CoE 211 ELECTRONIC DEVICE PHYSICS

Dr. Mohannad H. Al-Ali

Department of Computer Engineering

University of Basrah

Fall 2020

Chapter Two

Introduction to Quantum Mechanics

Chapter Objectives

- Give the basic principles of quantum mechanics,
- Illustrate Schrodinger's wave equation.
- Consider some applications of Schrodinger's wave equation to various potential functions.

2.1 Principles of Quantum Mechanics

- **Kinetic Energy**: It is the energy of an object that it possesses due to its motion.

$$KE = \frac{1}{2} m\nu^2 \,, \tag{1}$$

  -) m is the mass and ν is the velocity of the object.

- **Potential Energy**: It is the energy of an object that it possesses due its position relative to other objects.

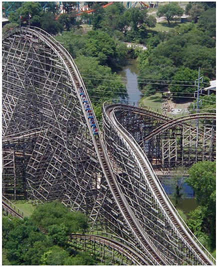


Figure: An example for kinetic energy.

Figure: An example for potential energy.

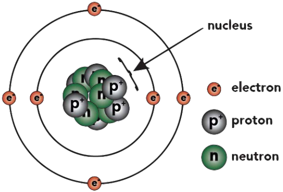


Figure: Kinetic and potential energies in an electron.

There are three principles for the quantum mechanics:

1) **Energy Packets**

- Photoelectric effect: Applying light beams with a certain intensity and frequency on a clean metal would free electrons.
  -) Newtons' laws: Electron kinetic energy should change with the light intensity and NOT with the frequency.
  -) Actual observation: At a constant intensity, electron kinetic energy is changing linearly with the light frequency with a limiting frequency, below which no electron is produced.

Figure: (a)Photoelectric effect. (b) Kinetic energy of the electrons versus frequency

- Interpretation: Light/electromagnetic waves consist of *discrete* units of energy called quanta or photon *that are proportional to the frequency*.
- Maximum kinetic energy of the released electron is

$$KE_{\text{max}} = hf - hf_0, \tag{2}$$

-) $h = 6.625 \times 10^{-34}$ J.s is Planck's constant, f is the frequency of the wave, f_0 is the limiting frequency, hf is the incident photon energy and hf_0 is the work function or the minimum energy required to remove an electron from the surface.

2) **Wave-Particle Duality**: Atomic particles do have *continuous* waves.

- In quantum mechanics, the photon momentum is

$$P = h/\lambda\,, \tag{3}$$

-) λ is the wavelength of the light wave.

- The wavelength of a particle is

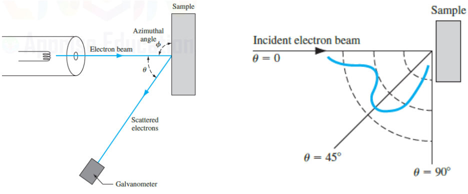
$$\lambda = h/P\,, \tag{4}$$

-) λ is called *de Broglie* wavelength of the matter wave and P is the momentum of the particle.

- In Newtons' classic mechanics, $P = m\nu$. The wavelength of the particle is then

$$\lambda = \frac{h}{m\nu}\,. \tag{5}$$

- **Davisson and Germer Experiment**: They used electron gun to hit a crystal of nickel and the electrons are scattered in a direction $\theta \in [0, 90]$. The peak of scattering intensity is due to the constructive addition of electron waves.



(a) (b)

Figure: Experimental arrangement of Davisson and Germer experiment.

Example 2.1: A metal has a work function of 4.3 V.
What is the minimum photon energy in Joule to emit an electron from this metal through the photo-electric effect?
What are the photon frequency in Terahertz and the photon wavelength in micrometer?
What is the corresponding photon momentum?
What is the velocity of a free electron with the same momentum?

3) **Uncertainty Principle**

- It is not possible to simultaneously describe with absolute accuracy the *position* and *momentum* of atomic particles.

$$\Delta x \Delta P \geq \hbar\,, \tag{6}$$

-) Δx is the uncertainty in position, ΔP is the uncertainty in momentum, $\hbar = \frac{h}{2\pi}$ is the modified Planck's constant.

- It is not possible to simultaneously describe with absolute accuracy the time and the energy of atomic particles.

$$\Delta t \Delta E \geq \hbar\,, \tag{7}$$

-) Δt is the uncertainty in time and ΔE is the uncertainty in energy.

- Probability is used to describe finding a particle of specific momentum at a particular position or of specific energy at a particular time.
- We need to develop a probability density function (pdf) to know the statistical distribution of P over x or E over t.

2.2 Schrodinger's Wave Equation

- Schrodinger's wave equation describes the space-time motion of an electron in a crystal. It incorporates the energy packets, wave-particle duality and uncertainty principles.
- The 1d Schrodinger's wave equation is

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}+V(x)\Psi(x,t)=j\hbar\frac{\partial\Psi(x,t)}{\partial t}\,, \tag{8}$$

  -) $\Psi(x,t)$: The wave function for the particle. It is the solution of (8),
  -) $V(x)$: The potential energy that particle experiences as particle moves in the x direction. $V(x)$ is known,
  -) j: It is the imaginary constant, $j=\sqrt{-1}$.

