Semiconductor Physics and Devices

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1 Quantum Mechanics of Semiconductors

After reading this chapter you will be able to appreciate the following:

- Limitation of classical mechanics and the need for a new mechanics
- Basic postulates and theory of quantum mechanics
- Schrödinger equation and its applications
- Concepts of bands, Brillouin zone, and reduced zone scheme in solids

Introduction

The beginning of the twentieth century heralded an unprecedented era of turnover and re-evaluation of the classical theory that had governed physics since pre-Newtonian times. In the late nineteenth century and the early twentieth century it was becoming clear that the science of physics was due for a major revision. An increasing number of phenomena and observations such as the blackbody radiation problem, photoelectric effect, $H_2$ spectrum, Compton effect, etc. failed to be adequately, or even approximately, described by the laws of classical physics. Problems arose especially in attempts to provide an explanation for phenomena involving small particles such as electrons and atoms and their interaction with electromagnetic fields. At first these deficiencies in physics were patched up with ad hoc hypotheses and postulates. However, as their number grew, it became clear that physics needed a complete reformation—especially the physics of small systems. The result was quantum mechanics—a towering intellectual achievement of human kind.

This chapter begins with a brief discussion on the essence of quantum mechanics and then moves on to an explanation of the basic postulates of the theory leading to a statement of the Schrödinger equation. Several problems, whose solutions can be obtained by solving Schrödinger equation in closed form, are presented to demonstrate methods of obtaining these solutions and of investigating the properties of the solutions. Finally, it has been shown that the one-dimensional wave mechanical treatment of an electron in a periodic potential characteristic of a crystal lattice results in the prediction of allowed energy bands for the electron. This concept is essential for understanding most modern solid-state materials and devices such as transistors and integrated circuits, tunnel diodes, and semiconductor lasers.
1.1 Essence of Quantum Mechanics

Classical physics relies directly on the reality that one can see and touch, on which one can act. It is basically casual, to the extreme of determinism. On the other hand, quantum physics deals with a world inaccessible to our senses and our common sense—a world that can only be described by abstract mathematics. The well-known physicist Richard Feynman suggested about quantum mechanics that even the experts do not understand it the way they would like to, and it is perfectly reasonable that they should not, because all of the direct human experience and intuition applies to large objects. So we have learnt about it in a sort of abstract or imaginative fashion and not by our direct experience with it.

In classical mechanics, the behaviour of a particle is completely determined by its initial position together with the force that can act upon it. In quantum mechanics, the act of measurement interferes with the system and modifies it. The resulting perturbation is negligible in ‘large’ (classical) systems but assumes major importance in small systems such as atoms, electrons, and nucleons (demonstration shown in Fig. 1.1). The most common place objects have a shadow of wave functions, simple quantities become matrices, operators, pure constructs of pure mathematics. In place of an excessive certainty of determinism, one faces absolute randomness. The quantities whose relationships quantum mechanics explores are probabilities. Instead of asserting, for example, that the radius of the electron’s orbit in a ground state hydrogen atom is always exactly $5.3 \times 10^{-11}$ m, as Bohr’s theory does, quantum mechanics states that this is the most probable radius.

In classical physics, particles and waves are two entities that are understood by their own set of equations that lead to a well-defined behaviour. In quantum mechanics particles and waves are described by one set of equations, creating a duality of being that defies intuitive understanding. Particles are described by a wave-like equation, and physical observables are quantized.

**Classical Physics**

<table>
<thead>
<tr>
<th>Particles</th>
<th>Waves</th>
</tr>
</thead>
<tbody>
<tr>
<td>Obey Newton’s equations.</td>
<td>Obey wave equations.</td>
</tr>
<tr>
<td>Have a well-defined position, velocity, momentum, energy, etc.</td>
<td>Are everywhere; uncertainty in position, well-defined momentum and energy.</td>
</tr>
<tr>
<td>Are not quantized.</td>
<td>May be quantized.</td>
</tr>
</tbody>
</table>

**Quantum Physics**

- Particle and wave duality.
- Uncertainty in physical observables.
- Obey a wave-like equation.
- Quantize physical observables.

1.1.1 Energy Quanta

On December 14, 1900, at the meeting of the German Physical Society, Max Planck stated that paradoxes pestering the classical theory of the emission and
absorption of light by material bodies could be removed if one assumed that radiant energy can exist only in integral multiples of the form of discrete packages such as \textit{quanta}. Planck called these packages \textit{light quanta}. The basic amount of the quantum of energy was given by

\[ E = h\nu \]  

(1.1)

where \( \nu \) is the frequency of the radiant energy and \( h \) is a constant now associated with Planck’s name. These steps in energy values were in sharp contrast with classical radiation theory, in which all energy values are permitted.

Five years later, Albert Einstein successfully applied the idea of light quanta to explain the empirical laws of photoelectric effect, that is, the emission of electrons from metallic surfaces irradiated by violet and ultraviolet light. Still later, Arthur
Compton performed his classical experiment, which showed that the scattering of x-rays by free electrons followed the same law as the collision between two elastic spheres. Thus, within a few years the novel idea of quantization of radiant energy firmly established itself in both theoretical and experimental physics.

In the year 1913, Niels Bohr extended Planck’s idea of quantization of radiant energy to the description of mechanical energy of electrons within an atom. Although his physics was a strange mixture of the old and new physics, the prediction of the major sharp spectral lines was indisputably in excellent agreement with accurate spectroscopic observations made at that time. Hence, in spite of some inherent contradictions in the theory, it appeared to have some element of truth.

1.1.2 Wave–Particle Duality

In 1925, Louis de Broglie, a French physicist, published a paper in which he gave a quite unexpected interpretation of Bohr quantum orbits. According to de Broglie, the motion of each electron is governed by some mysterious pilot waves, whose propagation velocity and length depend on the velocity of the electron in question. Assuming that the length of these pilot waves is inversely proportional to the electron’s velocity, de Broglie could show that the various quantum orbits in Bohr’s model of the hydrogen atom were those that could accommodate an integral number of pilot waves. Thus, the model of an atom began to look like some kind of musical instrument with a basic tone (the innermost orbit with the lowest energy) and various overtones (outlying orbits with higher energy).

A wave does not have momentum in classical sense, but, since a particle can exhibit wave-like properties, de Broglie suggested the opposite must be true also: a wave can exhibit particle-like behaviour and therefore must have a momentum. The momentum of a wave with a given wavelength $\lambda$ is

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

(1.2)

This is a logical consequence of assigning a particle such as a photon with a wavelength:

$$E = h\nu = mc^2 = pc = p\nu$$

<table>
<thead>
<tr>
<th>Particle</th>
<th>Wave</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E = mc^2$</td>
<td>$E = h\nu$</td>
</tr>
<tr>
<td>$P = mc$</td>
<td>$p = h\nu$</td>
</tr>
</tbody>
</table>

The fact that particles (such as electrons) do, indeed, exhibit wave properties and undergo diffraction by a grating was demonstrated by Davisson and Germer in 1927. The diffraction grating used was not the ruled grating that was commonly used for light, but a periodic array of atoms in a nickel crystal provided by nature. This choice was necessary because of the small wavelength of the electron predicted by de Broglie and the requirement that the periodicity be of the order of this wavelength to obtain a strong diffraction pattern. This observation finally resolved the nineteenth century debate between Isaac Newton, who favoured a corpuscular theory of light, and Christian Huygens, who emphasized its wave nature. There exists, in fact, a wave–particle duality.
One year after the publication (1926), de Broglie’s ideas were extended and brought into more exact mathematical form by the Austrian physicist Erwin Schrödinger, whose theory became known as wave mechanics. In fact, wave mechanics provided a complete and perfectly self-consistent theory of all atomic phenomena and, as was shown in the late twenties, could explain also the phenomena of radioactive decay and artificial nuclear transformation. Simultaneously with Schrödinger’s paper on wave mechanics, there appeared a paper by a young German physicist, W. Heisenberg, who developed the treatment of quantum problems by using the so-called ‘non-commutative algebra’, a mathematical discipline in which $a \times b$ is not necessarily equal to $b \times a$. The simultaneous appearance of Schrödinger’s and Heisenberg’s papers in two different German magazines astonished the world of theoretical physics. These two papers looked as different as they could be, but led to exactly the same results concerning atomic structure and spectra. A new mechanics, called quantum mechanics, took a proper shape after these two great minds.

1.2 Heisenberg’s Uncertainty Principle

In classical mechanics a position function of time $x(t)$ and a momentum function of time $p(t)$ describe the one-dimensional motion of a particle. According to Newton, we can determine the motion of a particle, such as an electron, given its initial momentum and position and the mechanical laws which describe its motion. This is sometimes referred to as a deterministic or casual point of view. Quantum mechanics, on the other hand, takes a probabilistic or statistical point of view, that is, it is not possible to predict a definite trajectory and motion of a particle but only the probability that it will behave in a specific way.

This may be expressed in terms of the uncertainty or indeterminacy principle of Werner Heisenberg, which states that it is not possible to measure simultaneously the position and momentum of a particle with arbitrary accuracy for the purpose of predicting behaviour. If the position is precisely identified, then the momentum will be somewhat uncertain, and vice versa. Mathematically, this is expressed as follows: Given that the position of a particle can be measured within $\Delta x$, its momentum uncertainty in the $x$-direction, $\Delta p_x$, cannot be ascertained to any greater accuracy than

$$\Delta p_x = \frac{h}{\Delta x} \quad (1.3)$$

The indeterminacy concept can be demonstrated by noting the disturbance (uncertainty) introduced into the motion of a particle by the instrument used to study its trajectory: Consider shining light on a particle in an attempt to locate it accurately. The momentum of the light photon disturbs the particle and changes its position and momentum. We cannot reduce this influence by lowering the light intensity in a continuous manner to zero, since the smallest quantity of light is still one photon with discrete energy $\hbar \nu$. Hence the quantization hypothesis and the uncertainty principle follow from each other. Obviously, this idea has serious consequences when we deal with small particles, such as electrons, with small energy.
1.2.1 Demonstration of the Uncertainty Principle

Bohr proposed a ‘gedanken’ (or thought) experiment to demonstrate the Heisenberg principle exactly. Imagine that we have a powerful microscope that is used to determine the x-position of an electron (Fig. 1.2).

Suppose the objective lens of the microscope subtends an angle $2\theta$ from the point where the electron is located. The classical theory of optics dictates that the minimum separation $\Delta x$ between two adjacent positions of the electron that can be resolved by observing with light of wavelength $\lambda$ is

$$\Delta x = \frac{\lambda}{\sin \theta} \quad (1.4)$$

That is, the uncertainty in locating the electron position in this experiment is $\lambda/\sin \theta$. Since the light used in viewing the electron may be considered to be composed of photons, these particles interact with the electron, cause it to recoil (Compton effect), and are correspondingly deflected into the microscope objective lens; and we see the electron. By conservation of momentum, the electron recoil momentum in the $x$-direction must just equal in magnitude the maximum interacting photon $x$-component momentum. If the photons, which are seen, enter the objective anywhere within an angle $2\theta$, the range of the $x$-component of their momenta (de Broglie) is between $(+h/\lambda)\sin \theta$ and $(-h/\lambda)\sin \theta$. Hence, the electron recoil momentum total range is given by

$$\Delta p_x = \frac{2h}{\lambda} \sin \theta$$

By combining Eqs (1.3) and (1.4), we get

$$\Delta p_x \Delta x = 2h > h \quad (1.5)$$

This demonstrates the uncertainty principle.

