

PHYS2901 Problem set 2

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Problem 3.4)

$$\begin{aligned}
 3.4) \quad & \frac{d}{dt} \int_{-\infty}^{\infty} \psi_1^*(x, t) \psi_2(x, t) dx = 0 \\
 & = \int_{-\infty}^{\infty} \frac{d}{dt} \psi_1^*(x, t) \psi_2(x, t) dx \\
 & \frac{d}{dt} \psi_1^*(x, t) \psi_2(x, t) = \frac{d\psi_1^*}{dt} \psi_2(x, t) + \frac{d\psi_2}{dt} \psi_1^*(x, t) \\
 & = \int_{-\infty}^{\infty} \frac{d\psi_1^*}{dt} \psi_2(x, t) + \frac{d\psi_2}{dt} \psi_1^*(x, t) dx \\
 & \frac{d\psi_1^*}{dt} = \frac{i\hbar}{2m} \frac{\partial^2 \psi_1^*}{\partial x^2} - \frac{i}{\hbar} V \psi_1^* \\
 & \frac{d\psi_2}{dt} = \frac{i\hbar}{2m} \frac{\partial^2 \psi_2}{\partial x^2} - \frac{i}{\hbar} V \psi_2 \\
 & = \int_{-\infty}^{\infty} \left(\frac{i\hbar}{2m} \frac{\partial^2 \psi_1^*}{\partial x^2} - \frac{i}{\hbar} V \psi_1^* \right) \psi_2 + \left(\frac{i\hbar}{2m} \frac{\partial^2 \psi_2}{\partial x^2} - \frac{i}{\hbar} V \psi_2 \right) \psi_1^* dx \\
 & \quad \text{cancel} \\
 & = \int_{-\infty}^{\infty} \left(\frac{i\hbar}{2m} \frac{\partial^2 \psi_1^*}{\partial x^2} \psi_2 - \frac{i\hbar}{2m} \frac{\partial^2 \psi_2}{\partial x^2} \psi_1^* \right) dx \\
 & \quad \text{Integrate by parts} \\
 & = \frac{i\hbar}{2m} \left(\left[\frac{\partial \psi_1^*}{\partial x} \psi_2 \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{\partial \psi_1^*}{\partial x} \frac{\partial \psi_2}{\partial x} dx - \left[\frac{\partial \psi_2}{\partial x} \psi_1^* \right]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \frac{\partial \psi_2}{\partial x} \frac{\partial \psi_1^*}{\partial x} dx \right) \\
 & = 0 \quad \text{QED}
 \end{aligned}$$

Problem 3.5)

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By first rearranging Schrödinger's equation, we find:

$$i\hbar \frac{\partial \Psi(x)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x)}{\partial x^2} + V \Psi(x)$$

As $\Psi(x)$ is time independent:

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

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

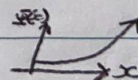
For the case $E < V_{\min}$, we find:

$$\frac{d^2 \Psi(x)}{dx^2} = \overset{\text{positive}}{\text{negative}} \quad \text{as } \frac{-2m}{\hbar^2} (E - V(x)) \text{ is } \overset{\text{positive}}{\text{negative}}.$$

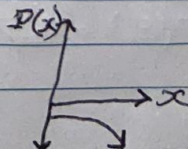
As $\frac{d^2 \Psi(x)}{dx^2}$ and $\Psi(x)$ ^{now} share the same

sign, regardless of whether it is negative or positive, $\Psi(x)$ will never converge to 0 as $x \rightarrow \infty$. To show this:

($\Psi(x)$ is positive): The function will be positive with a concave up motion:



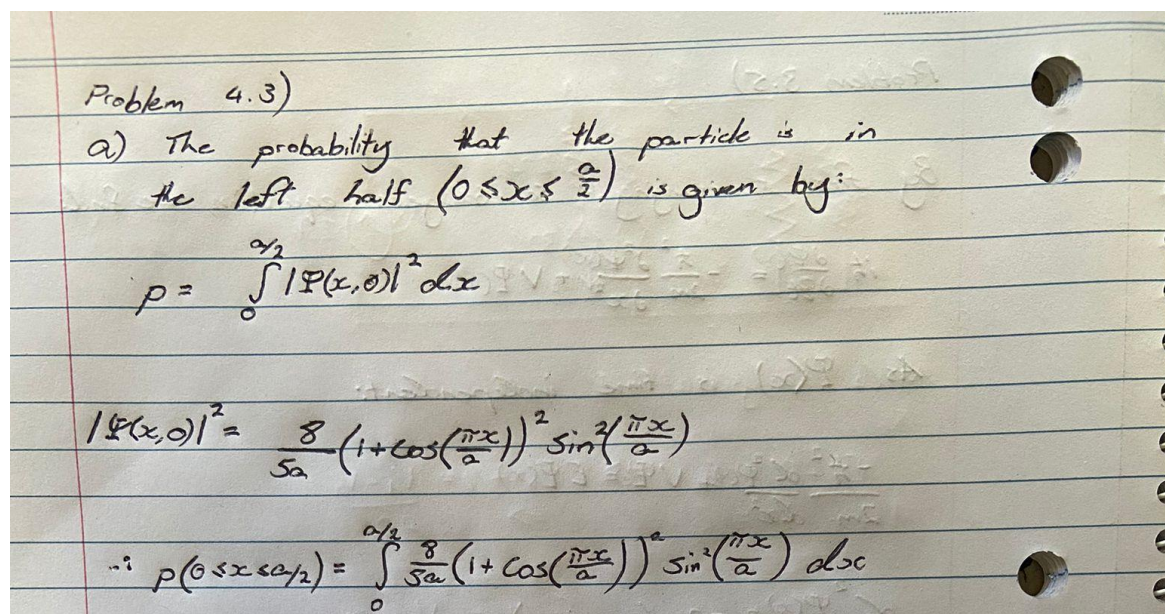
($\Psi(x)$ is negative): The function will be negative with a concave down motion:



Quantum vs Classical:

We have already investigated the case where a particle's energy is less than the minimum potential of $V(x)$, in which case, we found the wave function is not normalisable. This indicates that the energy of a particle must be greater than the minimum potential in order for its wavefunction to be normalisable. However, I now want you to consider the case where the energy of a particle is directly equal to the minimum potential. In such a case, there is the possibility for the energy of the particle to equal the minimum potential of $V(x)$. This indicates that somewhere in the square well, the particle may be stationary. However, we know this to violate Heisenberg's Uncertainty Principle, and as such, similarly proves that E must be greater than V_{\min} . However, in classical mechanics, the kinetic energy of an object can indeed be 0, thus we observe a major difference between classical and quantum mechanics.

Problem 4.3)



Problem 4.3)

a) The probability that the particle is in the left half ($0 \leq x \leq \frac{a}{2}$) is given by:

$$p = \int_0^{a/2} |\Psi(x,0)|^2 dx$$
$$|\Psi(x,0)|^2 = \frac{8}{5a} \left(1 + \cos\left(\frac{\pi x}{a}\right)\right)^2 \sin^2\left(\frac{\pi x}{a}\right)$$
$$\therefore p(0 \leq x \leq a/2) = \int_0^{a/2} \frac{8}{5a} \left(1 + \cos\left(\frac{\pi x}{a}\right)\right)^2 \sin^2\left(\frac{\pi x}{a}\right) dx$$

First, we further simplify the expression under the integral.

$$\begin{aligned}
 &= \frac{8}{5a} \left(1 + \cos\left(\frac{x\pi}{a}\right)\right)^2 \left(1 - \cos^2\left(\frac{x\pi}{a}\right)\right) \\
 &= \frac{8}{5a} \left(1 + 2\cos\left(\frac{x\pi}{a}\right) + \cos^2\left(\frac{x\pi}{a}\right)\right) \left(1 - \cos^2\left(\frac{x\pi}{a}\right)\right) \\
 &= \frac{8}{5a} \left(1 - \cos^2\left(\frac{x\pi}{a}\right) + 2\cos\left(\frac{x\pi}{a}\right) - 2\cos^3\left(\frac{x\pi}{a}\right) + \cos^2\left(\frac{x\pi}{a}\right) - \cos^4\left(\frac{x\pi}{a}\right)\right) \\
 &= \frac{8}{5a} \left(1 + 2\cos\left(\frac{x\pi}{a}\right) - 2\cos^3\left(\frac{x\pi}{a}\right) - \cos^4\left(\frac{x\pi}{a}\right)\right)
 \end{aligned}$$

This leaves:

$$\begin{aligned}
 &= \frac{8}{5a} \left(\int_0^{a/2} 1 dx + 2 \int_0^{a/2} \cos\left(\frac{\pi x}{a}\right) dx - 2 \int_0^{a/2} \cos^3\left(\frac{\pi x}{a}\right) dx - \int_0^{a/2} \cos^4\left(\frac{\pi x}{a}\right) dx \right) \\
 &= 0.8395
 \end{aligned}$$

Thus there is a ^{83.95}~~83.95~~% chance of finding it in the first half of the box.

b)

