FAQs & their solutions for Module 2:
Simple Solutions of the one-dimensional Schrodinger Equation

Question1: Determine the energy levels and the corresponding Eigen functions of a particle of mass μ in a one dimensional infinitely deep potential well characterized by the following potential energy variation

$$\begin{aligned} V(x) &= 0 \quad \text{for} \quad 0<x<a \\ &= \infty \quad \text{for} \quad x<0 \text{ and for } x>a \end{aligned} \tag{1}$$

Solution 1: For $0 < x < a$, the one dimensional Schrödinger equation becomes

$$\frac{d^2\psi}{dx^2} + k^2\psi(x) = 0 \tag{2}$$

where

$$k^2 = \frac{2\mu E}{\hbar^2} \tag{3}$$

The general solution of the Schrödinger equation is

$$\psi(x) = A\sin kx + B\cos kx \tag{4}$$

Since the boundary condition at a surface at which there is an infinite potential step is that ψ is zero, we must have

$$\psi(x=0) = \psi(x=a) = 0 \tag{5}$$

The above condition also follows from the fact that since the particle is inside an infinitely deep potential well, it is always confined in the region $0 < x < a$ and therefore ψ must vanish for $x < 0$ and $x > L$; and for ψ to be continuous, we must have

$$\psi(x=0) = B = 0 \tag{6}$$

and

$$\psi(x=a) = A\sin ka = 0 \tag{7}$$

Thus, either

$$A = 0$$

or

$$ka = n\pi\,; \quad n = 1, 2, \ldots \tag{8}$$

The condition $A = 0$ leads to the trivial solution of ψ vanishing everywhere, the same is the case for $n = 0$. Thus the allowed energy levels are given by

$$E_n = \frac{\pi^2 n^2 \hbar^2}{2\mu a^2} \quad ; \quad n = 1, 2, 3, \tag{9}$$

The corresponding eigenfunctions are

$$\left.\begin{aligned} \psi_n &= \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) && 0 < x < a \\ &= 0 && x < 0 \text{ and } x > a \end{aligned}\right\} \tag{10}$$

where the factor $\sqrt{2/a}$ is such that the wave functions form an orthonormal set :

$$\int_0^a \psi_m^*(x)\psi_n(x)\ dx = \delta_{mn} \tag{11}$$

It may be noted that whereas $\psi_n(x)$ is continuous everywhere, $d\psi_n(x)/dx$ is discontinuous at $x = 0$ and at $x = a$. This is because of $V(x)$ becoming infinite at $x = 0$ and at $x = a$.

<u>Question2:</u> Consider the potential energy variation given by

$$V(x) = \begin{cases} \infty & x \le 0 \\ 0 & 0 < x < b \\ V_0 & x > b \end{cases} \tag{12}$$

<u>Solution 2:</u>

$$\begin{aligned} \psi(x) &= A \sin kx \\ &= A \sin kb\, e^{-\kappa(x-b)} \end{aligned}$$

Continuity of $d\psi/dx$ at $x = b$ will give us

$$-\xi \cot \xi = \sqrt{\alpha^2 - \xi^2} \tag{13}$$

where

$$\alpha^2 = \frac{2\mu V_0 b^2}{\hbar^2} \tag{14}$$

and

$$\xi^2 = \frac{2\mu E b^2}{\hbar^2} \tag{15}$$

Question3: In continuation of the previous problem, assume

$$\frac{2\mu V_0 b^2}{\hbar^2} = 9\pi^2 \qquad (16)$$

Calculate the number of bound states and also the corresponding values of

$\xi = \sqrt{\frac{2\mu E b^2}{\hbar^2}}$.

Solution3: If we numerically solve the equation

$$-\xi \cot \xi = \sqrt{\alpha^2 - \xi^2} \qquad (17)$$

We will find that there are three bound states with

$$\xi = 2.83595,\ \ 5.64146 \text{ and } \ 8.33877$$

Question4: Show that the function $\psi(x) = A\ \exp(-\kappa\,|x|)\ ;\ [\kappa > 0]$ satisfies the one-dimensional Schrodinger equation corresponding to $V(x) = -S\ \delta(x)$. Find the value of S and the corresponding value of the energy.

