi/\partial y + \partial\Psi/\partial z$) are continuous, finite, and single valued.

2. In dealing with classical quantities such as energy E and momentum p, we must relate these quantities with abstract quantum mechanical operators defined in the following way:

Classical variable	Quantum operator
x	x
$f(x)$	$f(x)$
$\mathrm{p}(x)$	$\frac{\hbar}{j}\frac{\partial}{\partial x}$
E	$-\frac{\hbar}{j}\frac{\partial}{\partial t}$

and similarly for the other two directions.



3. The probability of finding a particle with wave function Ψ in the volume $dx\,dy\,dz$ is $\Psi^*\Psi\,dx\,dy\,dz$.[2] The product $\Psi^*\Psi$ is normalized according to Eq. (2–20) so that

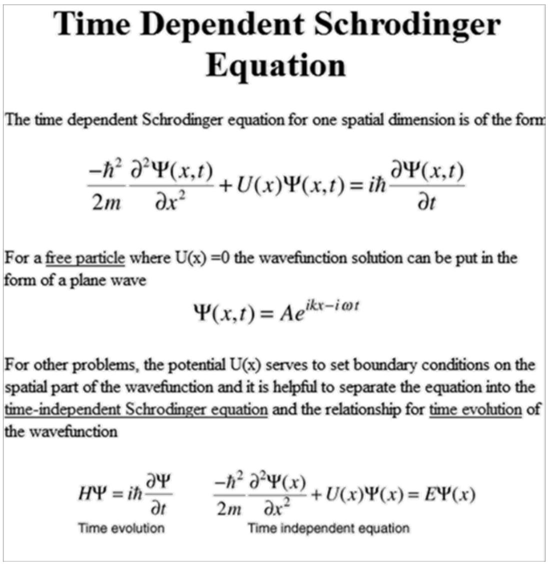
$$\int_{-\infty}^{\infty}\Psi^*\Psi\,dx\,dy\,dz = 1$$

and the average value $\langle Q\rangle$ of any variable Q is calculated from the wave function by using the operator form Q_{op} defined in postulate 2:

$$\langle Q\rangle = \int_{-\infty}^{\infty}\Psi^* Q_{op}\,\Psi\,dx\,dy\,dz$$

Once we find the wave function Ψ for a particle, we can calculate its average position, energy, and momentum, within the limits of the uncertainty principle. Thus, a major part of the effort in quantum calculations involves solving for Ψ within the conditions imposed by a particular physical system. We notice from assumption 3 that the probability density function is $\Psi^*\Psi$, or $|\Psi|^2$.

- The Schrodinger equation is a wave equation. Many experiments suggested that particles behave like waves and this behavior is more pronounced as the particles get smaller. A wave equation taking into account potential effects was introduced by Schrodinger as



Time Dependent Schrodinger Equation

The time dependent Schrodinger equation for one spatial dimension is of the form

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

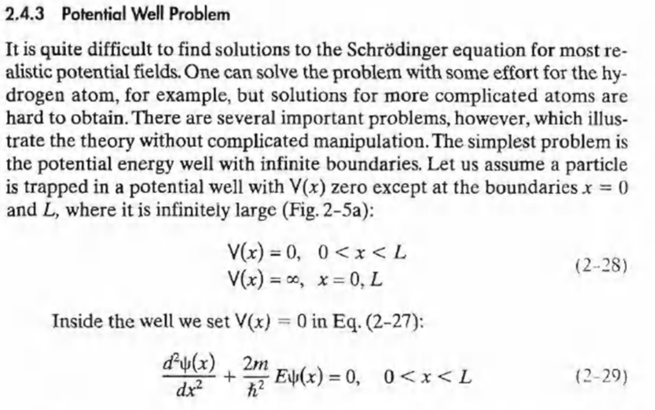
For a free particle where U(x) =0 the wavefunction solution can be put in the form of a plane wave

$$\Psi(x,t)=Ae^{ikx-i\omega t}$$

For other problems, the potential U(x) serves to set boundary conditions on the spatial part of the wavefunction and it is helpful to separate the equation into the time-independent Schrodinger equation and the relationship for time evolution of the wavefunction

$$H\Psi=i\hbar\frac{\partial\Psi}{\partial t} \qquad \frac{-\hbar^2}{2m}\frac{\partial^2\Psi(x)}{\partial x^2}+U(x)\Psi(x)=E\Psi(x)$$

Time evolution — Time independent equation



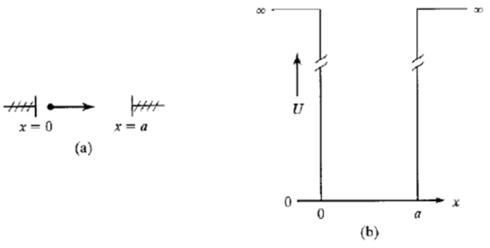
2.4.3 Potential Well Problem

It is quite difficult to find solutions to the Schrödinger equation for most realistic potential fields. One can solve the problem with some effort for the hydrogen atom, for example, but solutions for more complicated atoms are hard to obtain. There are several important problems, however, which illustrate the theory without complicated manipulation. The simplest problem is the potential energy well with infinite boundaries. Let us assume a particle is trapped in a potential well with $V(x)$ zero except at the boundaries $x = 0$ and L, where it is infinitely large (Fig. 2-5a):

$$\begin{aligned} V(x) &= 0, \quad 0 < x < L \\ V(x) &= \infty, \quad x = 0, L \end{aligned} \qquad (2\text{-}28)$$

Inside the well we set $V(x) = 0$ in Eq. (2-27):

$$\frac{d^2\psi(x)}{dx^2}+\frac{2m}{\hbar^2}E\psi(x)=0, \quad 0 < x < L \qquad (2\text{-}29)$$



$$A = \sqrt{\frac{2}{L}}, \quad \psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x$$