The physical quantities momentum and position comprise one set of variables governed by the principle. It turns out that the uncertainty principle also refers to a number of other sets of variables. One such set is energy and time, and it can be shown that

$$\Delta E \Delta t \geq h \quad (1.6)$$

Here $\Delta E$ can be uncertainty in the energy of a photon and $\Delta t$ the accuracy limits of time estimation of its emission. Combined with the Planck formula, this becomes

$$\Delta n \Delta t \geq 1 \quad (1.7)$$
This relation is useful in estimating the sharpness of a laser spectral line, where $\Delta \nu$ is the line width and $\Delta t$ is the electron transition time.

### 1.3 Schrödinger Equation

What has been discussed so far is a series of ideas and concepts which are peculiar to the modern physics of quantum mechanics. What is needed now is a mathematical formulation that will permit us to predict and explain the many subatomic processes that govern the behaviour of the electronic materials of interest to us. As previously indicated, the Schrödinger wave equation expresses the essence of this modern physics. Obtaining solutions to this equation for a variety of physically interesting cases will permit us to analyse problems that may be subject to experimental verification.

The Schrödinger equation refers to the motion of an electron in various force fields. It replaces for microscopic phenomena the Newtonian expression $F = ma$ for the motion of particles on a larger scale and permits a description of effects not previously explainable in classical terms. Since we have already indicated that the electron can be pictured as having a wavelength, it should not be surprising that the Schrödinger equation takes the form of a wave equation.

The time-dependent Schrödinger wave equation for an electron having a potential energy $V$, which in general can be a function of position and time, is

$$\frac{\hbar^2}{2m_0} \left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) - V\psi = \frac{\hbar}{i} \frac{d\psi}{dt} \tag{1.8}$$

(time-dependent Schrödinger equation)

Here $\hbar$ is the Planck constant, $m_0$ the electron mass, $i = \sqrt{-1}$, and $\psi$ is the wave function which depends in general on position and time, that is,

$$V = V(x, y, z, t)$$

and

$$\psi = \psi(x, y, z, t) \tag{1.9}$$

where $\psi$ is in general a complex quantity. This is a complicated second-order differential equation which can be solved in closed form in only a limited number of special cases. However, the equation may be greatly simplified in a large number of problems by dealing separately with position and time. This is possible when the potential energy depends only on position, and not on time. Let us introduce this condition into the one-dimensional Schrödinger equation, which we consider for additional simplicity, although the three-dimensional formulation may be handled similarly. The one-dimensional equation is

$$\frac{\hbar^2}{2m_0} \left( \frac{\partial^2 \psi(x, t)}{\partial x^2} \right) - V(x)\psi(x, t) = \frac{\hbar}{i} \frac{d\psi(x, t)}{dt} \tag{1.10}$$
Separation of variables Let us postulate a solution of the form

\[ \psi(x, t) = \psi(x) \phi(t) \]

assuming that the space and time parts of the wave function \( \psi \) can be separated. Substituting Eq. (1.11) into Eq. (1.10) gives

\[ \frac{\hbar^2}{2m_0} \frac{d^2 \psi(x)}{dx^2} \phi(t) - V(x) \psi(x) \phi(t) = \frac{\hbar}{i} \frac{d \phi(t)}{dt} \psi(x) \]

Dividing the left- and right-hand sides of Eq. (1.12) by \( \psi(x) \) and \( \phi(t) \), respectively, we get

\[ \frac{\hbar^2}{2m_0} \frac{1}{\psi(x)} \frac{d^2 \psi(x)}{dx^2} - V(x) = \frac{\hbar}{i} \frac{1}{\phi(t)} \frac{d \phi(t)}{dt} \]

Notice that the left-hand side of the equation is a function of \( x \) only, while the right-hand side is a function of \( t \) only. A useful theorem of mathematical physics states that in such a case, where \( x \) and \( t \) are independent variables, each side of this equation must be separately equal to a constant. This is so because if we arbitrarily choose a value of \( x \), the left-hand side of Eq. (1.13) takes a value that is not necessarily equal to the right-hand side, since \( t \) can be chosen arbitrarily as any value. Hence for the equality to hold, both sides must be equal to a constant, which we will take as \( -E \). This then reduces Eq. (1.13) to two ordinary differential equations, one in position and one in time, whose solutions are more easily obtainable. That is,

\[ \frac{\hbar^2}{2m_0} \frac{d^2 \psi}{dx^2} + (E - V) \psi = 0 \]  

(time-independent Schrödinger equation)

and

\[ \frac{d \phi}{dt} = -\frac{2\pi i}{\hbar} E \phi \]

After some algebraic manipulation, the second equation integrates to

\[ \ln \phi = -\frac{i}{\hbar} \frac{E t}{\hbar} + A \]

We can take the integration constant \( A = 0 \) without loss of generality and introduce a constant later in reconstructing the product \( \psi = \psi \phi \). Then Eq. (1.15) becomes

\[ \phi = e^{-(2\pi i E \phi / \hbar) t} \]

which is oscillatory in time; \( E (= \hbar \nu) \) is the total electron energy.

The problem of finding the solution for the motion of an electron having potential energy \( V \) due to some force field now reduces to solving the second-order linear ordinary differential equation (1.14a), and the time-dependent solution can always be written by tacking on the results of Eq. (1.16).

1.3.1 The Free Electron Problem

Many of the quantum and wave mechanical ideas that have already been discussed
are contained intrinsically in the Schrödinger equation. A mathematically simple case, such as the motion of an electron in field-free space, will be used to illustrate this point.

The spatial (time-independent) part of the Schrödinger equation for an electron moving in one dimension with no forces acting on it \( V(x) = 0 \) reduces to

\[
\frac{d^2\psi}{dx^2} + \left( \frac{2m_0E}{\hbar^2} \right)\psi = 0
\]

(1.17)

or

\[
\frac{d^2\psi}{dx^2} + k^2\psi = 0
\]

(1.18)

where

\[
k^2 = \frac{2m_0E}{\hbar^2} \quad \text{or} \quad E = \frac{\hbar^2 k^2}{2m_0}
\]

(1.19)

Equation (1.19) represents a quadratic function of the wave vector. The plot of this function, which takes the form of a quadratic parabola, appears in Fig. 1.3. Since no limitations are set on \( k \), a free particle can carry any amount of energy. So its energy spectrum is continuous. Relation (1.19) is known as dispersion formula.

![Graphs](1.3)

**Fig. 1.3** (a) Energy, (b) group velocity, and (c) the effective mass of a free electron as functions of wave vector

The wave number \( k \) is introduced and relates directly to the energy of the wave. This may be recognized as the form of the differential equation describing the motion of a harmonic oscillator or the current oscillation in a lossless circuit
containing inductance and capacitance. The general solution of this equation is given by

$$\psi = A \exp(ikx) + B \exp(-ikx)$$  \hspace{1cm} (1.20)

where $A$ and $B$ are constant coefficients. Multiplying both sides of Eq. (1.20) by $\exp(-iEt/\hbar)$ gives the time-dependent particular solution of Eq. (1.10), where $[F(x) = 0]$ for the one-dimensional case is

$$\psi(x, t) = A \exp \left[ i \left( kx - \frac{E}{\hbar} t \right) \right] + B \exp \left[ -i \left( kx + \frac{E}{\hbar} t \right) \right]$$  \hspace{1cm} (1.21)

This is a formula for two travelling waves, one going in the positive $x$-direction and one going in the negative direction. For a wave moving along the $x$-axis, $B = 0$ and

$$\psi(x, t) = A \exp \left[ i (kx - \omega t) \right]$$  \hspace{1cm} (1.22a)

Similarly, for a wave moving in the direction opposite to the $x$-axis, $A = 0$ and

$$\psi(x, t) = A \exp \left[ -i (kx + \omega t) \right]$$  \hspace{1cm} (1.22b)

In the general case, where the direction of wave propagation is not coincident with the $x$-axis, the stationary solution of the Schrödinger equation is expressed in terms of the wave functions of the form

$$\psi(x, y, z, t) = C \exp[i(k \cdot \vec{r} - \omega t)]$$  \hspace{1cm} (1.23)

where $\vec{r}$ is the radius vector and $\vec{k}$ is the vector pointing in the direction of propagation of the de Broglie wave and is numerically equal to $k = \sqrt{2mE/\hbar}$ [from Eq. (1.19)]. The frequency and wavelength of the travelling waves are easily recognized as

$$\omega = \frac{E}{\hbar}, \quad \lambda = 2\pi/k$$  \hspace{1cm} (1.24)

We can calculate the momentum and energy in terms of the wave number from Eq. (1.23), one of the boundary conditions of $\psi$ (see Appendix C), and the definition of $k$:

$$p = \int_{-\infty}^{\infty} \psi \frac{\hbar}{i} \frac{d\psi}{dx} dx = \hbar k \int_{-\infty}^{\infty} |\psi|^2 dx = \hbar k = \frac{\hbar}{\lambda}$$  \hspace{1cm} (1.25)

$\psi$ concerns with the probability density of finding the body described by it. The integral of $|\psi|^2$ over all space must be finite, i.e., the body is somewhere, after all. If the particle exists, the integral $\int_{-\infty}^{\infty} |\psi|^2 dv$ must be equal to 1, otherwise 0. The last part of Eq. (1.25) confirms the relation between $E$ and $p$ in classical mechanics. In the derivation of the first part we have used the fact that the wave must be somewhere, so the integral over $x$ of $|\psi|^2$ is 1. The first part confirms the postulate of de Broglie, so both Schrödinger’s and de Broglie’s postulates are consistent.

The free particle wave function (1.22) relates to an electron with a strictly definite momentum $\hbar k$. In accordance with the uncertainty relations, the function has a constant amplitude in finite space: the probability of finding the wave/particle anywhere is the same. The wave is everywhere. This means that the particle is totally delocalized in infinite space. The discussion on the behaviour of such a
particle becomes rather a poor example. It is much more convenient to deal with a particle localized in a limited portion of space, i.e., to consider the so-called wave packet. Besides, it poses a theoretical problem, since the probability of finding a particle somewhere turns out to be zero if the limits of integration over $x$ are finite. This is only a theoretical problem: simply consider our universe limited in size and the probability has a small value everywhere.