- Schrodinger's Wave Equation is a 2nd order partial differential equation.
- Mathematically, $\Psi(x,t)$ is a complex function, but $|\Psi(x,t)|^2=\Psi(x,t)\times\ \Psi^*(x,t)$ is always a real function. Here, $\Psi^*(x,t)$ is the complex conjugate of $\Psi(x,t)$.
- The function $|\Psi(x,t)|^2$ represents the probability density function (pdf) for finding the particle at a specific time.

2.2 Schrodinger's Wave Equation (cont.)

- Separation of variables technique: $\Psi(x,t)$ is separated into two functions, one is dependent on position only and the other one time only.

$$\Psi(x,t) = \Psi(x)\Phi(t)\,. \tag{9}$$

- Plug (9) in (8) and divide by $\Psi(x,t) = \Psi(x)\Phi(t)$. We get two differential equations that both must equal to the total energy E.
- The time-dependent part of Schrodinger's equation: $j\hbar\frac{d\Phi(t)}{dt} = E\Phi(t)\,.$
  -) It is 1st order differential equation that has the solution:

$$\Phi(t) = e^{-j(E/\hbar)t} = e^{-j\omega t}\,.$$

  -) $\Phi(t)$ is a sinusoidal wave with radian *time* frequency, $\omega = E/\hbar = 2\pi f$.
- The time-independent part of Schrodinger's equation is

$$\frac{d^2\Psi(x)}{dx^2} + \frac{2m}{\hbar^2}\left(E - V(x)\right)\Psi(x) = 0\,. \tag{10}$$

- The solution of (10) has the form

$$\Psi(x) = Ae^{y_1 x} + Be^{y_2 x}\,, \tag{11}$$

  -) $y_{1,2}$ are the roots of the *characteristic equation*: $0 = y^2 + \frac{2m}{\hbar^2}(E - V)$,

$$y_{1,2} = \pm\sqrt{-\frac{2m}{\hbar^2}(E-V)}\,.$$

  -) A and B are constants that are obtained from the *boundary conditions*.

2.2.1 Boundary Conditions

-) Boundary conditions are different from initial conditions. In Boundary conditions, we know the values of the function and its derivatives at different points. In initial conditions, the values of the function and its derivatives are at the same point.

-) **Boundary conditions for the wave equation:**

1. The area under $|\Psi(x)|^2$ is

$$\int_{-\infty}^{\infty} |\Psi(x)|^2 dx = 1\,. \tag{12}$$

2. $\Psi(x)$ must be finite, single-valued, and continuous.
3. $d\Psi(x)/dx$, i.e., the slop, must be finite, single-valued, and continuous.

-) In fig. (a), the wave function and its derivative are continuous. In fig. (b), the wave function is continuous while its derivative is discontinuous.

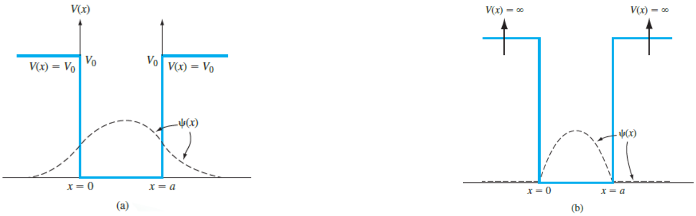


Figure: Potential functions and corresponding wave function solutions for the case (a) potential function is finite everywhere and (b) potential function is infinite in some regions.

2.3 Applications of Schrodinger's Wave Equation

i) **Electron in Free Space**

- Free particle with mass m, finite energy E and zero potential function $V(x) = 0$ over x. The particle wave propagates without barriers at constant speed and kinetic energy.
- Let $k = \sqrt{\frac{2mE}{\hbar^2}}$. The solution of (11) becomes

$$\Psi(x) = Ae^{jkx} + Be^{-jkx} .$$

- The total wave equation $\Psi(x, t)$ has the form

$$\Psi(x, t) = Ae^{j(kx-\omega t)} + Be^{-j(kx+\omega t)} .$$

  -) k is called the wave number and ω is the usual radian time frequency,
- $\Psi(x)$ has a traveling wave, $\exp(jkx)$, in the $+x$ direction and a traveling wave, $\exp(-jkx)$, in the $-x$ direction,
- Assume the particle is traveling in the $+x$ direction. Then, $B = 0$ and

$$\Psi(x) = Ae^{jkx} .$$

- Since $k = \sqrt{\frac{2mE}{\hbar^2}} = P/\hbar$ and the deBroglie wavelength $\lambda = 2\pi\hbar/P$, then $k = 2\pi/\lambda$.
- $|\Psi(x, t)|^2 = |A|^2$. This is uniform distribution which means that one can find the particle everywhere in the free space with equal probability.

ii) The Infinite Potential Well

- The particle motion is confined within the space, $0 \leq x \leq a$.