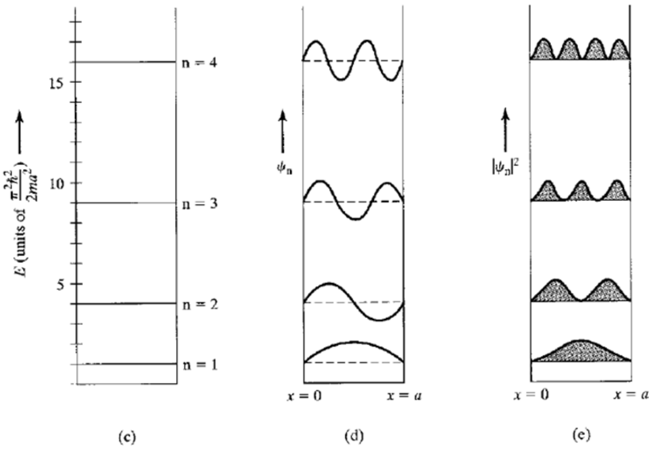


Figure 2.4 Particle in an infinitely deep one-dimensional potential well. (a) Spatial visualization of the particle confinement. (b) The assumed potential energy versus position dependence. (c) First four allowed energy levels. (d) Wavefunctions and (e) $|\psi|^2$ associated with the first four energy levels. $|\psi|^2$ is proportional to the probability of finding the particle at a given point in the potential well.

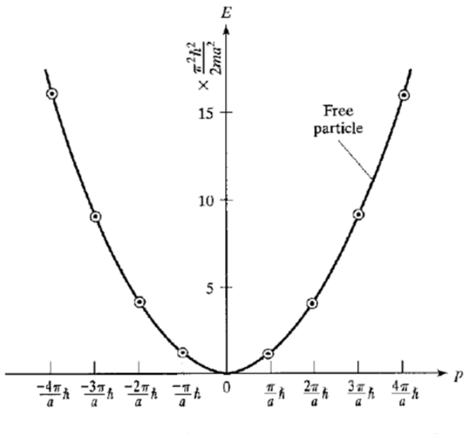
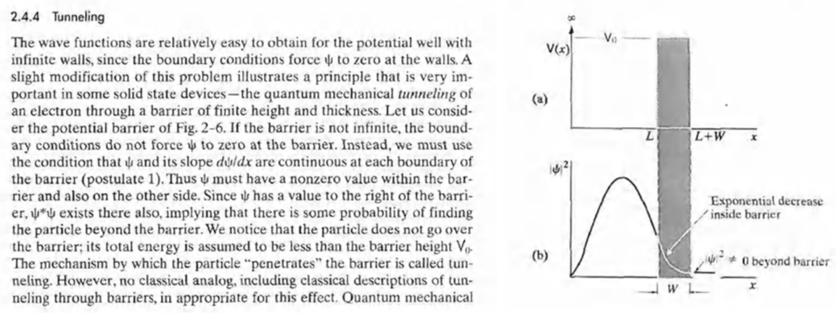
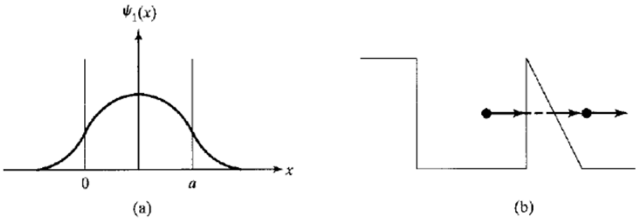


Figure 2.5 Allowed infinite-well particle energy versus counterpropagating wave momentum (discrete points) referenced against the free particle E–$\langle p \rangle$ relationship.



2.4.4 Tunneling

The wave functions are relatively easy to obtain for the potential well with infinite walls, since the boundary conditions force ψ to zero at the walls. A slight modification of this problem illustrates a principle that is very important in some solid state devices—the quantum mechanical *tunneling* of an electron through a barrier of finite height and thickness. Let us consider the potential barrier of Fig. 2-6. If the barrier is not infinite, the boundary conditions do not force ψ to zero at the barrier. Instead, we must use the condition that ψ and its slope $d\psi/dx$ are continuous at each boundary of the barrier (postulate 1). Thus ψ must have a nonzero value within the barrier and also on the other side. Since ψ has a value to the right of the barrier, $\psi^*\psi$ exists there also, implying that there is some probability of finding the particle beyond the barrier. We notice that the particle does not go over the barrier; its total energy is assumed to be less than the barrier height V_0. The mechanism by which the particle "penetrates" the barrier is called tunneling. However, no classical analog, including classical descriptions of tunneling through barriers, in appropriate for this effect. Quantum mechanical



(a) (b)

Figure 2.9 (a) Sketch of the wavefunction associated with the lowest energy state of a particle in a finite potential well. The sketch emphasizes the finite value of the wavefunction external to the well. (b) Visualization of tunneling through a thin barrier.

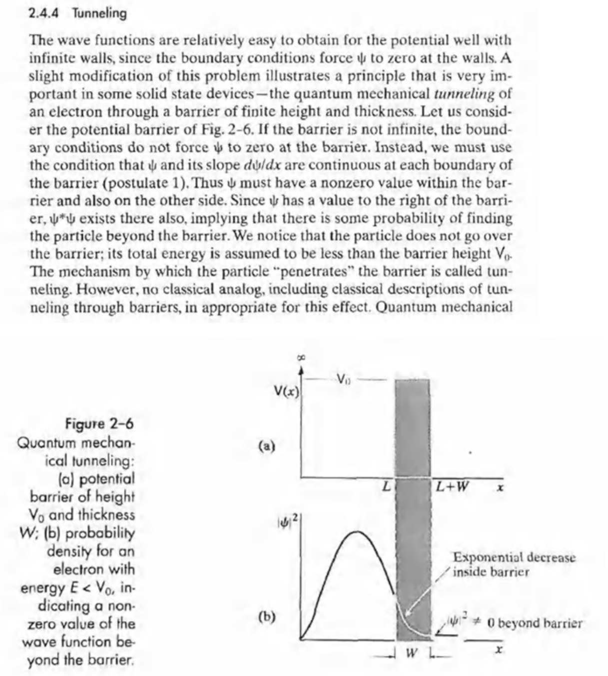


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Figure 2-6 Quantum mechanical tunneling: (a) potential barrier of height V_0 and thickness W; (b) probability density for an electron with energy $E < V_0$, indicating a nonzero value of the wave function beyond the barrier.