### 1.4 Electron as a Wave Packet

The wave–particle duality may be better understood by realizing that the electron can be represented by a combination of several wave trains having slightly different frequencies between $\omega$ and $\omega + \Delta \omega$ and different wave numbers between $k$ and $k + \Delta k$. The rigorous solution would require the summing of infinitely many such waves having slightly different wave vectors and frequencies. However, it turns out that the essence of the result is indicated effectively by our simplistic approach. Let us study this, assuming at first only two waves, which will be written as [from Eq. (1.21), considering only the real part]

$$
\psi_1 (x, t) = A \exp \left[ i (kx - \omega t) \right] = A \sin \left[ kx - \omega t \right] \tag{1.26}
$$

and

$$
\psi_2 (x, t) = A \exp \left[ i (k + \Delta k)x - (\omega + \Delta \omega)t \right] = A \sin \left[ (k + \Delta k)x - (\omega + \Delta \omega)t \right] \tag{1.27}
$$

Superposition of $\psi_1$ and $\psi_2$ yields a new wave $\psi$. With $\sin \alpha + \sin \beta = 2 \cos \left( \frac{\alpha - \beta}{2} \right) \sin \left( \frac{\alpha + \beta}{2} \right)$ we obtain

$$
\psi_1 + \psi_2 = \psi = 2A \cos \left( \frac{\Delta \omega}{2} t - \frac{\Delta k}{2} x \right) \sin \left[ \left( \frac{k + \Delta k}{2} \right) x - \left( \frac{\omega + \Delta \omega}{2} \right) t \right]
$$

Equation (1.28) describes a sine wave having a frequency intermediate between $\omega$ and $\omega + \Delta \omega$ whose amplitude is slowly modulated by a cosine function. (This familiar effect in acoustics can be heard in the form of beats when two strings of a piano have a slightly different pitch. The beats become less rapid the smaller the difference in frequency, $\Delta \omega$, between the two strings until they finally cease once both strings have the same pitch.) The wave packets become ‘larger’ the slower the beats, i.e., the smaller the $\Delta \omega$. The extreme conditions are as follows.

1. No variation in $\omega$ and $k$ (i.e., $\Delta \omega = 0$ and $\Delta k = 0$) yields an ‘infinitely long’ wave packet, i.e., a monochromatic wave. The wave has constant amplitude. This corresponds to the wave picture of an electron [Fig. 1.4(a)].

2. Alternatively, $\Delta \omega$ and $\Delta k$ could be assumed to be very large. This yields small wave packets. If a large number of different waves is considered (rather than $\psi_1$ and $\psi_2$), filling the frequencies between $\omega$ and $\omega + \Delta \omega$, the string of wave packets shown in Fig. 1.4(b) reduces to one wave packet only. The electron is then represented by a particle. $\Delta x$ is the distance over which the particle can be found.
1.4.1 Group Velocity and Phase Velocity

The velocity of the pilot wave, also known as matter wave, is called the wave velocity or phase velocity \( v \). As we saw in the preceding section, the matter wave is a monochromatic wave (or a stream of particles of equal velocity whose frequency \( \omega \), wavelength \( \lambda \), momentum \( p \), and energy \( E \) can be exactly determined [Fig. 1.4(a)]. The location of the particles, however, is undetermined. From the second part of Eq. (1.28) (marked ‘sine wave’), we deduce

\[
v = \frac{x}{t} = \frac{\omega + \Delta \omega}{2k + \Delta k/2} = \frac{\omega'}{k'}
\]

(1.29)

![Fig. 1.4](a) Monochromatic matter wave (\( \Delta \omega = 0 \) and \( \Delta k = 0 \)); (b) Combination of two waves of slightly different frequencies

Thus, we obtain the velocity of a matter wave that has a frequency \( \omega + (\Delta \omega/2) \) and a wave number \( k + (\Delta k/2) \). The phase velocities vary for different wavelengths, a phenomenon called dispersion.

It has already been mentioned that a particle can be understood to be composed of a group of waves or a ‘wave packet’. Each individual wave has a slightly different frequency, ranging in value between \( \omega \) and \( \omega + \Delta \omega \). Appropriately, the velocity of a particle is called ‘group velocity’, \( v_g \). The ‘envelope’ in Fig. 1.4(b) propagates with the group velocity \( v_g \).

From the left part of Eq. (1.28) (marked ‘modulated amplitude’) we obtain

\[
v_g = \frac{x}{t} = \frac{\Delta \omega}{\Delta k} = \frac{d\omega}{dk}
\]

(1.30)

Equation (1.30) is the velocity of a ‘pulsed wave’, i.e., of a moving particle (Fig. 1.5).

1.4.2 Particle in an Infinite Potential Well (\( E < V \) and \( V = \infty \))

Consider the motion of a particle such as an electron in a potential well with infinite sides, schematically shown in Fig. 1.6. Here the potential energy \( V \) is plotted as a
function of $x$. Note that the potential energy is taken as zero for $-a/2 < x < +a/2$. At $x = \pm a/2$, the potential energy takes on an infinite value. This will confine the electron within the ‘walls’ of the potential well because of the infinitely high barriers there. An analogy would be a ball moving with finite energy attempting to climb an infinitely ‘steep hill’ or a ball bouncing in a box with impenetrable walls. The particle does not lose energy when it collides with such walls, so its total energy remains constant. Hence the probability of an electron, once in the well, being found outside the walls is zero. In terms of Born’s hypothesis, this means that $|\psi_2| = 0$ there, and so $\psi = 0$ at $-a/2 < x < a/2$. For an electron, such a well can be a piece of metal; outside the metal the potential energy of a free electron is $U = 0$, and inside the metal this energy is equal to $U_0 = -qV_0$, where $V_0$ is the positive potential of a field produced by lattice sites. The electron cannot freely leave the metal. For this, it must do the work numerically to $U_0$.

**Solution of the Schrödinger equation** The one-dimensional time-independent Schrödinger equation for this case for $|x| < a/2$ is then

$$\frac{d^2\psi}{dx^2} + \frac{2m_0E}{\hbar^2}\psi = 0$$

(1.31)

Again this is similar to the equation of harmonic motion, and it is convenient here to write the solution as

$$\psi = A\sin\left(\sqrt{\frac{2m_0E}{\hbar^2}}x\right) + B\cos\left(\sqrt{\frac{2m_0E}{\hbar^2}}x\right)$$

(1.32)

To solve for the two constants of integration $A$ and $B$, the boundary condition $\psi = 0$ at $x = \pm a/2$ is applied. This gives, at $x = +a/2$,

$$\psi = A\sin\left(\sqrt{\frac{2m_0E}{\hbar^2}}\frac{a}{2}\right) + B\cos\left(\sqrt{\frac{2m_0E}{\hbar^2}}\frac{a}{2}\right) = 0$$

(1.33)

and, at $x = -a/2$,

$$\psi = -A\sin\left(\sqrt{\frac{2m_0E}{\hbar^2}}\frac{a}{2}\right) + B\cos\left(\sqrt{\frac{2m_0E}{\hbar^2}}\frac{a}{2}\right) = 0$$

(1.34)

Hence from Eq. (1.33) or (1.34) either $A = 0$ or $\sin\left(\sqrt{\frac{2m_0E}{\hbar^2}}(a/2)\right) = 0$, and either $B = 0$ or $\cos\left(\sqrt{\frac{2m_0E}{\hbar^2}}(a/2)\right) = 0$. To avoid the trivial solution $\psi = 0$ for all $x$, it must be true that either

$$A = 0, \quad \cos\left(\sqrt{\frac{2m_0E}{\hbar^2}}(a/2)\right) = 0$$

(1.35)
or

\[ B = 0, \quad \sin \left( \frac{\sqrt{2m_0E}}{\hbar} \frac{a}{2} \right) = 0 \] (1.36)

From Eq. (1.35), \[ \sqrt{\left(\frac{2m_0E}{\hbar}\right)} \frac{a}{2} = n\pi/2, \] where \( n \) is an odd integer. Similarly, from Eq. (1.36), \[ \sqrt{\left(\frac{2m_0E}{\hbar}\right)} \frac{a}{2} = n\pi/2, \] where \( n \) is an even integer. Hence the general solution can be obtained by summing solutions of the form

\[ \psi = B \cos \left( \frac{\sqrt{2m_0E}}{\hbar} \frac{a}{2} \right) x \] (1.37a)

where

\[ \frac{\sqrt{2m_0E}}{\hbar} \frac{a}{2} = \frac{n\pi}{a} \quad \text{for } n = 1, 3, 5, 7, \ldots \] (1.38a)

or

\[ \psi = A \sin \left( \frac{\sqrt{2m_0E}}{\hbar} \frac{a}{2} \right) x \] (1.37b)

where

\[ \frac{\sqrt{2m_0E}}{\hbar} \frac{a}{2} = \frac{n\pi}{a} \quad \text{for } n = 2, 4, 6, 8, \ldots \] (1.38b)

Finally, we can solve for the constants \( A \) and \( B \) by normalizing these solutions. This results from the Born probability interpretation of \( \psi \). One of the conditions of \( \psi \) previously stated was that the integral of \( |\psi|^2 \) over all space was required to be finite. Since the probability is normally a fractional quantity less than 1, the probability of finding the electron somewhere in space must be identically 1, and so in one dimension

\[ \int_{-\infty}^{\infty} |\psi|^2 \, dx = 1 \] (1.39)

Applying this normalization condition to Eqs. (1.37a) and (1.37b) and noting that \( \psi = 0 \) for \(-a/2 > x > a/2\) gives

\[ A = B = \left(\frac{2}{a}\right)^{1/2} \] (1.40)

Solving for \( E \) from Eqs. (1.37a) and (1.37b) yields

\[ E_n = \frac{n^2\hbar^2}{8m_0a^2} \] (1.41)

where \( n \) is an integer and \( E_n \) refers to an infinite number of discrete energy values or levels corresponding to each integral value of \( n \). These energy values are often referred to as eigenvalues and occur in all quantum mechanical problems concerning spatially bound or constrained particles; the number \( n \) is called the quantum number. The electron is then said to be in any of these energy states or eigenstates denoted by \( \psi_n \) at a given time, and it is expressed as
\[ \psi_n = \sqrt{\frac{2}{a}} \sin \left( \frac{\sqrt{2m_0E_n}}{\hbar} x \right) = \sqrt{\frac{2}{a}} \sin \left( \frac{n\pi x}{a} \right) \quad (1.42) \]

The lowest eigenstate is called the ground state, and the energy in this case is often referred to as the zero point energy; here \( E_1 = \hbar^2/(8m_0a^2) \). Hence at absolute zero all motion does not cease.

Note that as the particle is less constrained as the width of the well is increased, the energy levels come closer together, indicating that quantum mechanics predicts a continuum of energy values for nearly free electrons. One thus would also expect that the higher energy levels would become closer together as the electron is excited to these nearly free states. The one-dimensional model presented here does not predict this. The three-dimensional model corrects this dilemma and is the subject of a problem at the end of this chapter. Note too that as the particle mass becomes very large, a continuum of energy values is again predicted, in agreement with the correspondence principle.

