Quadrant II – Notes

Programme: Bachelor of Science (Third Year)

Subject: Physics

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Paper Title: Quantum Mechanics

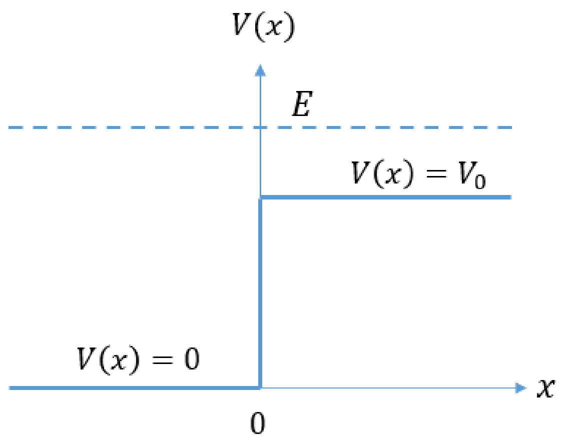
Unit 2: Applications of Schrödinger's Time Independent Wave Equation

Module Name: One dimensional finite square step potential of height Vo: Comparison of classical and quantum mechanical results for particle energy $E > V_0$ and $E < V_0 -$ Part II

Module No: 28

Name of the Presenter: Dr. Ashish M. Desai

Step Potential (Energy greater than Step Height)



Consider the motion of the particle under the influence of step potential where its total energy, E, is greater than the height of the potential step, V_0.

The potential energy of the step potential can be written as

$$V(x) = \begin{matrix} V_0 & \quad x > 0 \\ 0 & \quad x < 0 \end{matrix}$$

In classical mechanics a particle of total energy E travelling in the region $x < 0$ in the direction of increasing x will suffer in impulsive retarding force $F = -dV(x)/dx$ at the point $x = 0$. But the impulse will only slow the particle and the particle will continue its motion in the direction of increasing x.

Its momentum in region $x < 0$ is p_1, where $\frac{p_1^2}{2m} = E$; its momentum in region $x > 0$ is p_2, where $\mathrm{p}_2^2/2\mathrm{m} = E - V_0$

As per quantum mechanics we will see that if E is not too much larger than $V_0$the theory predicts that the particle has an appreciable chance of being reflected back even though the particle has enough energy to pass over the step into the region $x > 0$.

In the region $x < 0$ we have $V(x) = 0$.

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

In the region $x > 0$ we have $V(x) = V_0$.

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = (E - V_0)\psi(x)$$

These two equations can be solved separately and the eigenfunction for the entire range of x is constructed by joining the solutions together at $x = 0$.

Solutions of the Schrödinger Equation in the region $x < 0$

- The general solution of the Schrödinger equation

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2mE}{\hbar^2}\psi(x) = -k_1^2\psi(x)$$

in the region $x < 0$ is

$$\psi(x) = Ae^{ik_1x} + Be^{-ik_1x} \qquad ----(1)$$

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

Solutions of the Schrödinger Equation in the region $x > 0$

- The general solution of the Schrödinger equation

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = (E - V_0)\psi(x)$$

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2m(E - V_0)}{\hbar^2} = -k_2^2\psi(x)$$

in the region $x > 0$ is

$$\psi(x) = Ce^{ik_2x} + De^{-ik_2x} \quad - - - - - (2)$$

where $k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$

We do not need to take the second term of the general solution of Eq. 2 as this term describes wave travelling in a direction of decreasing x in the region $x > 0$ and there is nothing out there to cause a reflection.