2.5.1 The Hydrogen Atom

Finding the wave functions for the hydrogen atom requires a solution of the Schrödinger equation in three dimensions for a coulombic potential field. Since the problem is spherically symmetric, the spherical coordinate system is used in the calculation (Fig. 2–7). The term $V(x, y, z)$ in Eq. (2–24) must be replaced by $V(r, \theta, \phi)$, representing the Coulomb potential which the electron experiences in the vicinity of the proton. The Coulomb potential varies only with r in spherical coordinates

$$V(r, \theta, \phi) = V(r) = -(4\pi\epsilon_0)^{-1}\frac{q^2}{r} \qquad (2\text{–}36)$$

as in Eq. (2–14).

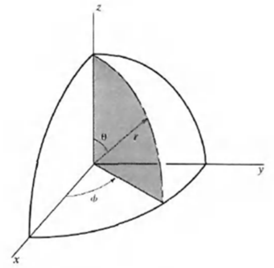


Figure 2–7
The spherical coordinate system.

When the separation of variables is made, the time-independent equation can be written as

$$\psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi) \qquad (2\text{–}37)$$

By similar treatments, the functions $R(r)$ and $\Theta(\theta)$ can be obtained, each being quantized by its own selection rule. For the r-dependent equation, the quantum number **n** can be any positive integer (not zero), and for the θ-dependent equation the quantum number $\boldsymbol{l}$ can be zero or a positive integer. However, there are interrelationships among the equations which restrict the various quantum numbers used with a single wave function ψ_{nlm}:

$$\psi_{nlm}(r, \theta, \phi) = R_n(r)\Theta_l(\theta)\Phi_m(\phi) \qquad (2\text{-}45)$$

These restrictions are summarized as follows:

$$\mathbf{n} = 1, 2, 3, \ldots \qquad (2\text{-}46a)$$

$$\boldsymbol{l} = 0, 1, 2, \ldots, (\mathbf{n} - 1) \qquad (2\text{-}46b)$$

$$\mathbf{m} = -\boldsymbol{l}, \ldots, -2, -1, 0, +1, +2, \ldots, +\boldsymbol{l} \qquad (2\text{-}46c)$$

In addition to the three quantum numbers arising from the three parts of the wave equation, there is an important quantization condition on the "spin" of the electron. Investigations of electron spin employ the theory of relativity as well as quantum mechanics; therefore, we shall simply state that the intrinsic angular momentum **s** of an electron with ψ_{nlm} specified is

$$\mathbf{s} = \pm\frac{\hbar}{2} \qquad (2\text{-}47)$$

That is, in units of $\hbar$, the electron has a spin of $\frac{1}{2}$, and the angular momentum produced by this spin is positive or negative depending on whether the electron is "spin up" or "spin down." The important point for our discussion is that each allowed energy state of the electron in the hydrogen atom is uniquely described by four quantum numbers: **n**, $\boldsymbol{l}$, **m** and **s**.[4]

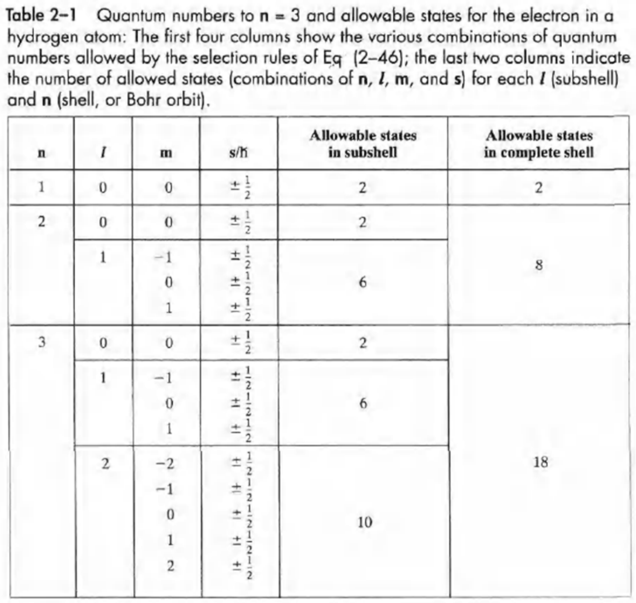
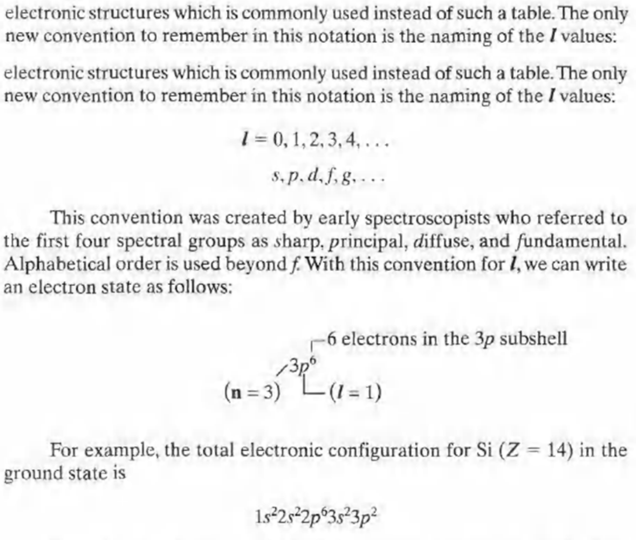


Table 2–1 Quantum numbers to **n** = 3 and allowable states for the electron in a hydrogen atom: The first four columns show the various combinations of quantum numbers allowed by the selection rules of Eq (2–46); the last two columns indicate the number of allowed states (combinations of **n**, ***l***, **m**, and **s**) for each ***l*** (subshell) and **n** (shell, or Bohr orbit).

