T03

Friday, 13 August 2021 12:58 PM

Problem 3.4:

Show that
$$\frac{d}{dt}\int_{-\infty}^{\infty} \psi_1^*(x,t)\psi_2(x,t) = 0$$
for any two ψ_1 and ψ_2.

Equation becomes
$$\int_{-\infty}^{\infty} \frac{\partial}{\partial t}\left(\psi_1^*\psi_2\right)dx = \int_{-\infty}^{\infty} \psi_1^*\frac{\partial \psi_2}{\partial t} + \psi_2\frac{\partial \psi_1^*}{\partial t}\,dx$$
(by chain rule)

but $\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2\psi}{\partial x^2} - \frac{i}{\hbar}V\psi$ and $\frac{\partial \psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2\psi^*}{\partial x^2} + \frac{i}{\hbar}V\psi^*$

$$\Rightarrow \quad = \int_{-\infty}^{\infty}\left(\frac{i\hbar}{2m}\frac{\partial^2\psi_2}{\partial x^2}\psi_1^* - \frac{i}{\hbar}V\psi_2\psi^* - \frac{i\hbar}{2m}\frac{\partial^2\psi_1^*}{\partial x^2}\psi_2 + \frac{i}{\hbar}V\psi_1^*\psi_2\right)dx$$
$$= \int_{-\infty}^{\infty}\frac{i\hbar}{2m}\left(\frac{\partial^2\psi_2}{\partial x^2}\psi_1^* - \frac{\partial^2\psi_1^*}{\partial x^2}\psi_2\right)dx$$
$$= \frac{i\hbar}{2m}\left(\frac{\partial\psi_2}{\partial x}\psi_1^* - \frac{\partial\psi_1^*}{\partial x}\psi_2\right)\Bigg|_{-\infty}^{\infty}$$

but ψ_2 must go to 0 as $x \to \pm\infty$ (since it's normalizable), and so
$$\frac{d}{dt}\int_{-\infty}^{\infty}\psi_1^*\psi_2\,dx = \frac{i\hbar}{2m}\left(\frac{\partial 0}{\partial x}\psi_1^* - \frac{\partial\psi_1^*}{\partial x}\cdot 0\right)$$
$$= 0$$

Problem 3.5:

Start with the time-independent Schrodinger Equation, and take ψ as a normalisable solution.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$$
$$\Rightarrow \quad V\psi - E\psi = \frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}$$
$$\Rightarrow \quad \frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(V-E)\psi$$

Now, suppose $E < V_{min}$, then $V - E = k > 0$

$$\Rightarrow \quad \frac{d^2\psi}{dx^2} = \frac{2mk}{\hbar^2}\psi$$

$\therefore$ ψ and its second derivative always have the same sign. Assuming ψ is real and nonnegative for all t and x, then ψ and its second derivative are always positive. That is, ψ is increasing at an increasing rate for all time and space.

For ψ to be a normalisable solution, however, $\psi \to 0$ as $x \to \pm\infty$. This is a contradiction, as ψ is increasing for all x, i.e. $\psi \to \infty$.

Therefore, the energy of a particle must be greater than V_{min} for ψ to be the normalisable solutions to the time-independent

Therefore, the energy of a particle must be greater than V_{min} for ψ to be a normalisable solution to the time-independent Schrodinger Equation.
This scenario is of the form of a harmonic oscillator.
In a classical harmonic oscillator, the energy of a particle can be equal to that of the potential. i.e. $E \geq V_{min}$, whereas a quantum harmonic oscillator must have $E > V_{min}$.