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

Notice that $\sin(2A) = 2\sin(A)\cos(A)$ Thus:

$$\Psi(x,0) = \sqrt{\frac{8}{5a}} \sin\left(\frac{\pi x}{a}\right) + \frac{1}{2} \sqrt{\frac{8}{5a}} \sin\left(\frac{2\pi x}{a}\right)$$

Given the two facts:

$$\Psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \text{ where } n=1,2,3,\dots$$

$$E = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

We know:

$$\sqrt{\frac{8}{5a}} \sin\left(\frac{\pi x}{a}\right) : \quad \frac{1}{2} \sqrt{\frac{8}{5a}} \sin\left(\frac{2\pi x}{a}\right) :$$

$$n=1$$

$$E_1 = \frac{\pi^2 \hbar^2}{2ma^2}$$

$$n=2$$

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

$$P(E_1) = |C|^2 = \frac{8}{5a}$$

$$P(E_2) = |k|^2 = \frac{8}{20a} = \frac{2}{5a}$$

$$\text{Since } P(E_1) + P(E_2) = 1 = \frac{8}{5a} + \frac{2}{5a}$$

$$\therefore P(E_1) = 4P(E_2) \text{ Thus}$$

$$E_1 = \frac{\pi^2 \hbar^2}{2ma^2}$$

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

$$P(E_1) = 0.8$$

$$P(E_2) = 0.2$$

c)

To solve for $\sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \psi_n(x) \Psi(x,0) dx$ we must remember the following:

$$\Psi(x,0) = \sum_{n=1}^{\infty} C_n \psi_n(x)$$

$$C_n = \int_{-\infty}^{\infty} \psi_n(x) \Psi(x,0) dx$$

Given $|C_n|^2$ is the probability that the wave function depicts some given $\psi_n(x)$, we know over a complete basis of eigenfunctions that:

$$\sum_{n=1}^{\infty} |C_n|^2 = 1$$

Thus we ~~notice~~ notice that.

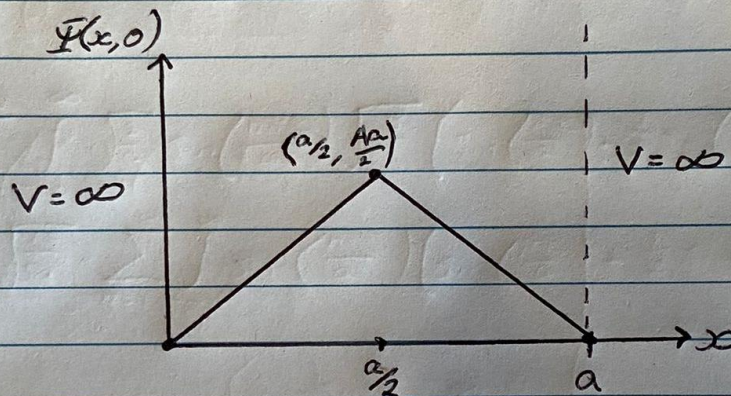
$$\sum_{n=1}^{\infty} C_n = \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \psi_n(x) \Psi(x,0) dx$$

In the same way that the sum of C_n squared ~~is~~ equalling 1 indicates that the particle must be somewhere, the sum of all projections of $\psi_n(x)$ onto $\Psi(x,0)$ must be 1 as by definition $\psi_n(x)$ forms a complete basis and $\Psi(x,0)$ is normalised.

Problem 4.4)

a)

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



To determine A , we recall:

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx \\ &= \int_0^{a/2} A^2 x^2 dx + \int_{a/2}^a A^2 (a-x)^2 dx \\ \frac{1}{A^2} &= \left[\frac{x^3}{3} \right]_0^{a/2} + \int_{a/2}^a (x^2 - 2ax + a^2) dx \\ &= \frac{1}{3} \left(\frac{a}{2} \right)^3 - 0 + \left[\frac{x^3}{3} - ax^2 + a^2 x \right]_{a/2}^a \\ &= \frac{a^3}{24} + \frac{a^3}{3} - a^3 + a^3 - \frac{1}{3} \left(\frac{a}{2} \right)^3 + a \left(\frac{a}{2} \right)^2 - a^2 \left(\frac{a}{2} \right) \\ &= \frac{a^3}{24} + \frac{a^3}{3} - \frac{a^3}{24} + \frac{a^3}{4} - \frac{a^3}{8} \\ &= \frac{a^3}{3/2} = \frac{1}{A^2} \quad \Rightarrow \quad A = \frac{2\sqrt{3}}{a^{3/2}} \end{aligned}$$

b) Given: $\Psi(x,0) = \sum_{n=1}^{\infty} C_n \Psi_n(x)$ and

$$C_n = \int_{-\infty}^{\infty} \Psi_n^* \Psi(x,0) dx$$

$$\Psi_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$$

Thus for $0 \leq x \leq \frac{a}{2}$ we find:

$$C_n = \int_0^{a/2} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) Ax dx$$