n	*l*	m	s/ħ	Allowable states in subshell	Allowable states in complete shell
1	0	0	$\pm\frac{1}{2}$	2	2
2	0	0	$\pm\frac{1}{2}$	2	8
	1	−1	$\pm\frac{1}{2}$	6	
		0	$\pm\frac{1}{2}$		
		1	$\pm\frac{1}{2}$		
3	0	0	$\pm\frac{1}{2}$	2	18
	1	−1	$\pm\frac{1}{2}$	6	
		0	$\pm\frac{1}{2}$		
		1	$\pm\frac{1}{2}$		
	2	−2	$\pm\frac{1}{2}$	10	
		−1	$\pm\frac{1}{2}$		
		0	$\pm\frac{1}{2}$		
		1	$\pm\frac{1}{2}$		
		2	$\pm\frac{1}{2}$		



electronic structures which is commonly used instead of such a table. The only new convention to remember in this notation is the naming of the ***l*** values:

electronic structures which is commonly used instead of such a table. The only new convention to remember in this notation is the naming of the ***l*** values:

$$\boldsymbol{l} = 0, 1, 2, 3, 4, \ldots$$
$$s, p, d, f, g, \ldots$$

This convention was created by early spectroscopists who referred to the first four spectral groups as *s*harp, *p*rincipal, *d*iffuse, and *f*undamental. Alphabetical order is used beyond *f*. With this convention for ***l***, we can write an electron state as follows:

$$\overset{\text{6 electrons in the } 3p \text{ subshell}}{3p^6} \quad (\mathbf{n} = 3) \quad (l = 1)$$

For example, the total electronic configuration for Si ($Z = 14$) in the ground state is

$$1s^2 2s^2 2p^6 3s^2 3p^2$$

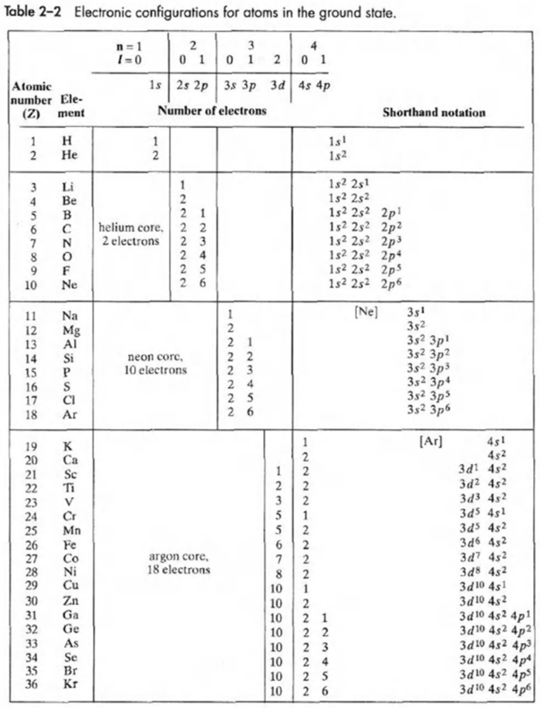


Table 2–2 Electronic configurations for atoms in the ground state.

Atomic number (Z)	Element	n = 1	2		3			4		Shorthand notation
		l = 0	0	1	0	1	2	0	1	
		1s	2s	2p	3s	3p	3d	4s	4p	
		Number of electrons								
1	H	1								$1s^1$
2	He	2								$1s^2$
3	Li	helium core, 2 electrons	1							$1s^2\ 2s^1$
4	Be		2							$1s^2\ 2s^2$
5	B		2	1						$1s^2\ 2s^2\ 2p^1$
6	C		2	2						$1s^2\ 2s^2\ 2p^2$
7	N		2	3						$1s^2\ 2s^2\ 2p^3$
8	O		2	4						$1s^2\ 2s^2\ 2p^4$
9	F		2	5						$1s^2\ 2s^2\ 2p^5$
10	Ne		2	6						$1s^2\ 2s^2\ 2p^6$
11	Na	neon core, 10 electrons			1					[Ne] $3s^1$
12	Mg				2					$3s^2$
13	Al				2	1				$3s^2\ 3p^1$
14	Si				2	2				$3s^2\ 3p^2$
15	P				2	3				$3s^2\ 3p^3$
16	S				2	4				$3s^2\ 3p^4$
17	Cl				2	5				$3s^2\ 3p^5$
18	Ar				2	6				$3s^2\ 3p^6$
19	K	argon core, 18 electrons						1		[Ar] $4s^1$
20	Ca							2		$4s^2$
21	Sc						1	2		$3d^1\ 4s^2$
22	Ti						2	2		$3d^2\ 4s^2$
23	V						3	2		$3d^3\ 4s^2$
24	Cr						5	1		$3d^5\ 4s^1$
25	Mn						5	2		$3d^5\ 4s^2$
26	Fe						6	2		$3d^6\ 4s^2$
27	Co						7	2		$3d^7\ 4s^2$
28	Ni						8	2		$3d^8\ 4s^2$
29	Cu						10	1		$3d^{10}\ 4s^1$
30	Zn						10	2		$3d^{10}\ 4s^2$
31	Ga						10	2	1	$3d^{10}\ 4s^2\ 4p^1$
32	Ge						10	2	2	$3d^{10}\ 4s^2\ 4p^2$
33	As						10	2	3	$3d^{10}\ 4s^2\ 4p^3$
34	Se						10	2	4	$3d^{10}\ 4s^2\ 4p^4$
35	Br						10	2	5	$3d^{10}\ 4s^2\ 4p^5$
36	Kr						10	2	6	$3d^{10}\ 4s^2\ 4p^6$

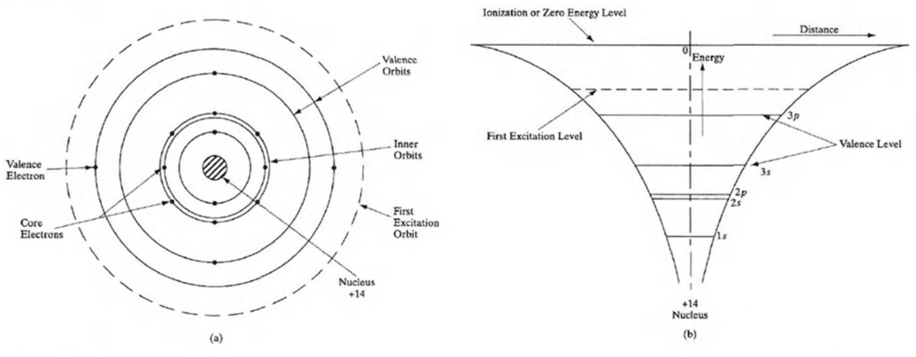


Figure 2–8
Electronic structure and energy levels in a Si atom: (a) The orbital model of a Si atom showing the 10 core electrons (**n** = 1 and 2), and the 4 valence electrons (**n** = 3); (b) energy levels in the coulombic potential of the nucleus are also shown schematically.

