University of Anbar

College of Science – Dept. of Physics

Lectures of Semiconductors #1

for 3th level of physics students
Lecture 3 : Introduction to Quantum Mechanics/1
by

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A second – Order linear differential equation solution:

Most differential equations in physics are linear equations of the second order, so it is important to must know how to solve this kind of equations

If the supposed continuous wave function ψ

$$a\psi'' + b\psi' + c\psi = 0 \quad \dots\dots\dots(1)$$ **; a, b, and c are const.**

We can suggest the following solution:

$$\psi = e^{rx} \quad \dots\dots\dots(2)$$

$$\psi' = re^{rx} \quad \dots\dots\dots(3)$$

$$\psi'' = r^2e^{rx} \quad \dots\dots(4)$$

By Substitute ψ, ψ' *and* ψ'' in eq.(1) with the results in eq.s (2), (3) and (4)

$$ar^2e^{rx} + bre^{rx} + ce^{rx} = 0 \quad \dots\dots\dots(5)$$

$$(ar^2 + br + c)e^{rx} = 0 \quad \dots\dots\dots(6)$$

$$(ar^2 + br + c) = 0 \quad \dots\dots\dots\dots\dots(7)$$

$$r = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \qquad : r = r_1 \, and \, r_2$$

$$\therefore \quad \psi = C_1 e^{r_1 x} + C_2 e^{r_2 x} \quad \dots\dots\dots (8)$$

$r_1 = r \;;\; r_2 = -r$

$$\therefore \quad \psi = C_1 e^{rx} + C_2 e^{-rx} \quad \dots\dots\dots (9)$$

$$e^{rx} = Cos(rx) + \; iSin(rx) \quad \dots\dots\dots (10)$$

$$e^{-rx} = Cos(rx) - \; iSin(rx) \quad \dots\dots\dots (11)$$

By Substitute eq.s (10) and (11) in eq. (9)

$$\boxed{\therefore \quad \psi = ACos(rx) + BSin(rx) \quad \dots\dots\dots (12)}$$

$$A = C_1 + C_2 \;\&\; B = i(C_1 - C_2)$$

The solution to be acceptable in physics, must be achieved the existence of the function

(2.2.1) : Physical Meaning of the Wave Function

The wave function $\psi(x,t)$ describes the behavior of an electron in a crystal.
We can describe the behavior of any particle by it's position $[(\text{probability})|\psi|^2]$ and momentum or energy.
Then ; the wave function may be written as :

$$\psi(x) = A \;\; Exp \left[i \sqrt{\frac{2m}{\hbar^2}\left(E - V(x)\right)} \;\; x \right] + B \; Exp \left[- i \sqrt{\frac{2m}{\hbar^2}\left(E - V(x)\right)} \;\; x \right]$$

Recall that the time-dependent portion of the solution is

$$\phi(t) = e^{-i\frac{E}{\hbar}t}$$

Wave function may be write as :

$$\psi(x,t) = A \;\; Exp \left[i \sqrt{\frac{2m}{\hbar^2}\left(E - V(x)\right)} \;\; x - Et \right] + B \; Exp \left[-i \sqrt{\frac{2m}{\hbar^2}\left(E - V(x)\right)} \;\; x + Et \right]$$

Position

momentum or energy : $E = \dfrac{P^2}{2m}$

2.3.2 Notes about the general solution of the wave function :

$$\psi(x,t) = A \;\; Exp\left[i\sqrt{\frac{2m}{\hbar^2}E}\;x \;- Et\right] + B\; Exp\left[-i\sqrt{\frac{2m}{\hbar^2}E}\;x + Et\right]$$

. If the wave function travels with + x direction , B constant must be zero , then the wave function is :

$$\psi(x,t) = A \;\; Exp \;\; i(kx - \;\omega t)$$ **with + x direction**

$$\psi(x,t) = B \;\; Exp[-i(kx - \;\omega t)]$$ **with − x direction**

where k is a wave number and is :

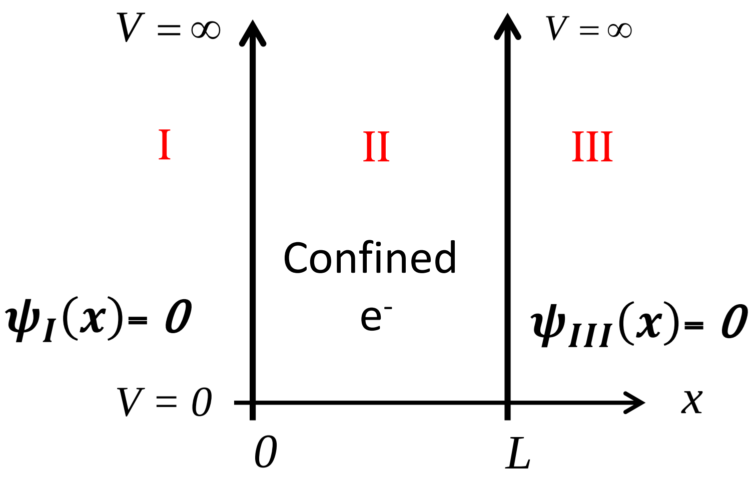
$$k = \frac{2\pi}{\lambda} \;\;, \; \lambda = \frac{h}{\sqrt{2mE}}$$ The parameter λ is the wavelength

From de Broghe's wave−particle duahty princeplet ,the wavelength is also given by

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

2.3.3 : The Infinite Potential Well

The problem of a particle in the infinite potential well is a classic example of a bound particle. The potential ***V(x)*** as a function of position for this problem is shown in figure



The time-independent Schrodinger's wave equation is again given by Equation :

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} - E\,\psi(x) = 0 \qquad \dots\dots\dots(33)$$

$E_I \;\; and \;\; E_{III} = ziro$; because of don't found of wave function in those regions

But , E_{II} $can\ be\ have\ a\ values\ as$:

$$E = E_n = \frac{n^2\pi^2\hbar^2}{2m\,a^2}$$

Example:

Calculate the first three energy levels of an electron in an infinite potential well. Consider an electron in an infinite potential well of width 5 Å .

