Solution for Exercise-sheet 3

I. Normalization of Schrödinger's wave function

(I.1) (a) Normalize the wave function to determine the constant A.
Solution

$$\int_0^a |\psi(x)|^2 \, dx = 1 = |A|^2 \int_0^a (\sin \frac{n\pi}{a} x)^2 dx \quad (1)$$

$$= |A|^2 \int_0^a \sin^2 \frac{n\pi}{a} x dx \quad (2)$$

$$= |A|^2 \int_0^a \frac{1 - \cos \frac{2n\pi}{a} x}{2} dx \quad (3)$$

$$= |A|^2 \left[\frac{1}{2} x - \frac{1}{4n\pi} \sin(\frac{2n\pi}{a} x) \right]_0^a \quad (4)$$

$$= |A|^2 \times \frac{a}{2} \quad (5)$$

This yields

$$|A| = \sqrt{\frac{2}{a}}. \quad (6)$$

Therefore $A = \pm\sqrt{\frac{2}{a}}, \pm j\sqrt{\frac{2}{a}}$ or any complex number having the magnitute of $\sqrt{\frac{2}{a}}$

(b) What would be the time-dependent wave function?
Solution:

$$\Psi(x,t) = \psi(x) e^{-i\frac{E}{\hbar}t} = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} e^{-i\frac{E}{\hbar}t} = \sqrt{\frac{2}{a}} \frac{\{e^{i(\frac{n\pi}{a}x - \frac{E}{\hbar}t)} - e^{-i(\frac{n\pi}{a}x + \frac{E}{\hbar}t)}\}}{2i} \quad (7)$$

II. time-independent Schrödinger equation

(II.1)
(a) Calculate the first two energy levels that the electron may occupy.
Solution: $E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2} = n^2 4.179 \times 10^{-20}\text{J} = 0.26 n^2\text{eV}$
The 1st energy level $n = 1$, $E_1 = 0.261\text{eV}$
The 2nd energy level $n = 1$, $E_2 = 1.04\text{eV}$
(b) If an electron drops from the second energy level to the first, what is the wavelength of the photon that might be emitted?
Solution: $\lambda = \frac{hc}{E_2 - E_1} = 1.59 \times 10^{-6}\text{m} = 1.59\mu\text{m}$

(II.2) Consider the particle in the infinite potential well as shown in Figure.1.
(a) Using a boundary condition, derive an expression of the wave functions.
(b) Using the normalization, determine a constant of the amplitude of the wave function. The following formula could be used;

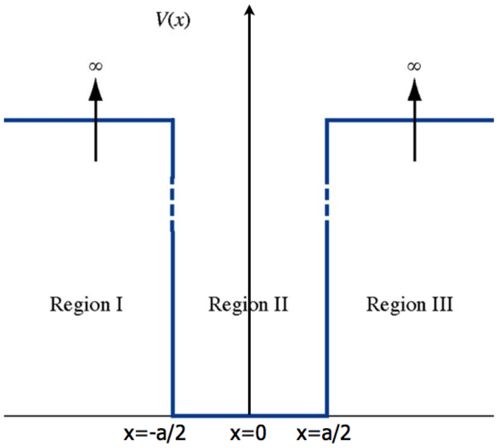

Figure 1: Potential function

$$\cos^2 x = \frac{\cos 2x + 1}{2} \tag{8}$$

III. TIME-INDEPENDENT SCHRÖDINGER EQUATION

(III.1) For the 1D step potential function shown in Figure 1, assume that the total energy of electrons $E > V_0$ and that the electrons are incident from the +x direction traveling in the -x direction.

(a) Write the general solutions of time-independent Schrödinger's equation for each region.

(b) By applying boundary conditions, derive expressions for the transmission T and reflection coefficients R, respectively.

Solution:

(a) For region II, $x > 0$

$$\frac{\partial \psi_2(x)}{\partial x^2} + \frac{2m(E - V_0)}{\hbar^2}\psi_2(x) = 0. \tag{9}$$

General form of the solution is

$$\psi_2(x) = A_2 e^{jK_2 x} + B_2 e^{-jK_2 x} \tag{10}$$

where

$$K_2 = \sqrt{\frac{2m}{\hbar^2}(E - V_0)} \tag{11}$$

Term with B_2 represents incident wave (⟵), and term with A_2 represents the reflected wave (⟶).

Region I, $x < 0$

$$\frac{\partial \psi_1(x)}{\partial x^2} + \frac{2m(E)}{\hbar^2}\psi_1(x) = 0. \tag{12}$$

The general solution is of the form

$$\psi_1(x) = A_1 e^{jK_1 x} + B_1 e^{-jK_1 x} \tag{13}$$

where

$$K_1 = \sqrt{\frac{2mE}{\hbar^2}} \tag{14}$$

The term involving B_1 represents the transmitted wave ($\leftarrow$). If a particle is transmitted into region I, it will not be reflected so that

$$A_1 = 0. \tag{15}$$

Then

$$\underline{\psi_1(x) = B_1 e^{-jK_1 x}} \tag{16}$$

$$\underline{\psi_2(x) = A_2 e^{jK_2 x} + B_2 e^{-jK_2 x}} \tag{17}$$

(b) Boundary conditions:

(1)

$$\psi_1(x = 0) = \psi_2(x = 0)$$

(2)

$$\left.\frac{\partial \psi_1(x)}{\partial x}\right|_{x=0} = \left.\frac{\partial \psi_2(x)}{\partial x}\right|_{x=0} \tag{18}$$

Applying the boundary conditions to the solutions, we find

$$B_1 = A_2 + B_2 \tag{19}$$

$$K_2 A_2 - K_2 B_2 = -K_1 B_1 \tag{20}$$

Combining these two equations, we find

$$A_2 = \left(\frac{K_2 - K_1}{K_2 + K_1} B_2\right) \tag{21}$$

$$B_1 = \left(\frac{2K_2}{K_2 + K_1} B_2\right) \tag{22}$$

The reflection coefficient is

$$R = \frac{A_2 A_2^*}{B_2 B_2^*} \to \underline{R = \left(\frac{K_2 - K_1}{K_1 + K_2}\right)^2} \tag{23}$$

The transmission coefficient is

$$T = 1 - R \to \underline{T = \frac{4K_1 K_2}{(K_1 + K_2)^2}} \tag{24}$$