- Thus, the operation of interchanging two particles is represented by multiplying the wave function by a phase factor, $e^{i\delta}$. However, if we interchange the particles twice, we get back to the exact situation we started with. This implies that:

  $e^{2i\delta} = 1$ and hence $e^{i\delta} = \pm 1$
- Both cases $e^{i\delta} = +1$ and $e^{i\delta} = -1$ are realized in nature: in the first case, we say that the wave function is symmetric with respect to the interchange of two particles; in the second case, we say that the wave function is anti symmetric. Note that the wave function only need be symmetric or anti symmetric if the two particles are indistinguishable.

- Particles for which the wave function is antisymmetric under interchange of any two of the particles are called fermions. Particles for which the wave function is symmetric under interchange of any two of the particles are called bosons.
- It can be shown, from quantum field theory, that particles with half-integer spin are always fermions, whereas particles with integer spin are always bosons.
- Conclusion: when 2 atoms with the same states come together the Schrodinger eqn. shows that the Pauli Exclusion principle is valid in that a band of 2 states is formed as shown by their two separate wave functions.

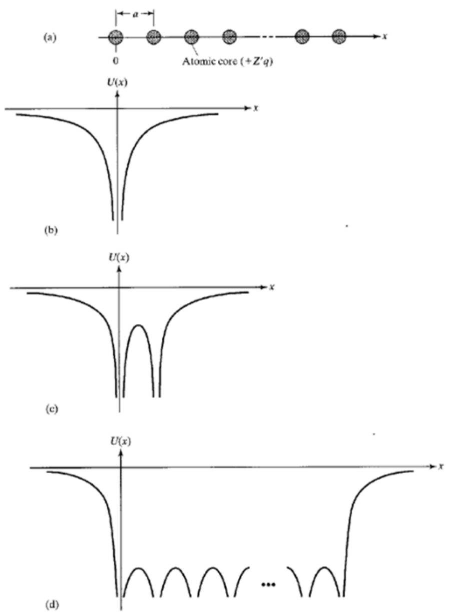


Figure 3.1 (a) One-dimensional crystalline lattice. (b–d) Potential energy of an electron inside the lattice considering (b) only the atomic core at $x = 0$, (c) the atomic cores at both $x = 0$ and $x = a$, and (d) the entire lattice chain.

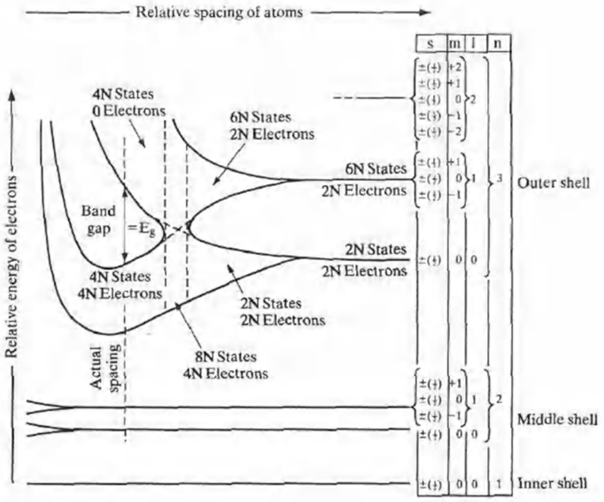
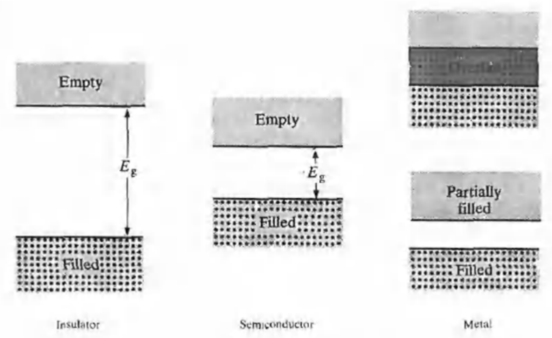


Figure 3–3

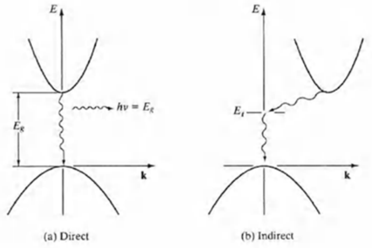
Energy levels in Si as a function of interatomic spacing. The core levels (**n** = 1,2) in Si are completely filled with electrons. At the actual atomic spacing of the crystal, the 2*N* electrons in the 3*s* subshell and the 2*N* electrons in the 3*p* subshell undergo sp^3 hybridization, and all end up in the lower 4*N* states (valence band), while the higher-lying 4*N* states (conduction band) are empty, separated by a band gap.

Figure 3–4
Typical band structures at 0 K.



Direct and Indirect Bandgaps

- The band gaps in semiconductors come in two flavors – direct and in direct. An indirect band gap material like Si usually releases energy as heat while a direct band gap material releases energy as light. In III – V ternary and quaternary alloys we can get both behaviors as the alloy composition is varied.