Solution4:

$$\psi(x) = A\ \exp(-\kappa\,|x|)\ ;\ [\kappa > 0]$$

Thus

$$\psi(x) = A\ e^{-\kappa x} \text{ for } x > 0$$

$$= A\ e^{\kappa x} \text{ for } x < 0$$

Thus

$$\psi'(x) = -A\kappa\, e^{-\kappa x} \text{ for } x > 0$$

$$= A\kappa\, e^{\kappa x} \text{ for } x < 0$$

The function $\psi'(x)$ has a discontinuity of $-2A\kappa$ at $x = 0$. Thus

$$\psi''(x) = \kappa^2 \psi - 2A\kappa\, \delta(x)$$

<u>Question5:</u> Solve the one-dimensional Schrodinger equation for

$$\begin{aligned} V(x) &= -V_0 \quad |x| < \frac{a}{2} \\ &= 0 \quad\quad |x| > \frac{a}{2} \end{aligned} \tag{18}$$

and derive the transcendental equations which would determine the energy eigenvalues.

(b) Show that if we let $a \to 0$ and $V_0 \to \infty$ such that

$$aV_0 \to S \tag{19}$$

we would obtain only one bound state with energy as given in the previous problem.

<u>Solution 5:</u> The transcendental equation determining the energy eigenvalues corresponding to symmetric states is given by

$$\xi \tan \xi = \sqrt{\sigma^2 - \xi^2} \tag{20}$$

where

$$\xi = \left[\frac{\mu}{2\hbar^2}(V_0 + E)a^2\right]^{1/2} \tag{21}$$

and

$$\sigma^2 = \frac{\mu}{2\hbar^2} V_0 a^2 \tag{22}$$

Notice that for bound states E is negative with $|E| < V_0$. When $V_0 \to \infty$ and $a \to 0$ such that $V_0 a \to S$ we obtain

$$\sigma^2 = \frac{\mu S}{2\hbar^2} a \tag{23}$$

which tends to zero. Thus the root of the equation

$\xi \tan \xi = \sqrt{\sigma^2 - \xi^2}$

will correspond to a very small value of ξ so that we may replace tan ξ by ξ to obtain

$$\xi^2 = \sqrt{\sigma^2 - \xi^2}$$

or

$$\xi^4 + \xi^2 - \sigma^2 = 0$$

or

$$\xi^2 = \frac{1}{2}\left[-1 \pm \sqrt{1 + 4\sigma^2}\right]$$

We neglect the minus sign and make a bionomial expansion to obtain

$$\xi^2 \approx \sigma^2 - \sigma^4$$

or

$$\frac{\mu}{2\hbar^2}\left[V_0 + E\right]a^2 \approx \frac{\mu V_0 a^2}{2\hbar^2} - \frac{\mu^2 V_0{}^2 a^4}{4\hbar^4}$$

or

$$E \approx -\frac{\mu S^2}{2\hbar^2}$$

<u>Question6:</u> Determine the normalized eigenfunctions of the momentum operator

$$p_{op} = -i\hbar \frac{d}{dx} \qquad (24)$$

and write the orthonormality and completeness conditions.

<u>Solution 6:</u> The eigen value equation for the operator

$$p_{op} = -i\hbar \frac{d}{dx}$$

will be

$$p_{op}u_p(x) = p\, u_p(x)$$

where p (on the RHS) is now a number. Thus

$$-i\hbar \frac{d}{dx} u_p(x) = p\, u_p(x)$$

Simple integration will give us

$$u_p(x) = \frac{1}{\sqrt{2\pi\hbar}}\, e^{\frac{i}{\hbar} p x} \quad ; \; -\infty < p < +\infty$$

where the factor $\frac{1}{\sqrt{2\pi\hbar}}$ is introduced so that

$$\int_{-\infty}^{+\infty} u_p^*(x) u_{p'}(x)\, dx = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} e^{-\frac{i}{\hbar}(p-p')x}\, dx = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-i(p-p')\xi}\, d\xi$$

$$= \delta(p-p')$$

which is the ortho-normaility condition. Similarly,

$$\int_{-\infty}^{+\infty} u_p^*(x) u_p(x')\, dp = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} e^{-\frac{i}{\hbar}(x-x')p}\, dp = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-i(x-x')\xi}\, d\xi$$

$$= \delta(x-x')$$

is the completeness condition.

<u>Question7:</u> In continuation of the previous problem show that the eigenfunctions of the operator

$$H = \frac{p_{op}^2}{2\mu} = -\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} \tag{25}$$

are the same as that of the operator

$$p_{op} = -i\hbar \frac{d}{dx}$$

Solution7:

$$H = \frac{p^2}{2m} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

It is easy to see that

$$u_p\left(x\right) = \frac{1}{\sqrt{2\pi\hbar}}\, e^{\frac{i}{\hbar}p\,x}$$

are eigenfunctions of H. Thus the functions $u_p\left(x\right)$ are also simultaneous eigenfunctions p_x , p_x^2 and H .