### 1.4.3 Particle in a Finite Potential Well (\( E < V \) and \( V = \) finite value):
Tunnelling Effect

We consider now an electron moving along the \( x \)-axis in a space where the potential energy changes abruptly in a step-like manner, as shown in Fig. 1.7. \( U = 0 \) in region I extending from \( -\infty \) to 0. In region II, extending from 0 to \( \infty \), the potential energy is \( U \). So, in going from region I to region II, the particle encounters an obstacle in the form of a potential barrier of height \( U \). This means that if electrons have energies \( E \) that are lower than the wall energy \( U \), then they will not be able to surmount the barrier; but for higher energies, they are free. This problem also deals with the problem of the motion of an electron in a periodic crystal lattice.

![Fig. 1.7 Passage of a particle across a potential barrier (a) extending to infinity, and (b) of finite thickness](image-url)
Solution of the Schrödinger equation The time-independent Schrödinger equation in region I, where \( U = 0 \), is
\[
\frac{d^2\psi}{dx^2} + \alpha^2 \psi = 0 \tag{1.43}
\]
where \( \alpha = [(2m_0E/\hbar^2)]^{1/2} \) is a constant quantity independent of \( x \). As before, it is convenient to write the solution of the form
\[
\psi = A \exp(j \alpha x) + B \exp(-j \alpha x) \tag{1.44}
\]
In region II the Schrödinger equation is
\[
\frac{d^2\psi}{dx^2} - \beta^2 \psi = 0 \tag{1.45}
\]
where \( \beta^2 = 2m_0 (U - E)/\hbar^2 \) is a real constant for \( x > 0 \). Now the solution of this equation may be written as
\[
\psi = C \exp(\beta x) + D \exp(-\beta x) \tag{1.46}
\]
The constants of integration, \( A, B, C, \) and \( D \), must be chosen to satisfy the boundary conditions, as follows:
\[
\begin{align*}
\psi & \text{ must be finite and continuous for all } x \tag{1.47} \\
\frac{d\psi}{dx} & \text{ must be finite and continuous for all } x \tag{1.48}
\end{align*}
\]
In Eq. (1.45) with \( \beta \) positive the first term on the right-hand side [Eq. (1.46)] grows infinitely large as \( x \to \infty \), which is in disagreement with condition (1.47). This term can be omitted by considering \( C = 0 \). Now, to maintain the continuity of \( \psi \) at \( x = 0 \) from Eqs (1.44) and (1.46),
\[
[A \exp(j \alpha x)]_{x = 0} + [B \exp(-j \alpha x)]_{x = 0} = [D \exp(-\beta x)]_{x = 0} \tag{1.49}
\]
which gives
\[
A + B = D \tag{1.50}
\]
Similarly, for \( d\psi/dx \) to be continuous at \( x = 0 \), Eqs (1.44) and (1.46) need to be differentiated to yield
\[
[j \alpha A \exp(j \alpha x)]_{x = 0} - [j \alpha B \exp(-j \alpha x)]_{x = 0} = [D \exp(x - \beta x)]_{x = 0} \tag{1.51}
\]
This gives
\[
\frac{j \beta D}{\alpha} = A - B \tag{1.52}
\]
Equations (1.50) and (1.52) are two equations and there are three unknowns; hence we can solve for \( A \) and \( B \) in terms of \( D \) as
\[
A = \frac{D}{2} \left(1 + \frac{j \beta}{\alpha} \right) \\
B = \frac{D}{2} \left(1 - \frac{j \beta}{\alpha} \right) \tag{1.53}
\]
Now that we know the integration constants, the complete wave function can be written by taking the time-dependent part as
\[ \psi(x, t) = D \left( \frac{1 + i \beta}{\alpha} \right) \exp \left[ j \left( \alpha x - \frac{Et}{\hbar} \right) \right] + \frac{D}{2} \left( 1 - i \beta \right) \exp \left[ -j \left( \alpha x + \frac{Et}{\hbar} \right) \right] \text{ for } x \leq 0 \]  

(1.54)

and

\[ \psi(x, t) = D \exp \left( -\beta x \right) \exp \left( -jEt/\hbar \right) \text{ for } x \geq 0 \]  

(1.55)

The first part of Eq. (1.54) corresponds to the wave travelling along the x-axis in region I. \((D/2)[1 + (j\beta/\alpha)]\) is the amplitude of this wave. The second part corresponds to the wave moving in region I in the direction opposite to the x-axis. This is the wave reflected from the barrier. \((D/2)[1 - (j\beta/\alpha)]\) is the amplitude of the reflected wave. Since the probability that the particle is present in one region of the space or another is proportional to the square of the de Broglie wave amplitude, the ratio \(R = |B|^2/|A|^2\) is the coefficient of reflection of a quantum mechanical particle from the barrier.

In region II, Eq. (1.55) indicates a standing wave, i.e., at any position \(x\), the wave oscillates harmonically with time. The square of the amplitude of this wave defines the probability of penetration of the particle into region II. The ratio \(D = |C|^2/|A|^2\) is the penetrability of the interface.

Using the mathematical identity \(\exp(j\theta) = \cos \theta + j \sin \theta\), the complete wave functions, Eqs (1.54) and (1.55), become

\[ \psi_1(x, t) = D \left( \cos \alpha x - \frac{\beta}{\alpha} \sin \alpha x \right) \exp(-jEt/\hbar) \text{ for } x \leq 0 \]

and

\[ \psi_2(x, t) = D[\exp(-\beta x)]\exp(-jEt/\hbar) \]

\[ = D \left[ \exp \left( -\frac{\sqrt{2m_0(U - E)}x}{\hbar} \right) \right] \exp(-jEt/\hbar) \text{ for } x \geq 0 \]  

(1.56)

Since the amplitude is not equal to zero, there is a probability that a particle can penetrate into the second region to a certain depth. This probability is in proportion to the square of the modulus of the wave function \(\psi_2\):

\[ w = |\psi_2|^2 = D^2 \exp \left[ -\frac{2x}{\hbar} \sqrt{2m_0(U - E)} \right] \]  

(1.57)

This probability is indicative of the fact that the particle is able to cross (penetrate) the potential barrier of finite width \(d\) [Fig. 1.7(b)]. Such penetration received the name tunnell effect. In accordance with Eq. (1.57), the penetrability of the barrier is

\[ D = D_0 \exp \left[ -\frac{2d}{\hbar} \sqrt{2m_0(U - E)} \right] \]  

(1.58)

where \(D_0\) is the proportionality factor close to unity. Table 1.1 lists the values of \(D\) for barriers of various widths but of the same height \(U - E = 5\) eV. As seen from the
data of Table 1.1, the barriers between crystal atoms exhibit a rather high penetrability. A remarkable thing is that the energy of the particle tunnelling across the potential barrier does not vary: particles leaving the barrier carry the same amount of energy as that with which they enter it.

<table>
<thead>
<tr>
<th>$d$, nm</th>
<th>0.1</th>
<th>0.15</th>
<th>0.2</th>
<th>0.5</th>
<th>1.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D$</td>
<td>0.1</td>
<td>0.03</td>
<td>0.008</td>
<td>$1.1 \times 10^{-6}$</td>
<td>$1.15 \times 10^{-10}$</td>
</tr>
</tbody>
</table>

The tunnel effect plays an important role in electronic devices. It governs such phenomena as the emission of electrons under the actions of strong field, passage of current through dielectric films, and breakdown of a $p$-$n$ junction. One of the most familiar of these devices is the tunnel diode, which is used as a high frequency (gigahertz) oscillator. Other devices whose operation can be explained by this effect are the zener diode and the Josephson junction.

1.4.4 Electron Motion in a Periodic Potential: Concept of Bands

Now we will discuss the motion of electrons in a solid where there is a periodic arrangement of atoms. In such solids the electrons are liberated from the atoms, making them ions; and the free electrons are wandering in an environment of periodic potential as shown in Fig. 1.8. It will be seen in our present discussion that electrons have a series of allowed bands separated by forbidden gaps. Within each allowed band the electron is described by a $k$ vector, very much as in the free space problem. As in free space, we have an energy versus $k$ vector relation and this relation is more complicated in the present situation. Later we will see that the properties of solid crystals such as metals, semiconductors, and insulators can be derived from this analysis.

1.4.4.1 Kronig–Penny Model

Kronig and Penny suggested a simple model to obtain a mathematical solution that confirms energy band formation, including the existence of forbidden bands. The model is drastically simplified in the sense that we reduce the problem to that of a single electron travelling in one dimension, impinging on a series, infinite in extent, of periodically spaced potential wells. Though it has a lot of similarity with the problems discussed in Section 1.4.2, the solution of Schrödinger’s equation using this model describes fairly accurately the effects that are observed in real solids.

It is important to be aware of the assumptions that are made in the model and its solution. These are as follows.

- Electron interaction with the core is purely coulombic in nature.
- Electron to electron interaction is precluded.
- Non-ideal effects such as collisions with the lattice and the presence of impurities are neglected.
- Atoms are fixed in position, although, in fact, they may be vibrating.
Fig. 1.8 (a) Potential energy function representing the force field created by periodically spaced ions. (b) Simplified mathematical representation of the periodic function of (a) assumed by Kronig and Penny.

Note that the $x$-space is broken down into regions of widths $a$ (region I) and $b$ (region II), with the distance between nuclei being $(a + b)$. The potential field $u(x)$ originating from the nuclei is periodic, and Bloch has stated a theorem that says that the wave function $\psi(x)$ will show the same periodicity as $u(x)$. In the solution to the Schrödinger equation this means that, unlike for the free electron, the solution will be periodic in $k$. If the lattice periodicity is $a$, then for a given $E$, $k$ values differing by a multiple of $2\pi/a$ will give the same wave function. These allowed wave functions are called Bloch waves, and these are the only waves allowed in the crystal.

**The Schrödinger equation** The rectangular representation is called the Kronig–Penny idealization of a crystal lattice and allows for an analytical solution of the Schrödinger equation. The time-independent Schrödinger equation in this case becomes

$$\frac{d^2\psi}{dx^2} + \frac{2m_h}{\hbar^2} [E - V(x)]\psi = 0 \quad (1.59)$$
where \( V(x) \) is given in Fig. 1.8 as

\[
V = V_0 \quad \text{for} \quad -b < x < 0, \quad a < x < a + b, \quad \text{etc.}
\]

\[
V = 0 \quad \text{for} \quad 0 < x < a, \quad a + b < x < 2a + b, \quad \text{etc.}
\]  \hspace{1cm} (1.60)

As per the Bloch theorem the wave function \( \psi(x) \) can be written in the form

\[
\psi(x) = u(x) \exp(jkx)
\]  \hspace{1cm} (1.61)

where \( k \) is a constant of motion and \( u(x) \) is a periodic function. If the Bloch function of Eq. (1.61) is a solution of the Schrödinger equation, then after substitution in Eq. (1.59) it leads to

\[
\frac{d^2u}{dx^2} + 2jk \frac{du}{dx} - \left[ k^2 - \alpha^2 + \frac{2m_0V(x)}{\hbar^2} \right] u = 0
\]  \hspace{1cm} (1.62)

where \( \alpha^2 = 2m_0E/\hbar^2 \); that is, the Bloch function is a solution of the Schrödinger equation if \( u(x) \) satisfies Eq. (1.62).