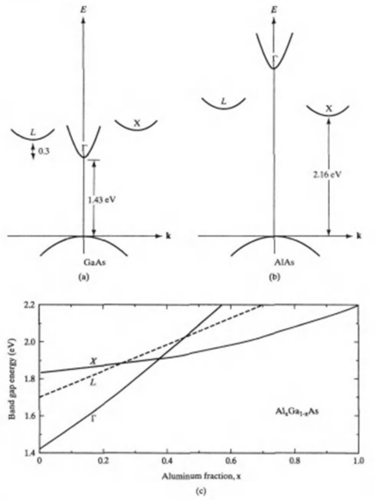


(a) Direct

(b) Indirect

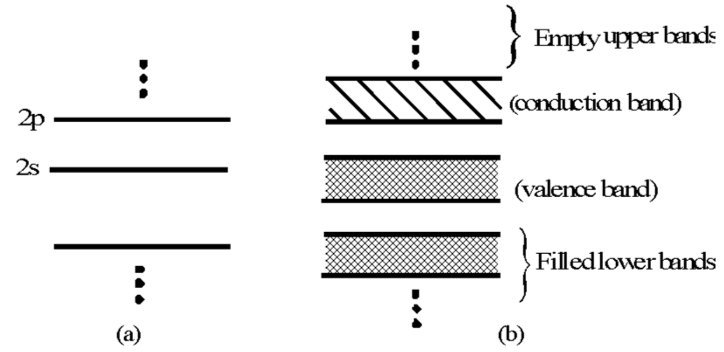
Figure 3–5
Direct and indirect electron transitions in semiconductors: (a) direct transition with accompanying photon emission; (b) indirect transition via a defect level.

- For GaAs and AlAs we can create a ternary compound $Al_xGa_{1-x}As$ and vary the % x to go from the first to the second giving



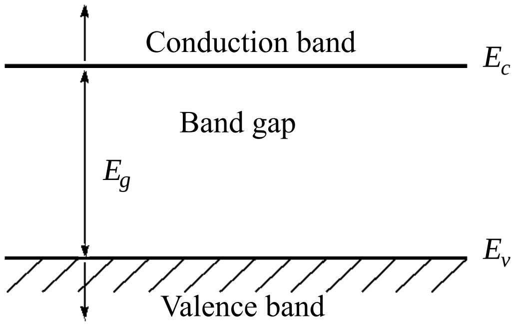
- For small Al % Γ is the min energy while at about 37% X becomes minimal.

Energy Band Model



- Energy states of Si atom (a) expand into energy bands of Si crystal (b).
- The lower bands are filled and higher bands are empty in a semiconductor.
- The highest filled band is the ***valence band.***
- The lowest empty band is the ***conduction band*** .

Energy Band Diagram



Conduction band

E_c

Band gap

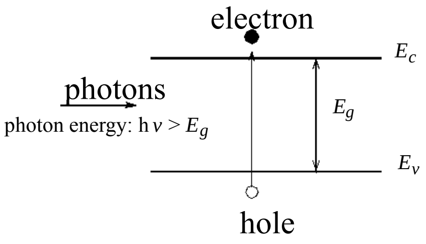
E_g

E_v

Valence band

- ***Energy band diagram*** shows the bottom edge of conduction band, E_c , and top edge of valence band, E_v .
- E_c and E_v are separated by the ***band gap energy, E_g*** .

Measuring the Band Gap Energy by Light Absorption



electron

E_c

photons

photon energy: $h\nu > E_g$

E_g

E_v

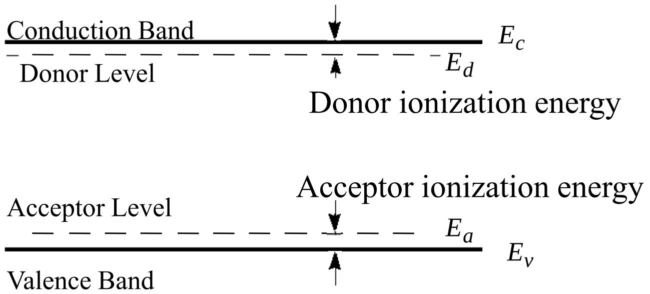
hole

- E_g can be determined from the minimum energy ($h\nu$) of photons that are absorbed by the semiconductor.

Bandgap energies of selected semiconductors

Semi-conductor	**InSb**	**Ge**	**Si**	**GaAs**	**GaP**	**ZnSe**	**Diamond**
Eg (eV)	**0.18**	**0.67**	**1.12**	**1.42**	**2.25**	**2.7**	**6**

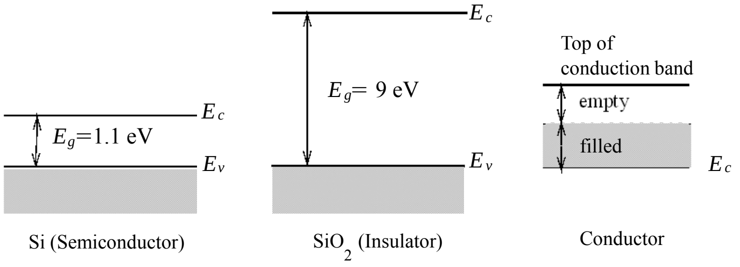
Donor and Acceptor in the Band Model



Ionization energy of selected donors and acceptors in silicon

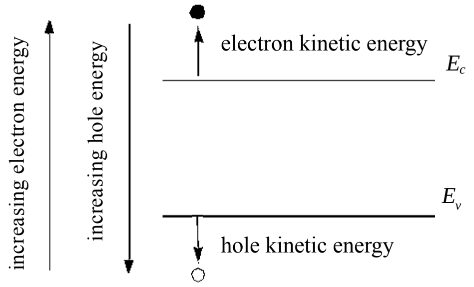
	Donors			Acceptors		
Dopant	Sb	P	As	B	Al	In
Ionization energy, $E_c - E_d$ or $E_a - E_v$ (meV)	39	44	54	45	57	160

Semiconductors, Insulators, and Conductors



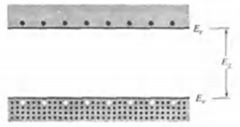
- Totally filled bands and totally empty bands do not allow current flow. (Just as there is no motion of liquid in a totally filled or totally empty bottle.)
- Metal conduction band is half-filled.
- Semiconductors have lower E_g's than insulators and can be doped.

Electrons and Holes



- Both electrons and holes tend to seek their lowest energy positions.
- Electrons tend to fall in the energy band diagram.
- Holes float up like bubbles in water.