Solution :

$$E = E_n = \frac{n^2\pi^2\hbar^2}{2m\,a^2}$$

$$E_n = n^2 \frac{3.14^{\,2} \times (1.054 \times 10^{-34})^{\,2}}{2 \times 9.1 \times 10^{-31} \times (5 \times 10^{-10})^2}$$

$$E_n \approx n^2 (2.49 \times 10^{-19}) \quad J$$

$$E_n = n^2 \frac{(2.4 \times 10^{-19})}{1.6 \times 10^{-19}} \approx 1.5 \ eV$$

n	E(eV)	E(J)
1	1.51	2.39×10^{-19}
2	6.02	9.55×10^{-19}
3	13.55	21.5×10^{-19}

This calculation : shows the order of magnitude of the energy levels of a bound electron

($H.W8$): The width of the infinite potential well in last example is doubled to 10 Å. Calculate the first three energy levels in terms of electron volts for an electron.

($H.W9$): 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 panicle?

2.3.3 : The Step Potential Function

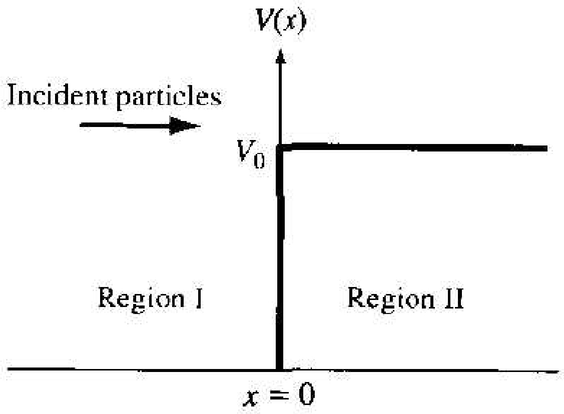
In this example, we will assume that a flux of particles is incident on the potential barrier. We will assume that the particles are traveling in the ***+x*** direction and that they originated at x = -∞. A particularly interesting result is obtained for the case when the total energy of the particle is less than the barrier height, or $E < V_o$.

First region (I)

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

2nd region (II)

$$k_2 = \sqrt{\frac{2m\,(V_o - E)}{\hbar^2}}$$



We can define a reflection coefficient, ***R ,*** as the ratio of the reflected flux to the incident flux, which is written as :

$$R = \frac{v_r}{v_i}\frac{(k_2{}^2 + 2i\,k_1 k_2 + k_1{}^2)(k_2{}^2 - 2i\,k_1 k_2 + k_1{}^2)}{(k_2{}^2 + k_1{}^2)}$$

And , transition coefficient, ***T ,*** as the ratio of the transition flux to the incident flux, which is written as :

$$\tau = = = \frac{2v_\tau k_1 (k_1 - i\,k_2)}{v_i}$$

where υ_i and υ_τ, are the incident and reflected particles velocities. respectively.

In region I, $V = 0$, so that $E = T$, where T is the kinetic energy of the particle. The kinetic energy is given by:

$$T = \frac{1}{2} m\upsilon^2$$

so that the constant K_1 written as:

$$k_1 = \sqrt{\frac{2m}{\hbar^2}\left(\frac{1}{2}\ m\upsilon^2\right)} = \frac{m\upsilon}{\hbar}$$

The incident velocity can then be written as

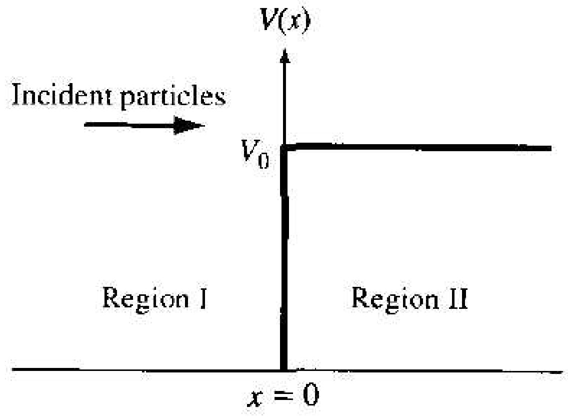
$$\upsilon_i = \frac{\hbar}{m} k_1$$

Since the reflected particle also exists in region I, the reflected velocity(magnitude) is given by:

$$\upsilon_r = \frac{\hbar}{m} k_1$$

then , reflection coefficient, *R in region I is :*

R = 1 **($H.W10$):** Prove that .



($H.W11$): E2.8, E2.9,and E2.10 in p.42 in Semiconductor Physics and Devices(Donald A. Neamen)