It is now necessary to introduce the proper potential energy values into this equation. Since the potential function repeats itself with period \( a + b \), it will be necessary to solve the equation in the interval \(-b < x < a\). The solution in other similar intervals will be identical with this one. Substituting the appropriate potential energy values from Eq. (1.60), we get

\[
\frac{d^2u_1}{dx^2} + 2jk \frac{du_1}{dx} - (k^2 - \alpha^2)u_1(x) = 0 \quad \text{(region I:} \quad 0 < x < a) \]  \hspace{1cm} (1.63a)

and

\[
\frac{d^2u_2}{dx^2} + 2jk \frac{du_2}{dx} - (k^2 - \beta^2)u_2(x) = 0 \quad \text{(region II:} \quad -b < x < a) \]  \hspace{1cm} (1.63b)

Here \( u_1(x) \) and \( u_2(x) \) are the values of \( u(x) \) in regions I and II, respectively, and \( \beta = 2m_0(E-V_0)/\hbar^2 \). Equations (1.63a) and (1.63b) resemble the differential equation for an electric circuit comprising resistance, inductance, and capacitance; they can be solved by the method of the Laplace transformation. One can show that the solutions of these two equations are of the form

\[
u_1(x) = A \exp j(\alpha - k)x + B \exp -j(\alpha + k)x \quad (0 < x < a) \]  \hspace{1cm} (1.64a)

\[
u_2(x) = C \exp j(\beta - k)x + D \exp -j(\beta + k)x \quad (-b < x < 0) \]  \hspace{1cm} (1.64b)

where \( A, B, C, \) and \( D \) are constants to be determined using boundary conditions.

**Boundary conditions** To determine the integration constants \( A, B, C, \) and \( D \), it is convenient to apply the conditions of finiteness and continuity of \( \psi \) and \( dy/dx \) at \( x = a, x = -b, \) and \( x = 0 \). It, therefore, follows that the functions \( u(x) \) obey these requirements since \( \exp(jkx) \) is known to be a bounded and continuous function for all \( x \). Also, because of the periodicity of \( u(x) \) in the distance \( a + b \) [see Eq. (1.61)], it follows that \( u_1(a) = u_2(-b) \) and \( u'_1(a) = u'_2(-b) \). Introducing these boundary conditions in a straightforward but somewhat tedious manner gives

\[
A + B = C + D \quad \text{[since} \quad u_1(0) = u_2(0)\text{]} \]

\[
j(\alpha - k)A - j(\alpha + k)B = j(\beta - k)C - j(\beta + k)D \quad \text{[since} \quad u'_1(0) = u'_2(0)\text{]} \]
\[
\exp \left[ j(\alpha - k)a \right] A + \exp \left[ -j(\alpha + k)a \right] B \\
= \exp \left[ -j(\beta - k)b \right] C + \exp \left[ j(\beta + k)b \right] D \\
\text{[since } u_1(a) = u_2(-b) ]}
\]
\[j(\alpha - k) A - j(\alpha + k) B \exp \left[ -j(\alpha + k)a \right] B \\
= j(\beta - k) \exp \left[ -j(\beta - k)b \right] C \\
- j(\beta + k) \exp \left[ j(\beta + k)b \right] D \\
\text{[since } u_1'(a) = u_2'(-b) ] \\
\] (1.65)

The simultaneous solution of these equations is very complicated and, in fact, unnecessary. A theorem of algebra states that in a set of simultaneous linear homogeneous equations [Eq. (1.65)] there is only a non-trivial solution if the determinant of the coefficients of \(A, B, C,\) and \(D\) equals to zero. The evaluation of this determinant leads to
\[
-\frac{\alpha^2 + \beta^2}{2\alpha \beta} \sin \alpha a \sin \beta b + \cos \alpha a \cos \beta b = \cos k(a + b) \\
\] (1.66)

Now the electron energy \(E\) can, in general, be less than or greater than \(V_0\). If \(E > V_0\), then \(\beta\) is previously defined as a real quantity. In cases where \(E < V_0\), it is convenient to introduce \(\beta = j\chi\) and then Eq. (1.66) becomes, with the use of \(\cos i x = \cosh x\) and \(\sin i x = j \sinh x\),
\[
\frac{\gamma^2 - \alpha^2}{2\alpha \gamma} \sinh \gamma b \sin \alpha a + \cosh \gamma b \cos \alpha a = \cos k(a + b) \\
\] (1.67)

Here \(\gamma^2\) is real and positive for electron energies such that \(0 < E < V_0\). \(\beta^2\) is real and positive for energies such that \(V_0 < E < \infty\), where Eq. (1.66) is most conveniently applied.

**Allowed energy bands** Equations (1.66) and (1.67) are complicated transcendental equations involving the electron energy \(E\) through the quantity \(\chi\). To solve for \(\chi\), the method of graphical solution is suitable. However, to obtain an equation more susceptible to solution, Kronig and Penny suggested a special case. The potential barrier in Fig. 1.8 will be of the kind such that \(b\) shrinks to zero and \(V_0\) is very large. It is further assumed that the product \(V_0 b\), i.e., the area of the potential barrier, remains finite. In other words, if \(V_0\) grows, \(b\) diminishes accordingly. The product \(V_0 b\) is called the potential barrier strength. Then Eq. (1.67) is most appropriate and, as \(\chi \to \infty\), Eq. (1.67) reduces to
\[
\frac{p \sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka \\
\] (1.68)

where \(p = m_0 V_0 b/a \hbar^2\) is sometimes referred to as the scattering power of the potential barrier. It is a measure of the strength with which electrons in a crystal are attracted to the ions on the crystal lattice sites.

Equation (1.68) has only two variables—\(p\) and \(k\). One can calculate energy \(E\) through \(p\) by plotting the function \(p \sin \alpha a/\alpha a + \cos \alpha a\) versus \(\alpha\). The plot is shown in Fig. 1.9 with \(p = 3 \pi/2\). The right-hand side of Eq. (1.68) is bounded between values \(+1\) and \(-1\). The allowed values of the function \(p \sin \alpha a/\alpha a + \cos \alpha a\) are marked by the solid line.
Fig. 1.9 Graph of $p \sin \alpha a/\alpha a + \cos \alpha a$ versus $\alpha a$ with $p = 3\pi/2$. The allowed values of $\alpha a$ are indicated by the cross-hatched regions.

We arrive at the following very important results.

- $\alpha a$ is a function of energy. The above-mentioned limitation means that an electron which moves in a periodically varying potential field can only occupy certain allowed energy zones. Energy outside these allowed zones or ‘bands’ is prohibited. In practical sense, the regularity of the crystal and the finite potential well have prohibited waves where only certain wavelengths can occur. The ones that are allowed to occur are called Bloch waves.
- The allowed bands get broader for larger energies and start overlapping for very large energies.
- The size of the allowed and forbidden energy bands varies with the variation of $p$. Some special cases are discussed below.

**Case I** $p \to$ large, i.e., the potential barrier strength $V_0b$ is also large, the curves in Fig. 1.9 become more steep. The allowed bands are narrow.

**Case II** $p \to$ small, i.e., the potential barrier strength $V_0b$ tends to be small, the allowed bands become wider.

**Case III** $p \to 0$, i.e., the potential barrier strength $V_0b$ is about to disappear completely, then one obtains from Eq. (1.68)

$$\cos \alpha a = \cos ka$$

(1.69)

or $\alpha = k$. From this it follows with $\alpha^2 = 2m_0E/h^2$ that

$$E = \hbar^2k^2/2m_0$$

(1.70)

This is the well known equation for a free electron as derived earlier.
Case IV $p \to \infty$, i.e., the left-hand side of Eq. (1.68) must remain bounded and hence finite, $\sin \alpha a = 0$. The solution of this latter equation is $\alpha a = \pm n\pi$, where $n$ is any integer; then the permitted energies reduce to unique values

$$E_n = \frac{n^2 \hbar^2}{8m_0 a^2} \quad (1.71)$$

Equation (1.71) is recognized as the eigenvalue for the electron in a box with impenetrable walls. This seems reasonable, since in this case the electron is prohibited from leaving its ion attachment. Finite values of $p$ lead to smearing out of these discrete levels into energy bands.

**Brillouin zones** Figure 1.10 shows the plot of $E$ versus $k$ for a value of $0 < p < \infty$. The dashed curve refers to the case $p = 0$, is parabolic, and corresponds to the $E(k)$ relationship for a free electron. The plot indicates energy discontinuities at

$$k = n\pi/a \quad (1.72)$$

where $n = 1, 2, 3, \ldots$. These are referred to as the Brillouin zone boundaries and correspond to those values of electron momenta where discontinuities in the relation of energy to the wave vector occur. Equation (1.72) physically indicates the condition for a standing wave due to an electron wave impinging and being reflected from the potential barrier represented by $p$. Since the electron momentum is given by $p = \hbar k$ and $p = h/\lambda$ by the de Broglie formula, $k$ is identified with the electron

![Fig. 1.10](image_url)

Fig. 1.10 The permitted values of energy for an electron travelling in one-dimensional periodic potential field are indicated by the solid lines. The $E$-$k$ relationship for a free electron is indicated by the dashed parabola.
wavelength as \( k = \frac{2\pi}{\lambda} \). Then the Brillouin zone boundaries defined by Eq. (1.72) correspond to \( \lambda = 2a/n \). That is, the maximum interaction with the lattice ions occurs when the electron wavelength is twice the lattice spacing, equal to the lattice spacing, etc.

1.4.4.2 \( E-k \) Diagram in Extended and Reduced Zone Schemes

In the free electron model we were able to discuss the energy and wave vector irrespective of the crystallography of the solid. The various Brillouin zone surfaces in \( k \)-space become important as soon as periodic potentials have to be taken into account. In the case of free electrons, the Bloch solutions are plane waves, i.e., \( \psi = \exp (ijkr) \) with the wave vector and energy related simply by Eq. (1.70). For this free electron limit, any energy is possible for some real values of \( k \). Figure 1.11(a) plots the \( E-k \) relationship of Eq. (1.70) for a one-dimensional solid of lattice constant \( a \) and a vanishingly small periodic potential. This figure shows both the extended zone and reduced zone representations of the solution. For the latter type of representation, a portion of the \( E-k \) solution has been moved horizontally through a reciprocal lattice vector to bring the range of \( k \) used within the first Brillouin zone, because, for a one-dimensional solid of lattice constant \( a \), any reciprocal lattice vector is an integral multiple of \( (2\pi/a) \).

This delightful simplicity is lost once we consider the Bloch functions, their wave vectors, and their permitted energies for a finite periodic potential energy \( V(r) \). It turns out that whatever the form of this periodic \( V(r) \) there exist some forbidden energy gaps in the \( E-k \) diagram and are represented in extended and reduced zone schemes, shown in Fig. 1.12(b).