T04

Friday, 20 August 2021 1:00 PM

Problem 4.3:

$$\Psi(x,0) = \sqrt{\frac{8}{5a}}\left(1+\cos\left(\frac{\pi x}{a}\right)\right)\sin\left(\frac{\pi x}{a}\right)$$

Infinite square well of potential $V(x)=0$ for $0 \le x \le a$

$$\Psi(x,0) = \sqrt{4}\sqrt{\frac{2}{5a}}\left(\sin\left(\frac{\pi x}{a}\right) + \cos\left(\frac{\pi x}{a}\right)\sin\left(\frac{\pi x}{a}\right)\right)$$

Using the trig identity $\sin(2\theta) = 2\cos(\theta)\sin(\theta)$,

$$\Psi(x,0) = \frac{1}{\sqrt{5}}\sqrt{\frac{2}{a}}\left(2\sin\left(\frac{\pi x}{a}\right) + \sin\left(\frac{2\pi x}{a}\right)\right)$$

$$= \frac{1}{\sqrt{5}}\left(2\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{2}{a}}\sin\left(\frac{2\pi x}{a}\right)\right)$$

Which is of the form

$$\Psi(x,0) = A\left(2\psi_1(x) + \psi_2(x)\right)$$

where $A = \frac{1}{\sqrt{5}}$ and ψ_1, ψ_2 are the first two solutions.

a. The probability of finding the particle between $0 \le x \le \frac{a}{2}$ at $t \neq 0$ is

$$\int_0^{a/2} |\Psi(x,0)|^2\,dx = \int_0^{a/2} \Psi^*\Psi\,dx$$

since Ψ has no complex components, $\Psi^* = \Psi \Rightarrow \Psi^*\Psi = \Psi^2$

$$\Rightarrow \quad = \int_0^{a/2} A^2\left(4\psi_1^2 + 2\psi_1\psi_2 + \psi_2^2\right)dx$$

since $\int \psi_n^*\psi_n = 1$ and $\int \psi_m^*\psi_n = 0 \ (m \neq n)$,

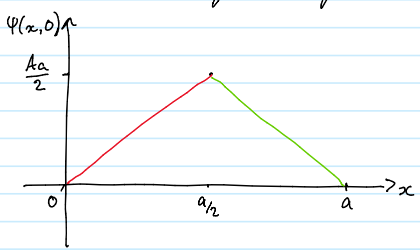
$$\Rightarrow P = A^2(4+1) = \frac{1}{5}\times 5 = 1$$

Problem 4.4:

$V(x) = 0$ for $0 \le x \le a$

$$\Psi(x,0) = \begin{cases} Ax & 0 \le x \le a/2 \\ A(a-x) & a/2 \le x \le a \end{cases}$$

a. Sketch $\Psi(x,0)$ as a function of x. Determine A



Determine A by normalization between 0 and a:

$$\int_0^a |\Psi(x,0)|^2\,dx = 1$$

$$\int_0^{a/2} |\Psi(x,0)|^2\,dx + \int_{a/2}^a |\Psi(x,0)|^2\,dx = 1 \qquad \text{(since } \Psi \text{ piecewise)}$$

$$\int_0^{a/2} A^2x^2\,dx + \int_{a/2}^a A^2(a-x)^2\,dx = 1 \qquad \left(\text{since no complex components, } \Psi^* = \Psi \Rightarrow \Psi^*\Psi = \Psi^2\right)$$

$$\left(A^2\frac{x^3}{3}\right)\Big|_0^{a/2} + \left(-\frac{A^2}{3}(a-x)^3\right)\Big|_{a/2}^a = 1$$

$$A^2\frac{a^3}{24} - \frac{A^2}{3}\left((a-a)^3 - \left(a-\frac{a}{2}\right)^3\right) = 1$$

$$A^2\frac{a^3}{24} + \frac{A^2}{3}\frac{a^3}{8} = 1 \quad \Rightarrow A^2 = \frac{12}{a^3}$$

$$A = \sqrt{\frac{12}{a^3}} = \frac{2\sqrt{3}}{\sqrt{a^3}}$$

b. The nth coefficient is expressed as

$$c_n = \sqrt{\frac{2}{a}}\int_0^a \sin\left(\frac{n\pi}{a}x\right)\Psi(x,0)\,dx$$

