Tutorial - 3 : Quantum Mechanics

To be discussed on 19 November 2018

1. Consider a particle in a one-dimensional box of length a, defined by the potential,

$$\begin{aligned} V(x) &= 0, \quad \text{for} \quad (0 \leq x \leq a) \\ &= \infty, \quad \text{for} \quad (0 > x, \quad x > a) \end{aligned}$$

The energy eigenvalues of the particle are given by $\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right)$, where $n = 1,\ 2,\ 3,\ \cdots$.

(a) At time $t = 0$, the state of the particle is $\psi(x, t = 0) = \sqrt{\frac{1}{3}}\ \psi_1(x) + \sqrt{\frac{2}{3}}\ \psi_2(x)$ at time $t = 0$.

i. What is the average energy, $\langle E \rangle$ of the particle at $t = 0$?

ii. In a measurement of energy, what is the probability to get the value $E_1 = \frac{\pi^2 \hbar^2}{2ma^2}$?

iii. What is its state $\psi(x, t)$ at a later time t?

iv. What is the value of $\langle E \rangle$ of the particle at time t?

(b) Consider a particle with energy E_1 in the box.

i. What is the expectation value of the position of the particle?

ii. What is the probability to find it in the region $0 \leq x \leq \frac{a}{2}$?

(c) Repeat the above for the particle of energy E_2.

Solution:

(a) i. We have $H\psi_n = E_n \psi_n$ with $E_n = \frac{n^2 \phi^2 \hbar^2}{2ma^2}$. The average value of energy at $t = 0$,

$$\begin{aligned} \langle E \rangle &= \int_0^a \psi(x, t = 0)^* H \psi(x, t = 0)\ dx \\ &= \int_0^a \left(\sqrt{\frac{1}{3}}\ \psi_1(x) + \sqrt{\frac{2}{3}}\ \psi_2(x) \right)\ H\ \left(\sqrt{\frac{1}{3}}\ \psi_1(x) + \sqrt{\frac{2}{3}}\ \psi_2(x) \right)\ dx \\ &= \int_0^a \left(\sqrt{\frac{1}{3}}\ \psi_1(x) + \sqrt{\frac{2}{3}}\ \psi_2(x) \right) \left(\sqrt{\frac{1}{3}}\ E_1\ \psi_1(x) + \sqrt{\frac{2}{3}}\ E_2\ \psi_2(x) \right)\ dx \\ &= \frac{E_1}{3} + \frac{2E_2}{3} \end{aligned}$$

ii. The probability to yield E_1 in a measurement is given by

$$\mathcal{P}_{E1} = \left| \int_0^a \psi_1^* \ \psi(x, t = 0) \ dx \right|^2 = \frac{1}{3} \tag{1}$$

iii. Time evolution of the energy eigenstates are $\psi_n(x, t) = e^{\frac{-iE_n t}{\hbar}} \ \psi_n(x)$. That gives

$$\psi(x, t) = \sqrt{\frac{1}{3}} \ \psi_1(x) e^{\frac{-iE_1 t}{\hbar}} + \sqrt{\frac{2}{3}} \ \psi_2(x) e^{\frac{-iE_2 t}{\hbar}} \tag{2}$$

iv. $\langle E \rangle_t = \langle E \rangle_{t=0}$.

(b) i.

$$\langle x \rangle = \frac{2}{a} \int_0^a x \sin^2\left(\frac{\pi x}{a}\right) \ dx = \frac{a}{2}$$

ii.

$$\mathcal{P}_{0 \le x \le \frac{a}{2}} = \frac{2}{a} \int_0^a \sin^2\left(\frac{\pi x}{a}\right) \ dx = \frac{1}{2}$$

(c) i.

$$\langle x \rangle = \frac{2}{a} \int_0^a x \sin^2\left(\frac{2\pi x}{a}\right) \ dx = \frac{a}{2}$$

ii.

$$\mathcal{P}_{0 \le x \le \frac{a}{2}} = \frac{2}{a} \int_0^a \sin^2\left(2\frac{\pi x}{a}\right) \ dx = \frac{1}{2}$$

2. The wave function of a particle in a one-dimensional box (described in Question 1) has the wave function $\psi(x) = A \ x^2(a - x)$. What is the probability to find the particle in energy state E_1 in a measurement?