1.4.4.3 \( E-k \) Diagrams in Semiconductors

In three-dimensional crystals with three-dimensional reciprocal lattices, the use of a reduced zone representation is no longer merely a convenience; it is essential, otherwise the representation of the electronic states becomes too complex. How then can we display the band structure information from a three-dimensional crystal, which needs of course four dimensions \( (E, k_x, k_y, k_z) \) to describe it? The answer is to make representations of certain important symmetry directions in the three-dimensional Brillouin zone in one-dimensional \( E \) versus \( k \) plots. Only by doing so can we get all the important information onto a two-dimensional page. Therefore, when looking at an \( E-k \) diagram, one is looking at different sections cut out from the \( k \)-space.

The \( E-k \) diagram for Si, Ge, C, GaAs, InAs, InP, and GaP materials are illustrated in Appendix B. Other properties (electrical, optical, and thermal) are also mentioned therein. For detailed information about \( E-k \) diagrams and explanations, the readers may consult textbooks mentioned in the Bibliography.
Fig. 1.11 (a) Energy as a function of the wave vector for electrons in a one-dimensional crystal of lattice constant \( a \) when the amplitude of the periodic potential is zero. Energy is then a continuous function of the wave vector. Energy is shown as a multi-valued function of \( k \) in the shaded first Brillouin zone. (b) The extended and reduced zone representations of energy versus wave vector of electrons in a one-dimensional solid of lattice constant \( a \), where the periodic potential is of finite amplitude. Well-behaved non-localized wave functions can be constructed (i.e., wave functions for real \( k \)) only within the shaded regions of eigenenergies. These are the allowed electron bands, separated from each other by forbidden energy gaps.
1.5 Simple Harmonic Oscillator

The solution of the Schrödinger equation for a particle moving with a restoring force that increases linearly with displacement from an equilibrium position is also possible. In this problem, the particle executes a harmonic vibration about its equilibrium position. The best example can be vibrating atoms in a solid at any temperature except \( T = 0 \) K.

As the particle deviates for a distance \( x \), a restoring force appears, which is proportional to \( x \) and directed towards the equilibrium position, \( F = \beta x \), where \( \beta \) is the restoring force constant. The oscillator oscillates with a frequency

\[
v = \frac{1}{2\pi} \sqrt{\frac{\beta}{m_0}} \quad \text{or} \quad \omega = \sqrt{\frac{\beta}{m_0}}
\]

Classically, the particle carries a potential energy

\[
V(x) = \frac{1}{2} \beta x^2 \quad (1.74)
\]

The dependence of \( V(x) \) is shown in Fig. 1.12. As seen from the plot, we deal here with a peculiar potential box having reflecting walls. A particle with energy \( E \) oscillates between these walls, without going outside the confines of the box. In the stationary state, this motion is described by the Schrödinger time-independent equation. Substitution of Eq. (1.74) into Eq. (1.14a) and solving subject to the appropriate boundary conditions again yield the eigenvalue (energy) of the form

\[
E_n = \left( n + \frac{1}{2} \right) \hbar \nu \quad (1.75)
\]

where \( \hbar \) is the Planck constant and \( n = 0, 1, 2, 3, \ldots \). Note that the bound particle has the discrete energy values spaced at equal intervals of \( \hbar \nu \). From a light emission viewpoint, this means that an electron in a higher or excited state can drop to the ground state with the radiation of an integral number of photons of energy \( \hbar \nu \). The lowest value of energy in the series corresponds to \( n = 0 \) and is equal to

\[
E_0 = \frac{1}{2} \hbar \nu \quad (1.76)
\]

This energy is known as zero-point energy, since it does not vanish at the temperature of absolute zero too. The existence of the zero-point energy is the immediate consequence of the uncertainty principle: if at \( T = 0 \) K, the vibrations of an oscillator were to stop completely, it would prove possible to determine precisely at the same time the coordinates \((x = 0)\) of a particle.
1.6 The Central Field Problem: Hydrogen-like Atom

In a hydrogen-like atom, the only electron moves around the nucleus having charge \( Z q \), where \( Z \) is the atomic number of the element in the periodic table. If the zero-point energy level is taken to be the energy of a quiescent electron infinitely remote from the nucleus, then at a distance \( r \) from the nucleus the potential energy of interaction of the electron with the nucleus becomes

\[
U(r) = \frac{-Zq^2}{4\pi\varepsilon_0 r}
\]  

(1.77)

where \( q \) is the electronic charge, \( \varepsilon_0 \) is the permittivity of free space, and \( r \) is the distance from the central nucleus to the electron. Figure 1.13 shows the curve \( U(r) \). It is seen from the figure that the hydrogen-like atom can be regarded as a potential well for an electron.

![Fig. 1.13 The interaction energy \( U \) between an electron and a hydrogen-like nucleus as a function of separation](image)

Substituting Eq. (1.77) into the Schrödinger time-independent equation, we obtain

\[
\nabla^2 \psi + \frac{2m_0}{\hbar^2} \left( E + \frac{Zq^2}{4\pi\varepsilon_0 r} \right) \psi = 0
\]  

(1.78)

Note that Eq. (1.78) is written in spherical coordinates \( (r, \theta, \Phi) \) because of the spherical form of the potential-energy function. The solution is somewhat lengthy and is not presented here. It can be shown for this case that the three-dimensional partial differential Schrödinger equation can be separated into three ordinary differential equations involving \( r \), \( \theta \), and \( \Phi \) individually. One quantum number is derived from each of these equations, with the quantum numbers \( n \), \( l \), and \( m_l \) corresponding to the spherical coordinates \( r \), \( \theta \), and \( \Phi \). The solution of Eq. (1.78) leads to the following basic results.

1. The electron in the hydrogen-like atom has a discrete energy spectrum. The eigenvalues of energy are given by

\[
E_n = -\frac{Z^2q^4m_0}{8\varepsilon_0^2\hbar^2} \frac{1}{n^2}
\]  

(1.79)

where \( n \) is the principal quantum number.
2. The electron orbital angular momentum \( L_i \) can take only the following set of discrete values:

\[
L_i = \hbar \sqrt{l(l + 1)}
\]

where \( l \) is the orbital quantum number. It can take any value out of the following integral series of \( n \):

\[ l = 0, 1, 2, \ldots, (n - 1) \]

3. The orbital angular momentum can orient itself about the chosen direction, such as the direction of a magnetic field \( H \), only in such a manner that its projection on this direction is an integral multiple of \( \hbar \) (Fig. 1.13). Here only certain discrete directions are permitted; this constitutes *spatial quantization* and \( m_i \) can take the following discrete values:

\[ m_i = 0, \pm 1, \pm 2, \pm 3, \ldots, \pm l_i \]

![Fig. 1.14 Orientation of the orbital angular momentum](image)

4. The electron, besides its known orbital angular momentum, has an additional intrinsic angular momentum. The fact that the electron acts like a spinning solid body leads to the association of a quantum number \( m_s \) with the intrinsic angular momentum or spin having the values

\[ m_s = \pm 1/2 \]

The last number corresponds to the two spatial quantizations of the electron spin, ‘up’ or ‘down’. The famous Pauli exclusion principle states that each electron state can be occupied by no more than one electron either with spin +1/2 or −1/2.

**Solved Problems**

1.1 Calculate the de Broglie wavelength of an electron that is orbiting in the second Bohr orbit of the singly ionized helium atom.

**Solution**

For the singly ionized (He\(^+\)) helium atom, \( Z = 2 \) and \( E_2 = -(13.6)Z^2/4 = -13.6 \text{ eV} \).

Hence the kinetic energy of the electron is 13.6 eV. Therefore,
\[
\frac{1}{2} m_0 c^2 = 13.6 \text{ eV} \\
p^2/2m_0 = 13.6 \text{ eV}
\]

and

\[
p = \sqrt{2 \times 13.6 \times m_0} = \sqrt{27.2 \times m_0}
\]

Hence the de Broglie wavelength,

\[
\lambda = \frac{\hbar}{p} = 6.6 \times 10^{-34} / \sqrt{27.2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19} m_0} = 0.33 \text{ nm}
\]

1.2 (a) An unstable elementary particle, called the eta meson, has a rest mass of 549 MeV and a mean lifetime of \(7 \times 10^{-19}\) s. Find the uncertainty in its rest mass. (b) A proton’s position is to be determined without changing its kinetic energy by more than 1 keV. Find the maximum accuracy with which its position can be determined.

**Solution**

(a) Rest mass energy \(= 549 \text{ MeV}\)

\[m_0 c^2 = 549 \times 1.6 \times 10^{-13} \text{ J}\]

Hence

\[m_0 = (549 \times 1.6 \times 10^{-13})/c^2 = (549 \times 1.6 \times 10^{-13})/(9 \times 10^{16}) \text{ kg}\]

Average life of the particle = \(7 \times 10^{-19}\) s. This can be taken as the uncertainty \(\Delta t\) in the lifetime of the particle.

If \(\Delta E\) is the corresponding uncertainty in the rest-mass energy of the particle, then we have

\[\Delta E = (\Delta m_0) c^2\]

and

\[\Delta E \times \Delta t \geq \hbar/(2\pi)\]

Hence we have

\[\Delta m_0 \times \Delta t \geq \hbar/(2\pi c^2)\]

\[\Delta m_0 \geq \hbar/(\Delta t \times 2\pi \times c^2) = (1.055 \times 10^{-34})/(7 \times 10^{-19} \times 3 \times 10^{16}) \text{ kg}\]

\[= 0.05 \times 10^{-31} \text{ kg}\]

Expressed in terms of its rest mass, the uncertainty is

\[\Delta m_0/m_0 = (0.05 \times 10^{-31})/(9.76 \times 10^{-28}) = 0.5 \times 10^{-5}\]

(b) The kinetic energy has an uncertainty of 1 keV. If \(p\) is the momentum and \(\Delta p\) the maximum uncertainty in it, we have

\[p^2/2m_0 = K\]

\[(p + \Delta p)^2/2m_0 = K + (10^{3} \times 1.6 \times 10^{-19})\]

Hence we have

\[(p + \Delta p)^2 - p^2 = 2m_0 \times 10^{3} \times 1.6 \times 10^{-19}\]

where \(m_0\) is the mass of the proton. This gives the dependence of \(\Delta p\) on \(p\), the initial momentum of the proton. The maximum uncertainty in \(\Delta p\) will occur when \(p = 0\) (i.e., initially the proton is at rest). Putting \(p = 0\) in the above,

\[(\Delta p)^2 = 2m_0 \times 10^{3} \times 1.6 \times 10^{-19}\]
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If $\Delta x$ is the minimum uncertainty (hence maximum accuracy) of the position of the proton, we have

$$\Delta p \Delta x \geq \hbar/2\pi$$

Hence

$$\Delta x = \hbar/[2\pi(\Delta p)]$$

$$= 1.055 \times 10^{-34}/\sqrt{2 \times 1.672 \times 10^{-27} \times 10^3 \times 1.6 \times 10^{-19}}$$

$$= 1.055 \times 10^{-34}/\sqrt{5.35 \times 10^{-43}}$$

$$= 1.055 \times 10^{-34}/(0.731 \times 10^{-21}) \text{ m}$$

$$= 1.44 \times 10^{-13} \text{ m}$$

1.3 (a) Assuming that the average nuclear radius is $5 \times 10^{-15}$ m. Find the minimum energy that an electron can have, if it were to be a part of the nucleus. (b) Given that the radius of a hydrogen atom is $5.3 \times 10^{-11}$ m, estimate the minimum energy that an electron can have in this atom. Explain the disparity that you observe between this value and that of the electron in the ground state of the hydrogen atom.

