PHY F242 QUANTUM MECH I

ASSIGNMENT-01

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Q :

Given a 1D electron in a box of length a = 0.1m, the wavefunction is made up of three stationary states defined by n1, n2 and n3. Find the wavefunction of the electron and plot the following :

- Ψ(x, 0) vs x
- Ψ(x, t) vs x for a given time t
- $|\Psi(x, 0)|^2$ vs x
- $|\Psi(x, t)|^2$ vs x

SOL:

The wavefunction for electron in nth stationery state is :

$$\psi_n(x,t) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)e^{-\frac{iE_n t}{\hbar}} \quad ; \quad E_n = \frac{n^2\pi^2\hbar^2}{2ma}$$

Where, E_n = energy associated with nth state
a = length of the box = 0.1m
m = mass of electron = 9.109×10^{-31}kg
ħ = (modified) Planck's constant = 1.054×10^{-34} J.s

General expression for wavefunction of *k* (here, k =3) number of stationery states is :

$$\psi_n(x,t) = \sum_{k=1}^{3} c_k \sqrt{\frac{2}{a}}\sin\left(\frac{n_k\pi x}{a}\right)e^{-\frac{iE_{n_k} t}{\hbar}}$$

Where, $c_k \in \mathbb{C}$ *(constant).*

Now, we know that for the set of coefficients $\{c_1, c_2, c_3\}$,

$$\sum_{k=1}^{3} |c_k|^2 = 1$$

Assuming that coefficients are equal, i.e. $c_1 = c_2 = c_3 = c$ (say), we get

$$|c|^2+|c|^2+|c|^2 = 1$$

$$3|c|^2 = 1$$

$$|c| = \frac{1}{\sqrt{3}}$$

Assuming that $c \in \mathbb{R}$ *(real)*, we get $c = \frac{1}{\sqrt{3}}$.

Given: $n_1 = 14$, $n_2 = 12$, $n_3 = 17$ the 14^{th},12^{th} and 17^{th} stationery states are:

$$\psi_{14}(x,t) = \sqrt{20}\sin(140\pi x)\, e^{-\frac{iE_{14}t}{\hbar}} \quad ; \quad E_{14} = \frac{980\,\pi^2\hbar^2}{m}$$

$$\psi_{12}(x,t) = \sqrt{20}\sin(120\pi x)\, e^{-\frac{iE_{12}t}{\hbar}} \quad ; \quad E_{12} = \frac{720\,\pi^2\hbar^2}{m}$$

$$\psi_{17}(x,t) = \sqrt{20}\sin(170\pi x)\, e^{-\frac{iE_{17}t}{\hbar}} \quad ; \quad E_{17} = \frac{1445\,\pi^2\hbar^2}{m}$$

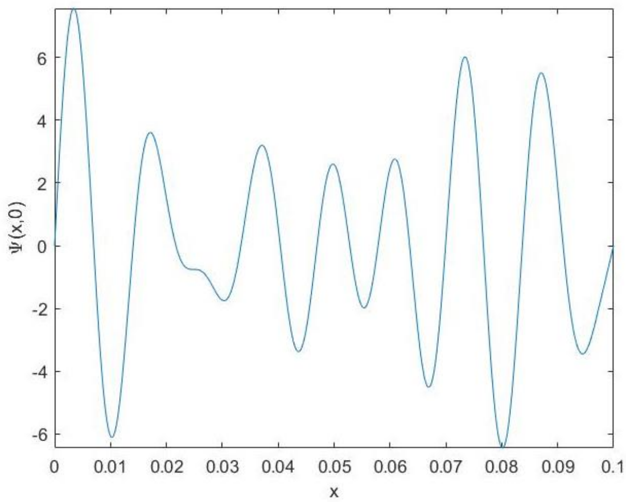
Thus,

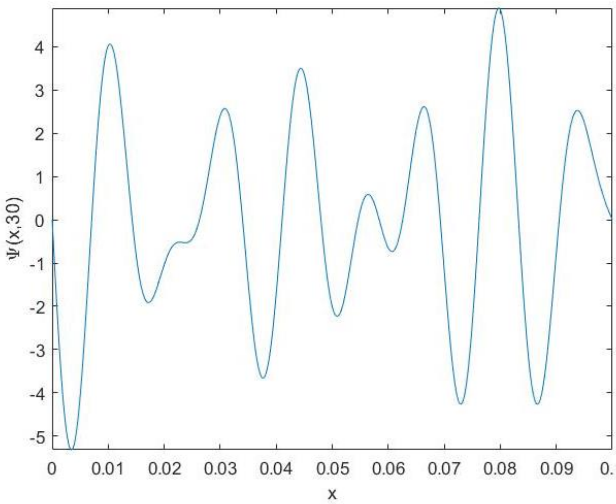
- $\psi(x,0) = \frac{1}{\sqrt{3}}(\sqrt{20}\sin(140\pi x) + \sqrt{20}\sin(120\pi x) + \sqrt{20}\sin(170\pi x))$
- $\psi(x,t) = \frac{1}{\sqrt{3}}\Re e[\sqrt{20}\sin(140\pi x)e^{-\frac{iE_{14}t}{\hbar}} + \sqrt{20}\sin(120\pi x)e^{-\frac{iE_{12}t}{\hbar}} + \sqrt{20}\sin(170\pi x)\, e^{-\frac{iE_{17}t}{\hbar}}]$

(For $\psi(x,t)$, only the real part of the wavefunction has been considered for plotting.)