- For a semiconductor like Si at 0°k, the valence band is full and the conduction band is empty. As we increase the temperature, some electrons will acquire enough energy (on avg.) to reach the conduction band leaving a hole behind. We have thus formed an electron-hole pair.

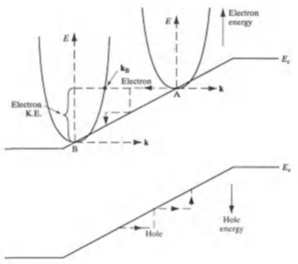


- If a field is applied

Electrons -> current in the conduction band

Holes -> - current in the valence band

- The one to one nature of things shows there is no net current in this situation.



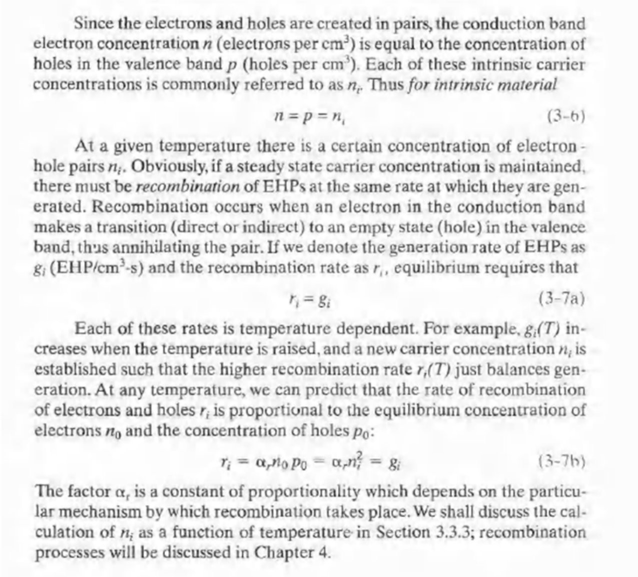
- Thus in Si at various temperatures there is an avg. number of Electron (n) – Hole (p) pairs formed and

$$n = p = n_i$$

where i stands for intrinsic (un doped) Si.

- Since we have said there is no net current this is not very helpful. To get a current requires doping - later.
- Some other thoughts on intrinsic Si are that the rate of generation of E-H pairs and their ultimate re combination rate should be equal at a given temp.
- Note the term generation means generation over and above the equilibrium value which would be the intrinsic number.
- As a side note it must be made clear that masses when used in the Quantum mechanical form are now effective masses. We should also note that effective masses are slightly different for electrons and holes but this difference is small enough such that we ignore it.

Intrinsic Material



Since the electrons and holes are created in pairs, the conduction band electron concentration n (electrons per cm^3) is equal to the concentration of holes in the valence band p (holes per cm^3). Each of these intrinsic carrier concentrations is commonly referred to as n_i. Thus *for intrinsic material*

$$n = p = n_i \qquad (3\text{-}6)$$

At a given temperature there is a certain concentration of electron-hole pairs n_i. Obviously, if a steady state carrier concentration is maintained, there must be *recombination* of EHPs at the same rate at which they are generated. Recombination occurs when an electron in the conduction band makes a transition (direct or indirect) to an empty state (hole) in the valence band, thus annihilating the pair. If we denote the generation rate of EHPs as g_i (EHP/cm^3-s) and the recombination rate as r_i, equilibrium requires that

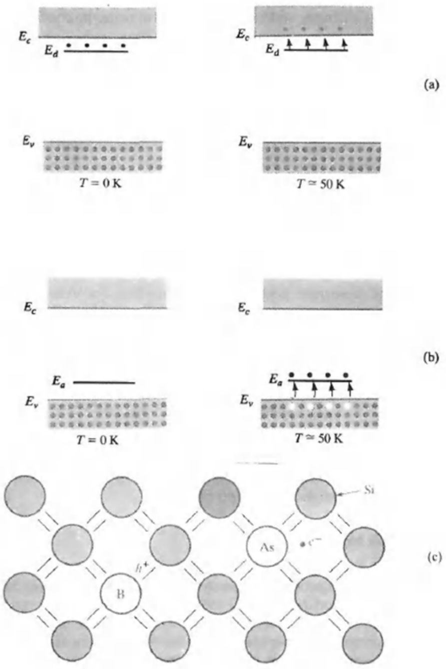
$$r_i = g_i \qquad (3\text{-}7a)$$

Each of these rates is temperature dependent. For example, $g_i(T)$ increases when the temperature is raised, and a new carrier concentration n_i is established such that the higher recombination rate $r_i(T)$ just balances generation. At any temperature, we can predict that the rate of recombination of electrons and holes r_i is proportional to the equilibrium concentration of electrons n_0 and the concentration of holes p_0:

$$r_i = \alpha_r n_0 p_0 = \alpha_r n_i^2 = g_i \qquad (3\text{-}7b)$$

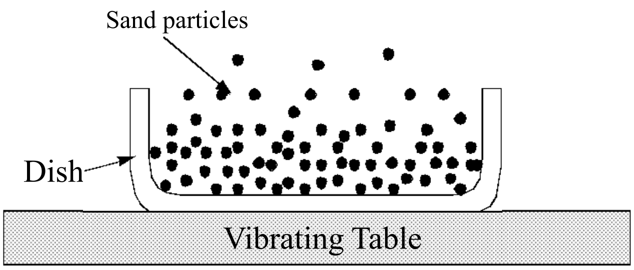
The factor α_r is a constant of proportionality which depends on the particular mechanism by which recombination takes place. We shall discuss the calculation of n_i as a function of temperature in Section 3.3.3; recombination processes will be discussed in Chapter 4.

Figure 3–12 Energy band model and chemical bond model of dopants in semiconductors: (a) donation of electrons from donor level to conduction band; (b) acceptance of valence band electrons by an acceptor level, and the resulting creation of holes; (c) donor and acceptor atoms in the covalent bonding model of a Si crystal.