**Solution**

(a) If $\Delta x$ is the uncertainty in the position of the electron in the nucleus, then

$$\Delta x = r = \text{radius of nucleus} = 5 \times 10^{-15} \text{ m}$$

Hence the uncertainty $\Delta p$ in the momentum is given by

$$\Delta p \geq \hbar/[4\pi(\Delta x)] = 1.055 \times 10^{-34}/(2 \times 5 \times 10^{-15}) = 1.1 \times 10^{-20} \text{ kg m/s}$$

If this is the uncertainty of the momentum of the electron, the value of the momentum itself will be much larger than this uncertainty. Now for the electron

$$m_ec^2 = \text{rest mass energy}$$

$$= 0.511 \times 1.6 \times 10^{-13} \text{ J}$$

and from above,

$$\Delta pc = 1.1 \times 10^{-20} \times 3 \times 10^8 = 3.3 \times 10^{-12} \text{ J}$$

Therefore, $\Delta pc > m_ec^2$ and the value of $pc$ must be very much larger than the rest mass energy $m_ec^2$ of the electron. Hence the relativistic expression for the total energy of the electron

$$E = \sqrt{(m_ec^2)^2 + (pc)^2}$$

may be validly approximated to $E = pc$. Hence the minimum value of $E$ (i.e., $pc$) must be $\Delta pc$, i.e.,

$$E_{\text{min}} = 3.3 \times 10^{-12}$$

$$= 20 \text{ MeV}$$

Since experimentally we find that the $\beta$-particle energies in beta-decay do never have more than a fraction of this energy, we may conclude that the electrons do not exist within the nuclei of atoms.

(b) With $\Delta x = 5.3 \times 10^{-11}$ m, we get

$$\Delta p \geq \hbar/(4\pi\Delta x) = 9.9 \times 10^{-25} \text{ kg m/s}$$
This is a sufficiently small momentum to be considered non-relativistic and hence the kinetic energy will have a minimum value given by

\[ K = \frac{p^2}{2m_0} \geq (\Delta p)^2/2m_0 = [(9.9)^2 \times 10^{-50}]/(2 \times 9.1 \times 10^{-31}) \text{ J} \]

\[ = 5.4 \times 10^{-19} \text{ J} = 5.4/1.6 \text{ eV} = 3.4 \text{ eV} \]

The electron bound to the proton in the hydrogen atom has a kinetic energy (= ionization energy), in the ground state, of 13.6 eV. The above value of 3.4 eV has been obtained as the minimum value of the KE as equated to the value obtained from \( \Delta p \). The actual value 13.6 eV is much larger because the actual momentum of the electron in the ground state is double the uncertainty we have calculated above so that the KE is four times as large.

1.4 (a) An excited atom takes a time of \( 10^{-8} \) s from the instant of its excitation to the time it radiates. Estimate the uncertainty in the frequency of the photon emitted in the radiation. (b) Making use of the uncertainty principle, evaluate the minimum permitted energy of an electron in a hydrogen atom and its corresponding distance from the nucleus.

**Solution**

(a) Uncertainty in time = \( \Delta t = 10^{-8} \) s. If \( \Delta E \) is the uncertainty in the corresponding energy and \( \Delta \nu \) the uncertainty in the frequency of emission, we have

\[ \Delta E \Delta t = \hbar \Delta \nu \Delta t \geq \hbar/4\pi \]

i.e.,

\[ \Delta \nu \geq 1/(4\pi \times \Delta t) = 1/(4 \times 3.14 \times 10^{-8}) \text{ Hz} \]

\[ = 10^9/1.256 = 8 \times 10^6 \text{ Hz} \]

(b) Let us take the minimum radius \( r \) and the minimum momentum \( p \) of the electron in the hydrogen atom to be equal to the uncertainties \( \Delta r \) and \( \Delta p \) in the radius and momentum, respectively, in the ground state of the atom. Thus,

\[ p = \Delta p = \hbar/(2\pi \Delta r) \quad \text{and} \quad r = \Delta r \]

The total energy of the electron is given by

\[ E = \frac{p^2}{2m_0} = -e^2/(4\pi \varepsilon_0 r) \quad \text{(1)} \]

The minimum of \( E \) will occur when \( dE/dr = 0 \), i.e., when

\[ dE/dr = -\hbar^2/(4\pi^2 m_0 e^2) + e^2/(4\pi^2 \varepsilon_0 r^2) = 0 \]

\[ r = (4\pi\varepsilon_0\hbar^2)/(4\pi^2 m_0 e^2) \]

\[ = [(1.054)^2 \times 10^{-68} \times 1]/[9.1 \times 10^{-31} \times (1.6)^2 \times 10^{-38} \times 9 \times 10^9] \text{ m} \]

\[ = 5.3 \times 10^{-11} \text{ m} \]

The corresponding minimum value of the energy from Eq. (1) is

\[ E_{\text{min}} = -m_0e^4 \times 4\pi^2/[2\hbar^2 \times (4\pi\varepsilon_0)^2] \]

\[ = -(9.1 \times 10^{-31} \times (1.6)^4 \times 10^{-76} \times 9^2 \times 10^{18})/[2 \times (1.054)^2 \times 10^{-68}] \text{ J} \]

\[ = -(9.1 \times 10^{-31} \times (1.6)^4 \times 10^{-76} \times 9^2 \times 10^{18}/[2 \times (1.054)^2 \times 10^{-68} \times 1.6 \times 10^{-15}] \text{ eV} \]

\[ = -13.6 \text{ eV} \]
1.5 Assuming the wave functions for a finite rectangular potential barrier, calculate the probability of transmission for a 1 MeV proton tunnelling through a potential of 4 MeV height and $10^{-14}$ m thickness.

**Solution**

For the penetration of a rectangular potential barrier, the transmission coefficient is given by

$$T = 16 \exp(-2\beta\nu/[(1 + \beta/\alpha)^2 (1 + \alpha/\beta)^2])$$

(1)

where

$$\alpha^2 = 4\pi^2 m_0 E/h^2; \quad \beta^2 = 4\pi^2 m_0 (V_0 - E)/h^2; \quad \text{and} \quad \alpha = \text{width of the barrier}$$

Here

$$E = 1 \text{ MeV}, \quad V_0 = 4 \text{ MeV}, \quad \alpha = 10^{-12} \text{ m}$$

Hence

$$\beta = \sqrt{4\pi^2 m_0 (V_0 - E)/h^2}$$

$$= \sqrt{[2 \times 1.67 \times 10^{-27} \times (4 - 1) \times 1.6 \times 10^{-13}] / [(1.055)^2 (10^{-68})]}$$

$$= 1.6 \times 10^{14}$$

$$\beta/ \sqrt{[V_0 - E/E]} = \sqrt{3}$$

and

$$\beta/ = \sqrt{[E/V_0 - E]} = \sqrt{1/3}$$

Putting values in Eq. (1),

$$T = 16 \exp(-2 \times 1.9 \times 10^{14} \times 10^{-12} \times 10^{-3} / (1 + \sqrt{3})^2 (1 + 1/\sqrt{3})^2)$$

$$= (48 \times 0.02237)/55.7$$

$$= 1.9\%$$

1.6 The mass of an electron in In$_{0.55}$Ga$_{0.47}$As is 0.04$m_p$. If a quantum well of size 50 Å is formed in this material, calculate the lowest energy of the electron.

**Solution**

The energy of an electron confined in a three-dimensional quantum well of cubic shape can be expressed as

$$E = \frac{\pi^2 \hbar^2}{2m_e L_X^2} + \frac{\pi^2 \hbar^2}{2m_e L_Y^2} + \frac{\pi^2 \hbar^2}{2m_e L_Z^2}$$

Since the particle is confined only in a one-dimensional quantum well, the confinement energy is

$$E = \frac{\pi^2 \hbar^2}{2m_e L_c^2} = \frac{9.87 \times (1.05 \times 10^{-34})^2}{2(0.04 \times 0.91 \times 10^{-30}) \times (50 \times 10^{-10})^2}$$

$$= 5.96 \times 10^{-20} \text{ J} = 0.373 \text{ eV}$$

1.7 When glass is manufactured, tiny particles of CdS semiconductor get embedded in it. These particles have small dimensions and their radii can be controlled to
some extent by adjusting the growth conditions. Assume that the electrons in the small semiconductor dots can be treated as if they were in a three-dimensional quantum well dot surrounded by an infinite potential. Estimate the first two levels of the dot if the dot is a cube of side 50 Å and the electron mass is $m_e^* = 0.1 m_0$.

**Solution**

The energy of an electron confined in a three-dimensional quantum well of cubic shape can be expressed as

$$E = \frac{\pi^2 \hbar^2}{2 m_e^* L_x^2} + \frac{\pi^2 \hbar^2}{2 m_e^* L_y^2} + \frac{\pi^2 \hbar^2}{2 m_e^* L_z^2}$$

Since the confinement is made in a three-dimensional cubic box, where $L_x = L_y = L_z = 50$ Å, we get

$$E = \frac{3\pi^2 \hbar^2}{2 m_e^* L^2} = \frac{(3 \times 9.87) \times (1.05 \times 10^{-34})^2}{2(0.01 \times 0.91 \times 10^{-30}) \times (50 \times 10^{-10})^2}$$

$$= 7.17 \times 10^{-20} \text{ J} = 0.45 \text{ eV}$$

1.8 Calculate the zero-point energy of a system of a mass of $10^{-3}$ kg attached to a spring of spring constant $10 \text{ N/m}$ oscillating along the x-axis, assuming the system to behave quantum mechanically.

**Solution**

The zero-point energy of a quantum mechanical harmonic oscillator is given by

$$E_0 = \hbar/(2\nu)$$

where $\nu$ is the frequency of the oscillator. For the given spring–mass system,

$$\nu = (2\pi)^{-1} \sqrt{k/m_0} = (2\pi)^{-1} \sqrt{(10/10^{-3})} = (50/\pi) \text{ Hz}$$

Hence, zero-point energy

$$E_0 = \left(\frac{\hbar}{2}\right) \left(\frac{50}{\pi}\right) \text{ J}$$

$$= 25 \hbar / \pi \text{ J}$$

$$= (25 \times 6.6 \times 10^{-34})/3.14 \text{ J}$$

$$= 5.27 \times 10^{-31} \text{ J}$$

1.9 A muon ($\mu^-$) is a lepton particle whose charge is that of an electron but which has a mass 106 times that of the electron rest mass. Assuming that a muon along with a proton forms a hydrogen-like atom, work out the solution of the Schrodinger wave equation for such an atom. Compare the energies of the muon and the electron in their ground states, and also the radii of the ground states.