- $|\psi(x,0)|^2 = \frac{20}{3}(\sin(140\pi x) + \sin(120\pi x) + \sin(170\pi x))^2$
- $|\psi(x,t)|^2 = \frac{20}{3}\Re e[\sin(140\pi x)e^{-\frac{iE_{14}t}{\hbar}} + \sin(120\pi x)e^{-\frac{iE_{12}t}{\hbar}} + \sin(170\pi x)\, e^{-\frac{iE_{17}t}{\hbar}}]^2$

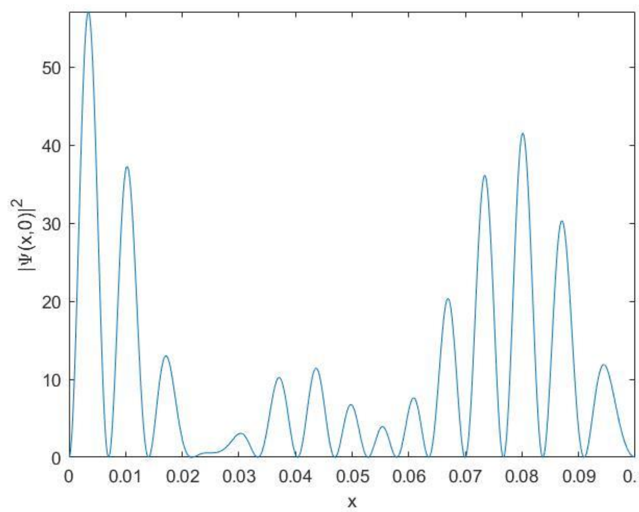
The wavefunctions were plotted using MATLAB, and the following were obtained.

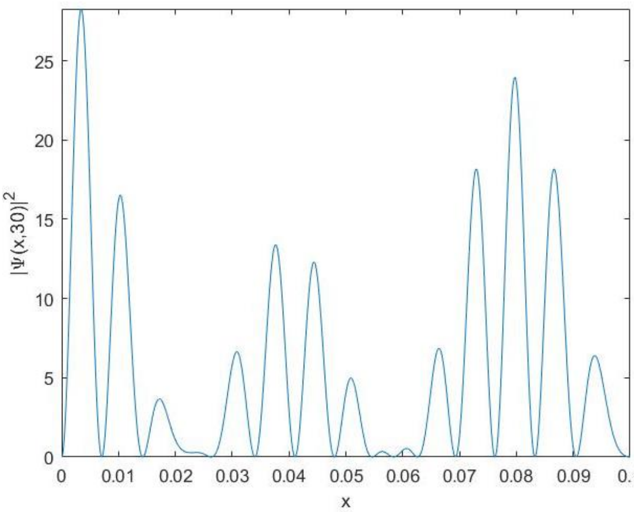




Ψ(x, 0) vs x

Ψ(x, t) vs x, for t = 30s





$|\Psi(x, 0)|^2$ vs x

$|\Psi(x, t)|^2$ vs x, for t = 30s

APPENDIX

MATLAB code :

```
x = 0:0.001:0.1;
a=0.1;                        %length of the box
m=9.102*10^-31;               %mass of electron
hbar = (6.602*10^-34)/(2*pi); %Planck's constant

syms psi(x,t)                 %create a function psi(x,t)
psi(x,t) = sqrt(1/3)*sqrt(2/a)*sin(14*pi*x/a)*exp((-i*(14^2)*(pi^2)*hbar*t)
/(2*m*a^2))) + sqrt(1/3)*sqrt(2/a)*sin(12*pi*x/a)*exp((-i*(122^2)*(pi^2)
*hbar*t)/(2*m*(a^2))) + sqrt(1/3)*sqrt(2/a)*sin(17*pi*x/a)*exp((-i*(17^2)
*(pi^2)*hbar*t)/(2*m*(a^2))); %define psi

fplot (psi(x,0), [0 0.1]), xlabel('x'), ylabel('\Psi(x,0)')
                              %plot psi(x,t) vs x for diff values of t; add
                              axis labels
fplot (real(psi(x,30)), [0 0.1]), xlabel('x'), ylabel('\Psi(x,30)')
fplot (abs(psi(x,0))^2, [0 0.1]), xlabel('x'), ylabel('|\Psi(x,0)|^{2}')
fplot (abs(real(psi(x,30)))^2, [0 0.1]), xlabel('x'),
ylabel('|\Psi(x,30)|^{2}')
```