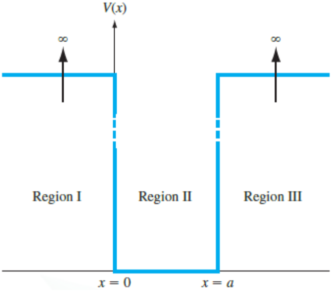


Figure: Potential function V versus the position x.

- The potential function is

$$V(x) = \begin{cases} 0, & 0 \leq x \leq a \\ \infty, & x < 0 \text{ and } x > a \end{cases}$$

- The probability of finding the particle in regions I and III is zero if E is finite. The boundary conditions are $\Psi(0) = \Psi(a) = 0$.
- In region II, time-independent wave equation: $\frac{d^2\Psi(x)}{dx^2} + \frac{2m}{\hbar^2 E}\Psi(x) = 0$. It has the solution

$$\Psi(x) = A\sin(kx) + B\cos(kx) \ , \quad \text{with } \Psi(0) = \Psi(a) = 0 \, . \qquad (13)$$

- Plugging the boundary conditions in (13). The constants A and B are

$$0 = A\sin(ka)$$
$$0 = B$$

The Infinite Potential Well (cont.)

- A cannot be zero since $\Psi(x)$ would be zero in the region $0 \leq x \leq a$. Therefore $\sin(ka) = 0$, which is equivalent to
$$k = \frac{\pi n}{a}\,, \tag{14}$$
$n = \pm 1, \pm 2, \pm 3, \cdots$ is an integer and called the quantum number.
- A is found from the normalization boundary condition $\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1$. Then,
$$A = \sqrt{2/a}$$
- The wave function for the particle in the infinite potential well becomes
$$\Psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi n x}{a}\right)\,, n = 1, 2, \cdots$$
- Since k must have discrete values from (14) and $k = \sqrt{\frac{2mE}{\hbar^2}}$. This gives
$$E = \frac{\pi^2 \hbar^2}{2ma^2} n^2\,. \tag{15}$$
- Particle energy is quantized and only certain values are allowed.

The Infinite Potential Well (cont.)

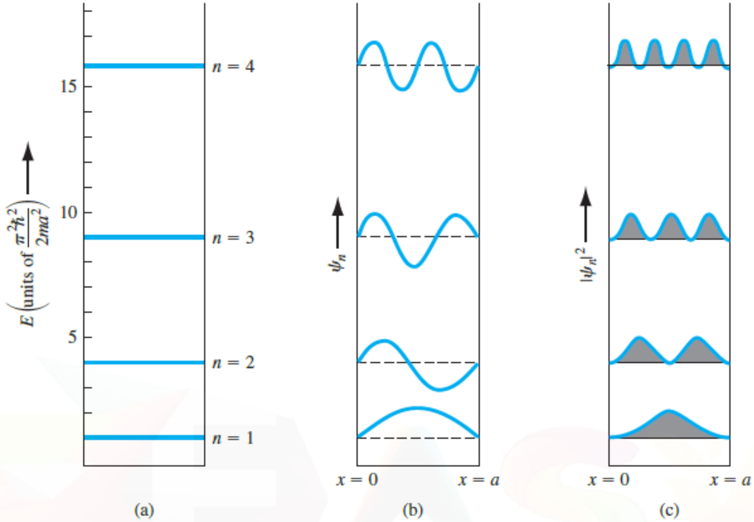


Figure: (a) The first four allowed energy levels, (b) wave functions $\Psi_n(x)$, and (c) $|\Psi_n(x)|^2$ is proportional to the pdf of finding a particle at a given point in the infinite potential well.

Example 2.2: Consider the step potential function shown below. Assume that a flux of particles is incident on a potential barrier with energy of V_0. The particles are traveling in the x direction and they are originated from $x = -\infty$. The total energy is fixed at E.
(i) Let the wavenumbers in regions I and II be k_1 and k_2. Provide expressions for k_1 and k_2.
(ii) Derive the time-independent wave solutions that apply in each region.
(iii) Write the set of equations that result from applying the boundary conditions.
(iv) Derive an expression, in terms of the constants k_1 and k_2, for the reflection coefficient R. The reflection coefficient is defined as the ratio of the reflected flux of particles in region II to the incident flux in region I.

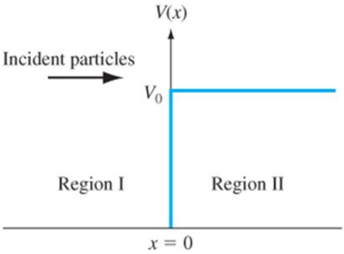


Figure: The step potential function.

End of Chapter Two