In the context of this wavefunction, this expands to:

$$c_n = \sqrt{\frac{2}{a}}\left(\int_0^{a/2} \sin\left(\frac{n\pi}{a}x\right) Ax\, dx + \int_{a/2}^{a} \sin\left(\frac{n\pi}{a}x\right) A(a-x)\, dx\right)$$

Solving each of these integrals individually,

1. $\displaystyle\int_0^{a/2} \sin\left(\frac{n\pi}{a}x\right) Ax\, dx$

Integrate by parts, with $u = x$, $dv = \sin\left(\frac{n\pi}{a}x\right)dx$

$$\Rightarrow A\int \sin\left(\frac{n\pi}{a}x\right) x\, dx = A\left(-\frac{ax}{n\pi}\cos\left(\frac{n\pi}{a}x\right) + \int \frac{a}{n\pi}\cos\left(\frac{n\pi}{a}x\right)dx\right)$$
$$= A\left(\frac{a^2}{(n\pi)^2}\sin\left(\frac{n\pi}{a}x\right) - \frac{ax}{n\pi}\cos\left(\frac{n\pi}{a}x\right)\right)$$
$$= \frac{Aa\left(a\sin\left(\frac{n\pi}{a}x\right) - n\pi x\cos\left(\frac{n\pi}{a}x\right)\right)}{(n\pi)^2}$$

$$\Rightarrow \int_0^{a/2} \sin\left(\frac{n\pi}{a}x\right) Ax\, dx = \frac{Aa\left(a\sin\left(\frac{n\pi}{a}x\right) - n\pi x\cos\left(\frac{n\pi}{a}x\right)\right)}{(n\pi)^2}\Bigg|_0^{a/2}$$
$$= \frac{Aa\left(a\sin\left(\frac{n\pi}{2}\right) - \frac{n\pi a}{2}\cos\left(\frac{n\pi}{2}\right)\right)}{(n\pi)^2}$$
$$= \frac{Aa^2}{(n\pi)^2}\left(\sin\left(\frac{n\pi}{2}\right) - \frac{n\pi}{2}\cos\left(\frac{n\pi}{2}\right)\right)$$

2. $\displaystyle\int_{a/2}^{a} \sin\left(\frac{n\pi}{a}x\right) A(a-x)\, dx = A\left(\int_{a/2}^{a} a\sin\left(\frac{n\pi}{a}x\right)dx - \int_{a/2}^{a} x\sin\left(\frac{n\pi}{a}x\right)dx\right)$

2.a. $\displaystyle a\int \sin\left(\frac{n\pi}{a}x\right)dx = a\left(-\frac{a}{n\pi}\cos\left(\frac{n\pi}{a}x\right)\right) = -\frac{a^2}{n\pi}\cos\left(\frac{n\pi}{a}x\right)$

2.b. $\displaystyle\int x\sin\left(\frac{n\pi}{a}x\right)dx = \frac{a\left(a\sin\left(\frac{n\pi}{a}x\right) - n\pi x\cos\left(\frac{n\pi}{a}x\right)\right)}{(n\pi)^2}$ (calculated in integral 1.)

$$\Rightarrow \int_{a/2}^{a} \sin\left(\frac{n\pi}{a}x\right) A(a-x)\, dx = -A\left(\frac{a^2}{n\pi}\cos\left(\frac{n\pi}{a}x\right) + \frac{a\left(a\sin\left(\frac{n\pi}{a}x\right) - n\pi x\cos\left(\frac{n\pi}{a}x\right)\right)}{(n\pi)^2}\right)\Bigg|_{a/2}^{a}$$
$$= -A\left(\frac{a^2}{n\pi}\left(\cos(n\pi) - \cos\left(\frac{n\pi}{2}\right)\right) + \frac{a^2\left(\sin(n\pi) - \sin\left(\frac{n\pi}{2}\right)\right)}{(n\pi)^2} + \frac{\left(\frac{a^2 n\pi}{2}\cos\left(\frac{n\pi}{2}\right) - a^2 n\pi\cos(n\pi)\right)}{(n\pi)^2}\right)$$
$$= -\frac{Aa^2}{(n\pi)^2}\left(n\pi\left(\cos(n\pi) - \cos\left(\frac{n\pi}{2}\right)\right) + \sin(n\pi) - \sin\left(\frac{n\pi}{2}\right) + \frac{n\pi}{2}\cos\left(\frac{n\pi}{2}\right) - n\pi\cos(n\pi)\right)$$
$$= -\frac{Aa^2}{(n\pi)^2}\left(\sin(n\pi) - \sin\left(\frac{n\pi}{2}\right) - \frac{n\pi}{2}\cos\left(\frac{n\pi}{2}\right)\right)$$