Solution:

$$\begin{aligned} \psi(x) &= \sum_{n=0}^{\infty} c_n \ \sin\left(\frac{n\pi}{a} x\right) \\ c_n &= A \int_0^a x^2 \ (a - x) \ \sin\left(\frac{n\pi}{a} x\right) \\ &= \begin{cases} -\frac{2Aa^4}{n^3\pi^3}, & \text{for } n = 1, \ 3, 5, \ \cdots \\ \frac{6Aa^4}{n^3\pi^3}, & \text{for } n = 2, \ 4, \ 6, \ \cdots \end{cases} \end{aligned}$$

Probability to find the particle in state of energy E_1, $\mathcal{P}_{E_1} = |c_1|^2 = \left(\frac{2Aa^4}{\pi^3}\right)^2$.

3. Consider the one-dimensional potential,

$$\begin{aligned} V(x) &= \infty, && \text{for } (x<0) \\ &= -V_0, && \text{for } (0 \le x \le a) \\ &= 0, && \text{for } (x > a). \end{aligned}$$

Find the wave function of a particle of energy $-V_0 < E < 0$ in all the three regions.

Solution:

In region 1: $x < 0$, $\psi_1(x) = 0$.

In region 2: $0 \le x \le a$, we have the Schrödinger eqnation,

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi - V_0\psi &= E\psi. \\ \frac{\partial^2}{\partial x^2}\psi &= -\frac{2m(E+V_0)}{\hbar^2}\psi \end{aligned}$$

Note that $E + V_0 > 0$. This give the solution: $\psi_2(x) = A\cos(kx) + B\sin(kx)$, with $k = \frac{\sqrt{2m(E+V_0)}}{\hbar}$

In region 3: $x > a$. We have $V(x) = 0$. That leads to $\frac{\partial^2}{\partial x^2}\psi = -\frac{2mE}{\hbar^2}\psi = +\kappa^2\psi$, where $\kappa = \frac{\sqrt{-2mE}}{\hbar} > 0$.

$\Longrightarrow$ $\psi_3(x) = C\,e^{-\kappa x} + D\,e^{\kappa x}$, but $D = 0$, lest $\psi \to \infty$ as $x \to \infty$.

That is,

$$\begin{aligned} \psi_1(x) &= 0, && \text{for } (x<0) \\ \psi_2(x) &= A\cos(kx) + B\sin(kx), && \text{for } (0 \le x \le a) \\ \psi_3(x) &= C\,e^{-\kappa x}, && \text{for } (x > a). \end{aligned}$$

Boundary conditions: $\psi_1(0) = \psi_2(0)$, $\psi_2(a) = \psi_3(a)$, $\left.\frac{\partial \psi_2}{\partial x}\right|_{x=a} = \left.\frac{\partial \psi_3}{\partial x}\right|_{x=a}$

$\Longrightarrow$

$$\begin{aligned} A &= 0 \\ B\sin(ka) &= Ce^{-\kappa a} \\ k\ B\ \cos(ka) &= -\kappa\ Ce^{-\kappa a} \\ \Longrightarrow \qquad \tan(ka) &= -\frac{k}{\kappa} \end{aligned} \tag{3}$$

In k and κ, E is the parameter. Energy cannot be any value, but those that satisfy the above equation. Redefine the parameter:

$z = ka$.

Notice that $k^2 + \kappa^2 = \frac{2mV_0}{\hbar^2}$. $\Longrightarrow$ $\kappa a = \sqrt{z_0^2 - z^2}$.

Eqn.3 is now: $\tan(z) = -\frac{z}{\sqrt{z_0^2 - z^2}}$. Plot below shows $\tan z$ (blue) and $-\frac{z}{\sqrt{z_0^2-z^2}}$ (orange) with z along the horizontal axis. The intersection points are the allowed values of z, and therefore (the corresponding) E.