Thus we take the arbitrary constant D to have the value

$$D = 0$$

Hence,

$$\psi(x) = Ce^{ik_2x} \qquad x > 0 \quad - - - - - (3)$$

- The two forms of eigenfunction should join in such a way that $\psi(x)$ and $d\psi(x)/dx$ must be continuous at the point $x = 0$. As the eigenfunction must be continuous at $x = 0$, we have

$$A\left(e^{ik_1x}\right)_{x=0} + B\left(e^{-ik_1x}\right)_{x=0} = C\left(e^{ik_2x}\right)_{x=0}$$

This relation yields

$$A + B = C \qquad - - - (4)$$

As the derivative of eigenfunction must be continuous at $x = 0$, we have

$$\frac{d\psi(x)}{dx} = ik_2Ce^{ik_2x} \qquad x > 0 \; - - - - - - (5)$$

and

$$\frac{d\psi(x)}{dx} = ik_1Ae^{ik_1x} - ik_1Be^{-ik_1x} \qquad x < 0 \; - - - - - - (6)$$

Equating the derivatives at $x = 0$ we get

$$ik_1A\left(e^{ik_1x}\right)_{x=0} - ik_1B\left(e^{-ik_1x}\right)_{x=0} = ik_2C\left(e^{ik_2x}\right)_{x=0}$$

Thus

$$k_1(A - B) = k_2C \quad - - - - - - - - (7)$$

Adding Eqns. (4) and (7) gives

$$B = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)A$$

and

$$C = \left(\frac{2k_1}{k_1 + k_2}\right)A$$

Thus the eigenfunction for the step potential for the energy $E > V_0$ is

$$\psi(x) = \begin{array}{ll} Ae^{ik_1x} + A\left(\frac{k_1 - k_2}{k_1 + k_2}\right) e^{-ik_1x} & x \le 0 \\ A\left(\frac{2k_1}{k_1 + k_2}\right) e^{-k_2x} & x \ge 0 \end{array}$$

The ratio of the intensity of the reflected wave to the intensity of the incident wave gives the probability that the incident particle is reflected back into $x < 0$ region

$$R = \frac{B^*B}{A^*A} = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^* \left(\frac{k_1 - k_2}{k_1 + k_2}\right) = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2$$

We see that $R < 1$ when $E > V_0$.

The result is surprising that $R > 0$ as a classical particle would definitely not be reflected if it had enough energy to pass the potential discontinuity.

The transmission coefficient specifies the probability that the particle will be transmitted past the potential step from the region $x < 0$ into the region $x > 0$. As the velocity of the particle is different in two regions the evaluation of the transmission coefficient is more complicated. Transmission and reflection coefficient are actually defined as ratio of probability fluxes. The probability flux is the probability per second that the particle will be found crossing some reference point travelling in a particular direction.

Incident probability flux is the probability per second that the particle will be found crossing a point at $x < 0$ travelling in a direction of increasing x. Reflected probability flux is the probability per second that the particle will be found crossing a point at $x < 0$ travelling in a direction of decreasing x. Transmitted probability flux is the probability per second that the particle will be found crossing a point at $x > 0$ travelling in a direction of increasing x.

The probability flux is not only proportional to the intensity of the wave but also proportional to the velocity of the particle. (Refer Ref. 1 , Appendix L for more detailed discussion)

According to this definition

$$R = \frac{v_1 B^*B}{v_1 A^*A} = \frac{B^*B}{A^*A}$$

where v_1 is the velocity of the particle in the region $x < 0$. Since the velocity cancels this formula is identical to the one obtained previously.

For $T,$ the velocities do not cancel and we have

$$T = \frac{v_2 C^*C}{v_1 A^*A} = \frac{v_2}{v_1}\left(\frac{2k_1}{k_1 + k_2}\right)^2$$

Where v_2 is the velocity of the particle in the region $x > 0$.

Now

$$v_1 = \frac{p_1}{m} = \frac{\hbar k_1}{m} \text{ and } v_2 = \frac{p_2}{m} = \frac{\hbar k_2}{m}$$

The above expression becomes

$$T = \frac{k_2}{k_1}\left(\frac{2k_1}{k_1 + k_2}\right)^2 = \frac{4k_1 k_2}{(k_1 + k_2)^2}$$

It can be easily verified that $\boldsymbol{R + T = 1}$.