$$\Rightarrow c_n = \sqrt{\frac{2}{a}}\int_0^a \sin\left(\frac{n\pi}{a}x\right)\Psi(x,0)\,dx = \sqrt{\frac{2}{a}}\frac{Aa^2}{(n\pi)^2}\left(\sin\left(\frac{n\pi}{2}\right) - \frac{n\pi}{2}\cos\left(\frac{n\pi}{2}\right) + \sin(n\pi) - \sin\left(\frac{n\pi}{2}\right) - \frac{n\pi}{2}\cos\left(\frac{n\pi}{2}\right)\right)$$
$$= \sqrt{\frac{2}{a}}\frac{Aa^2}{(n\pi)^2}\left(\sin(n\pi) - n\pi\cos\left(\frac{n\pi}{2}\right)\right)$$

$$\Rightarrow c_1 = \sqrt{\frac{2}{a}}\frac{Aa^2}{\pi^2}(0 - \pi\cdot 0) = 0$$
$$c_2 = \sqrt{\frac{2}{a}}\frac{Aa^2}{4\pi^2}(0 - 2\pi\cdot -1) = \sqrt{\frac{2}{a}}\frac{Aa^2}{(n\pi)^2}(n\pi)$$
$$c_3 = \sqrt{2/a}\,\frac{Aa^2}{9\pi^2}(0 - 3\pi\cdot 0) = 0$$
$$c_4 = \sqrt{\frac{2}{a}}\frac{Aa^2}{16\pi^2}(0 - 4\pi\cdot 1) = -\sqrt{\frac{2}{a}}\frac{Aa^2}{n\pi}$$

$\Rightarrow$ if n is odd, $c_n = 0$
n is even, $c_n = \sqrt{\frac{2}{a}}\frac{Aa^2}{n\pi}\cos\left(\frac{n\pi}{2}\right)$

but $A = \frac{2\sqrt{3}}{\sqrt{a^3}}$ $\Rightarrow \sqrt{\frac{2}{a}}A = \sqrt{\frac{2}{a}}\frac{2\sqrt{3}a^2}{\sqrt{a^3}} = \sqrt{\frac{6}{a^4}}2a^2 = 2\sqrt{6}$

$$\Rightarrow c_n = \begin{cases} 0 & n \text{ odd} \\ \frac{2\sqrt{6}}{n\pi}\cos\left(\frac{n\pi}{2}\right) & n \text{ even} \end{cases}$$

c. By eq 2.20 in the textbook,

$|c_n|^2$ is the probability of getting the particular energy E_n.

$$\Rightarrow |c_n|^2 = \begin{cases} 0 & n \text{ odd} \\ \frac{24}{n^2\pi^2}\cos^2\left(\frac{n\pi}{2}\right) & n \text{ even} \end{cases}$$

Since $|c_n|^2$ is inversely proportional to n^2, lower energy states are more likely. Since the lowest state, $n=1$, has no probability, the next lowest, $n=2$, must be the most likely state.

$$|c_2|^2 = \frac{24}{4\pi^2}\cos^2(\pi) = \frac{6}{\pi^2} \simeq 0.61$$

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$$|c_2|^2 = \frac{24}{4\pi^2}\cos^2(\pi) = \frac{6}{\pi^2} \simeq 0.61$$

The E_2 value is thus

$$E_2 = \frac{4\pi^2\hbar^2}{2ma^2}$$

with a probability of approx 0.61.