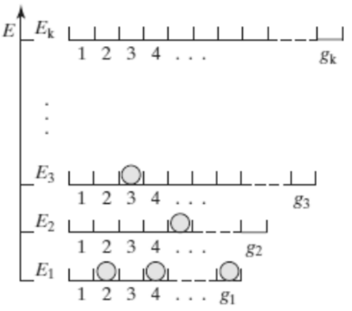
Thermal Equilibrium and the Fermi Function

An Analogy for Thermal Equilibrium



- There is a certain probability for the electrons in the conduction band to occupy high-energy states under the agitation of thermal energy.

Probability of a State at *E* being Occupied



•There are g_1 states at E_1, g_2 states at E_2… There are N electrons, which constantly shift among all the states but the average electron energy is fixed at 3kT/2.

•There are many ways to distribute N among n_1, n_2, n_3….and satisfy the 3kT/2 condition.

•The equilibrium distribution is the distribution that maximizes the number of combinations of placing n_1 in g_1 slots, n_2 in g_2 slots…. :

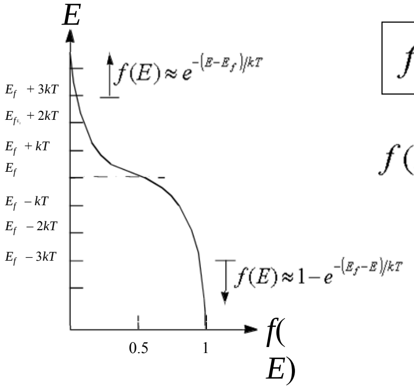
$$\boxed{n_i/g_i = \frac{1}{1 + e^{(E-E_F)/kT}}}$$

E_F is a constant determined by the condition $\sum n_i = N$

Fermi Function–The Probability of an Energy State Being Occupied by an Electron

$$f(E) = \frac{1}{1+e^{(E-E_f)/kT}}$$

E_f is called the ***Fermi energy*** or the ***Fermi level.***



Boltzmann approximation:

$$\boxed{f(E) \approx e^{-(E-E_f)/kT}} \qquad E - E_f >> kT$$

$$f(E) \approx 1 - e^{-(E_f-E)/kT} \qquad E - E_f << -kT$$

Remember: there is only one Fermi-level in a system at equilibrium.

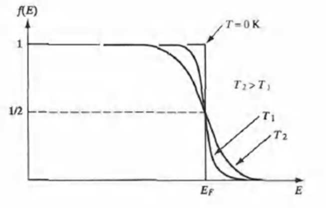
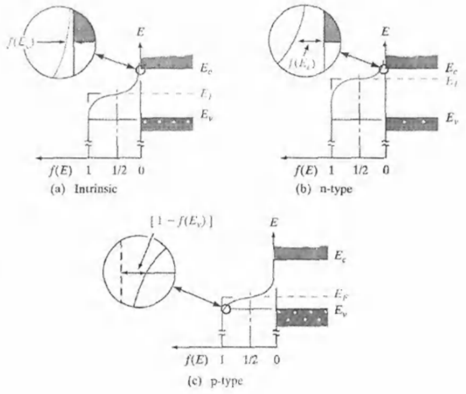


Figure 3–14 The Fermi-Dirac distribution function.



(a) Intrinsic

(b) n-type

(c) p-type

Figure 3–15 The Fermi distribution function applied to semiconductors: (a) intrinsic material; (b) n-type material; (c) p-type material.

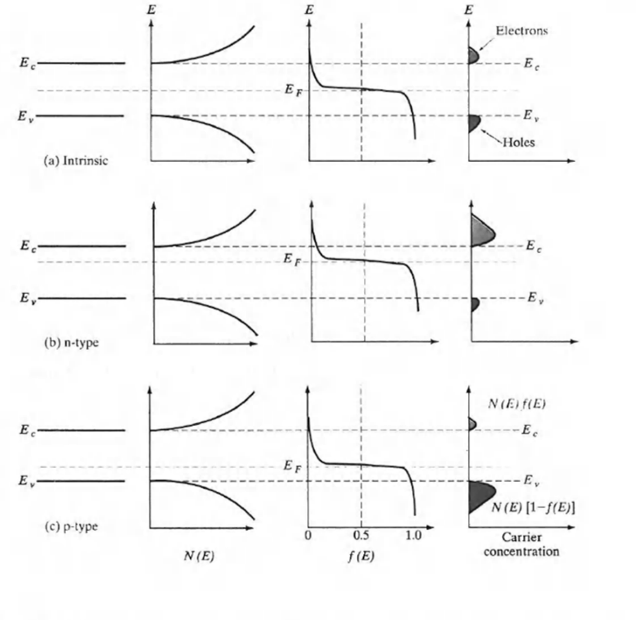


Figure 3–16
Schematic band diagram, density of states, Fermi–Dirac distribution, and the carrier concentrations for (a) intrinsic, (b) n-type, and (c) p-type semiconductors at thermal equilibrium.

Effective Mass

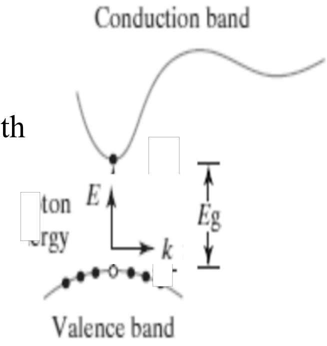
The electron wave function is the solution of the three dimensional Schrodinger wave equation

$$-\frac{\hbar^2}{2m_0}\nabla^2\psi + V(r)\psi = \psi$$

The solution is of the form exp(± **k**· **r**)
k = wave vector = 2π/electron wavelength
For each k, there is a corresponding E.

$$\text{acceleration} = -\frac{q\varepsilon}{\hbar^2}\frac{d^2E}{dk^2} = \frac{F}{m}$$

$$\text{effective mass} \equiv \frac{\hbar^2}{d^2E/dk^2}$$



In an electric field, ***E***, an electron or a hole accelerates.

$$a = \frac{-q\mathcal{E}}{m_n}$$ electrons

$$a = \frac{q\mathcal{E}}{m_p}$$ holes

Electron and hole effective masses

	Si	Ge	GaAs	InAs	AlAs
m_n/m_0	0.26	0.12	0.068	0.023	2
m_p/m_0	0.39	0.3	0.5	0.3	0.3