**Solution**

The solution will follow a procedure similar to that for an electron in the hydrogen atom. However, since the mass of the muon is 106 times the electronic mass, it becomes significant to the mass of the proton. So one has to use the reduced mass of the (muon, proton) system given by $\mu = [m_m m_p / (m_m + m_p)]$, where $m_i$ is the mass
of the muon and \( m_p \) that of the proton. Otherwise, the solutions will be similar to that of the electron. For the ground state energy, for the muon, one gets
\[ E_1 = -(4\pi^2\mu e^4)/(32\pi^2\varepsilon_0^2\hbar^2) \]
and the radius of the ground state muon orbit will be
\[ r_1 = (4\pi\varepsilon_0\hbar^2)/(4\pi\mu e^2) \]
Thus the ratio of the energies of the ground states for the muon and electron will be \( \mu : 1 \) (\( \approx 100 \)) and that of the radii of their ground states will be 1: \( \mu \) (\( \approx 0.01 \)).

1.10 Doubly ionized lithium (\( \text{Li}^{++} \)) is a hydrogen-like atom. Compute the first three energy levels of this atom. Find the wavelengths of the first three lines of the \( K \) series \( (n_e = 1, n_m = 2, 3, 4) \).

**Solution**

For the doubly ionized lithium atom, \( Z = 3 \) and the energies of the quantum states are given by
\[ E_n = -(13.6)Z^2/n^2 \]
where 13.6 eV is the ionization energy (= energy of the first Bohr orbit) and \( n \) is the quantum number for \( \text{Li}^{++} \) atom. The first three energy levels are
\[ \begin{align*}
    n &= 1, \text{ ground state, } E_1 = -(13.6) \times 9 \text{ eV} = -122.4 \text{ eV} \\
    n &= 2, \text{ first excited state } E_2 = -122.4/4 = -30.6 \text{ eV} \\
    n &= 3, \text{ second excited state } E_3 = -122.4/9 = -13.6 \text{ eV}
\end{align*} \]

The frequencies \( \nu_1, \nu_2, \) and \( \nu_3 \) of the first three lines of the \( K \) series will be given by
\[ h\nu_1 = -(122.4)[-1 + (1/4)] = 91.8 \text{ eV} \]
\[ \nu_1 = (91.8 \times 1.6 \times 10^{-10})/(6.6 \times 10^{-34}) \text{ Hz} \]
and the corresponding wavelengths
\[ \begin{align*}
    \lambda_1 &= c/\nu_1 = (3 \times 10^{8})/91.8 = 13.46 \times 10^{-9} \text{ m} \\
    \nu_2 &= (108.8 \times 1.6 \times 10^{-10})/(6.6 \times 10^{-34}) \text{ Hz} \\
    \lambda_2 &= c/\nu_2 = 11.37 \text{ nm} \\
    \nu_3 &= (114.75 \times 1.6 \times 10^{-10})/(6.6 \times 10^{-34}) \text{ Hz} \\
    \lambda_3 &= c/\nu_3 = 10.78 \text{ nm}
\end{align*} \]

**Review Questions and Problems**

1.1 Compare the following:
(a) Wave nature of the electron and particle nature of the electron.
(b) Planck’s law and de Broglie’s law.
(c) Phase velocity and group velocity.
(d) Wave mechanics and Newtonian mechanics.

1.2 Find the de Broglie wavelength for an electron, a proton, and a 100-gm bowling ball each having 2 eV of kinetic energy. Find the uncertainty in the position of each particle taking \( \Delta p = p \).

[Ans. 0.69 Å, 0.016 Å, 2.07 \times 10^{-25} \text{ m}]
1.3 The average duration of an excited state of an atom in a gas laser is about $10^{-8}$ s. This laser emits a spectral line whose central wavelength is 6328 Å.
(a) Compute the minimum frequency variation of the emitted red light according to the uncertainty principle.
(b) Express the possible sharpness of the spectral line by the ratio of the frequency variation to the fundamental radiated frequency in parts per million. 
[Ans. (a) $10^8$ Hz, (b) 0.21 ppm]

1.4 When light of wavelength 4000 Å shines on the surface of barium, electrons of kinetic energy 0.63 eV are emitted. Calculate the wavelength of light needed so that photoelectrons of de Broglie wavelength 10 Å are emitted from the surface of barium.
[Ans. 3120 Å]

1.5 Assume the wave function $\psi (x, t) = A (\sin \pi x) \exp (-i\omega t)$. Find $|\psi|^2$. Choose $A$ such that $\int |\psi|^2 dx = 1$ for $0 \leq x \leq 1$ 
[Ans. $\sqrt{2}$, $-\sqrt{2}$, $\sqrt{2}i$, $-\sqrt{2}i$]

1.6 Assume that $\psi_1(x, t)$ and $\psi_2(x, t)$ are solutions of a one-dimensional time-dependent Schrödinger equation.
(a) Prove the superposition principle by showing that $\psi_1 + \psi_2$ is also a solution.
(b) Is $\psi_1 \psi_2$ a solution of the Schrödinger equation in general?

1.7 Consider the Schrödinger equation in time-dependent form

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi$$

where $\hat{H} = -\frac{\hbar^2}{2m_0} \frac{\partial^2}{\partial x^2} + V(x)$

Show that if we write $\psi (x, t) = \psi (x) \exp (-iEt/\hbar)$ we obtain $\hat{H}\psi = E\psi$, where $E$ is the energy of the system.

1.8 The wave function for a quantum particle of mass $m$ confined to move in the domain $0 \leq x \leq L$ is given by

$$\psi (x) = N \sin (4\pi x/L)$$

where $N$ is the normalization factor.
(a) Normalize the function.
(b) Calculate the probability of finding the particle in the region from $x = 0$ to $x = L/4$.
(c) Calculate the probability of finding the particle in the left two-thirds of the box.

[Ans. (a) $\left(\frac{2}{L}\right)^{1/2}$, (b) 0.25, (c) $\frac{2}{3} - \frac{1}{8\pi} \sin \frac{16\pi}{3}$]

1.9 The normalized ground state wave function for an isotropic three-dimensional harmonic oscillator of mass $m$ and natural frequency in spherical polar coordinates is given by

$$\langle r \rangle = \left(\frac{1}{\alpha^3 \pi^{3/2}}\right)^{1/2} \exp(-r^2/2\alpha^2)$$
where $\alpha = (\hbar/m_0\omega)^{1/2}$. Calculate $\langle r \rangle$ and $\langle 1/r \rangle$ for the oscillator.

\[
\text{Ans.} \frac{2\alpha}{\sqrt{\pi}}, \frac{2}{\alpha\sqrt{\pi}}
\]

1.10 The wave function for a quantum particle of mass $m$ confined to move in the domain $0 \leq x \leq L$ is given by $\psi(x) = N \sin(n\pi x/L)$, where $N$ is the normalization factor.

(a) Normalize the function.

(b) Calculate the probability of finding the particle in the left two-thirds of the box.

(c) For what value of $n$ is this probability a maximum?

\[
\text{Ans.} \quad N = \left( \frac{(2L)^{1/2}}{2n\pi a^2} \right)^{1/2}, \quad (b) \quad \frac{2}{3} \sin \left( \frac{4n\pi}{3} \right), \quad (c) \quad n = 1
\]

1.11 An electron is moving freely in a one-dimensional box of width $a$ having impenetrable walls. Write an expression for the force on the walls of the box due to the trapped electron in its lowest state.

1.12 The wave function of an electron, $\psi(x, t) = D \exp(-\beta x)(-iEt/\hbar)$, impinging on a barrier whose height is $V_0$, with an energy $E < V_0$, will penetrate the barrier. What is the probability of finding the electron at a distance of 3 Å beyond the barrier relative to its being 10 Å beyond the barrier? Assume the electron energy to be 0.6 eV and the barrier height 1.0 eV. \[\text{Ans. 105}\]

1.13 Consider the penetration of a potential barrier of height 3.0 eV by an electron whose energy is 1.0 eV. Determine the relative probability of finding the electron at the barrier compared to finding it (a) 10 Å beyond the barrier, (b) 100 Å beyond the barrier. \[\text{Ans. (a) 0.1, (b) 1.02 \times 10^{-10}}\]

1.14 (a) Show that the de Broglie wavelength of a particle of rest mass $m_0$ and kinetic energy $K$ is given by

\[
\lambda = \frac{\hbar}{\sqrt{K(K + 2m_0c^2)}}
\]

(b) Find the kinetic energy of an electron whose de Broglie wavelength is the same as that of a 100 keV x-ray. \[\text{Ans. 10 keV}\]

1.15 (a) Derive a relativistically correct formula for the de Broglie wavelength of a charged particle in terms of the potential difference $V$ through which it has been accelerated.

(b) What is the non-relativistic approximation of this formula valid for $eV \ll m_0c^2$.

1.16 (a) Show that for a particle whose positional uncertainty is $\Delta x = \lambda/(2\pi)$, where $\lambda$ is its de Broglie wavelength, the velocity uncertainty is of the same order of magnitude as the particle’s velocity itself.
(b) A particle of mass \( m \) moves in a unidimensional potential field \( U = kx^2/2 \) (harmonic oscillator). Using the uncertainty principle, estimate the minimum permitted energy of the particle in that field.

\[ \text{Ans.} \ E_{\text{min}} = \frac{h\omega}{2} \]

1.17 A free electron was initially confined within a region with linear dimension \( l = 0.10 \) nm. Using the uncertainty principle, evaluate the time over which the width of the corresponding group of waves becomes \( \eta = 10 \) times as large.

\[ \text{Ans.} \ t = 10^{-16} \text{ s} \]

1.18 (a) Verify that the uncertainty principle can be expressed in the form \( \Delta L \Delta \theta \geq \hbar/(4\pi) \), where \( \Delta L \) is the uncertainty in the angular momentum of a particle and \( \Delta \theta \) is the uncertainty in its angular position.

(b) At what uncertainty in \( L \) will the angular position of a particle become completely indeterminate?

1.19 The width of an infinite potential well is 10 Å. Calculate the first three energy levels in terms of eV for an electron.

\[ \text{Ans.} \ 0.376 \text{ eV, 1.50 eV, 3.38 eV} \]

1.20 The lowest energy of a particle in an infinite potential well with a width of 100 Å is 0.025 eV. What is the mass of the particle?

\[ \text{Ans.} \ 1.37 \times 10^{-31} \text{ kg} \]

1.21 A certain semiconductor device requires a tunnelling probability of \( 10^{-5} \) for an electron tunnelling through a rectangular barrier with a barrier height of \( V_0 = 0.4 \) eV. The electron energy is 0.04 eV. Determine the maximum barrier width.

\[ \text{Ans.} \ 19.3 \text{ Å} \]

1.22 Consider the penetration of a step potential function of height 2.4 eV by an electron whose energy is 2.1 eV. Determine the relative probability of finding the electron at a distance (a) 12 Å beyond the barrier, (b) 48 Å beyond the barrier.

\[ \text{Ans.} \ (a) \ 0.118\%, \ (b) \ 1.9 \times 10^{-10}\% \]