Integrate by parts: $u = Ax$ $du = A$

$$\frac{dv}{dx} = \sin\left(\frac{n\pi x}{a}\right) \quad v = \frac{-a}{n\pi} \cos\left(\frac{n\pi x}{a}\right)$$

$$= \left[\frac{-a}{n\pi} \cos\left(\frac{n\pi x}{a}\right) Ax \right]_0^{a/2} - \int_0^{a/2} A \frac{-a}{n\pi} \cos\left(\frac{n\pi x}{a}\right) dx$$

$$= \frac{-a}{n\pi} \cos\left(\frac{n\pi}{2}\right) \frac{Aa}{2} + \left[\frac{Aa^2}{n\pi^2} \sin\left(\frac{n\pi x}{a}\right) \right]_0^{a/2}$$

$$= \frac{Aa^2}{2n\pi} \cos\left(\frac{n\pi}{2}\right) + \frac{Aa^2}{n\pi^2} \sin\left(\frac{n\pi}{2}\right) - \frac{Aa^2}{n\pi^2} \sin\left(\frac{n\pi}{2}\right)$$

$$C_n = \left(\frac{-Aa^2}{2n\pi} \cos\left(\frac{n\pi}{2}\right) + \frac{Aa^2}{n^2\pi^2} \sin\left(\frac{n\pi}{2}\right) \right) \sqrt{\frac{2}{a}}$$

$$= A\sqrt{\frac{2}{a}} \left(\frac{a^2}{n^2\pi^2} \sin\left(\frac{n\pi}{2}\right) - \frac{a^2}{2n\pi} \cos\left(\frac{n\pi}{2}\right) \right)$$

Now for $a/2 \leq x \leq a$:

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

Integrate by parts: $u = A(a-x) \quad \frac{du}{dx} = -A$
 $\frac{dv}{dx} = \sin\left(\frac{n\pi x}{a}\right) \quad v = \frac{a}{n\pi} \cos\left(\frac{n\pi x}{a}\right)$

$$\frac{C_n}{\sqrt{\frac{2}{a}}} = \left[A(a-x) \frac{a}{n\pi} \cos\left(\frac{n\pi x}{a}\right) \right]_{a/2}^a - \int_{a/2}^a -A \frac{a}{n\pi} \cos\left(\frac{n\pi x}{a}\right) dx$$

$$= 0 + \frac{Aa^2}{2n\pi} \cos\left(\frac{n\pi}{2}\right) - \left[\frac{Aa^2}{n^2\pi^2} \sin\left(\frac{n\pi x}{a}\right) \right]_{a/2}^a$$

$$= \frac{Aa^2}{2n\pi} \cos\left(\frac{n\pi}{2}\right) - \frac{Aa^2}{n^2\pi^2} \sin(n\pi) + \frac{Aa^2}{n^2\pi^2} \sin\left(\frac{n\pi}{2}\right)$$

$$= A\sqrt{\frac{2}{a}} \left(\frac{a^2}{2n\pi} \cos\left(\frac{n\pi}{2}\right) + \frac{Aa^2}{n^2\pi^2} \sin\left(\frac{n\pi}{2}\right) \right)$$

With this we can now conclude:

$$C_n = C_n(0 \leq x \leq a/2) + C_n(a/2 \leq x \leq a)$$

$$= A\sqrt{\frac{2}{a}} \left(\frac{a^2}{n^2\pi^2} \sin\left(\frac{n\pi}{2}\right) - \frac{a^2}{2n\pi} \cos\left(\frac{n\pi}{2}\right) + \frac{a^2}{2n\pi} \cos\left(\frac{n\pi}{2}\right) + \frac{a^2}{n^2\pi^2} \sin\left(\frac{n\pi}{2}\right) \right)$$

$$= A\sqrt{\frac{2}{a}} \left(\frac{2a^2}{n^2\pi^2} \sin\left(\frac{n\pi}{2}\right) \right)$$

C)

Given these series of coefficient C_n , we understand that the probability $P(E)$ will be largest for a number that maximises the $\frac{2a^2}{n^2\pi^2}$ and $\sin\left(\frac{n\pi}{2}\right)$ terms given $P(E_n) = |C_n|^2$. This, by observation, indicates that the most probable energy level will be $n = 1$ which means:

$$E_1 = \frac{n^2\pi^2\hbar^2}{2ma^2} = \frac{\pi^2\hbar^2}{2ma^2}$$