PEU 323 Assignment 4

Mohamed Hussien El-Deeb (201900052)

Contents

1 Problem 1

(a) Yes, this wave function is physically acceptable if the normalization constant A is chosen such that $\int_{-a}^{a} |\psi(x)|^2 \, dx = 1$. The wave function is continuous and single-valued within $[-a, a]$, meeting the requirements for physical acceptability.

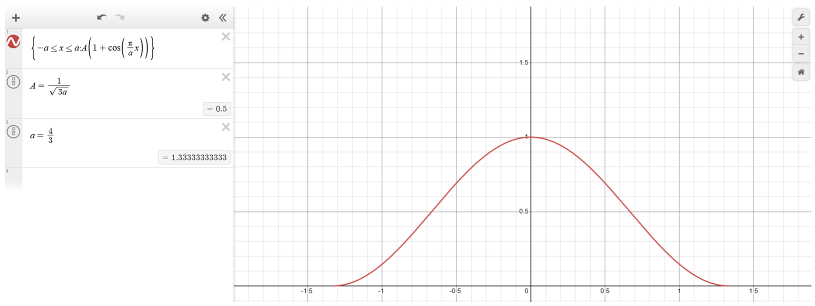


Figure 1: ψ

(b) The classically allowed region is:

$$[-a, a]$$

since the wave function $\psi(x) = 0$ outside this interval, meaning the classical particle cannot be found outside $[-a, a]$.

2 Problem 2

(a)

$$\psi(x,t) = \sin\left(\frac{n\pi}{a}x\right)e^{-i\omega t}$$

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

$$\begin{aligned}
V(x)\psi &= \frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + i\hbar\frac{\partial\psi}{\partial t} \\
&= \frac{\hbar^2}{2m}\frac{\partial^2(\sin\left(\frac{n\pi}{a}x\right))}{\partial x^2}e^{-i\omega t} + i\hbar\sin\left(\frac{n\pi}{a}x\right)\frac{\partial(e^{-i\omega t})}{\partial t} \\
&= -\frac{\hbar^2 n^2\pi^2}{2ma^2}\sin\left(\frac{n\pi}{a}x\right)e^{-i\omega t} + \omega\hbar\sin\left(\frac{n\pi}{a}x\right)e^{-i\omega t} \\
&= (\omega\hbar - \frac{\hbar^2 n^2\pi^2}{2ma^2})\sin\left(\frac{n\pi}{a}x\right)e^{-i\omega t} \\
&= (\omega\hbar - \frac{\hbar^2 n^2\pi^2}{2ma^2})\psi \\
V &= \omega\hbar - \frac{\hbar^2 n^2\pi^2}{2ma^2}
\end{aligned}$$

(b) To find the expectation value $\langle x\rangle$, we observe that the term $\sin^2\left(\frac{n\pi}{a}x\right)$ is symmetric around $x = \frac{a}{2}$. By shifting the domain of $\psi(x)$ as $\psi(x) \to \psi\left(x - \frac{a}{2}\right)$, we redefine the domain as $-\frac{a}{2} \leq x \leq \frac{a}{2}$.

Under this transformation, the shifted wave function becomes an even function, while x (as a variable) is odd with respect to $x = 0$. As a result, the integrand for $\langle x'\rangle = \int_{-\frac{a}{2}}^{\frac{a}{2}} x'|\psi(x')|^2\,dx'$ is an odd function over a symmetric interval, leading to:

$$\langle x'\rangle = 0.$$

To obtain $\langle x\rangle$ in the original coordinates, we perform the inverse transformation $x' = x - \frac{a}{2}$, which implies $x = x' + \frac{a}{2}$. Thus:

$$\langle x\rangle = \langle x' + \frac{a}{2}\rangle = \langle x'\rangle + \frac{a}{2} = 0 + \frac{a}{2} = \frac{a}{2}.$$

Therefore, the average position of the particle is:

$$\langle x\rangle = \frac{a}{2}.$$

3 Problem 3

Fourier transform:

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x) e^{-ikx} \, dx$$

Inverse Fourier transform:

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx} \, dk$$

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^*(x) \left(-i\hbar \frac{d}{dx} \right) \psi(x) \, dx$$

$$\langle p \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \phi^*(k') e^{-ik'x} \, dk' \left(-i\hbar \frac{d}{dx} \right) \int_{-\infty}^{\infty} \phi(k) e^{ikx} \, dk \, dx$$

$$-i\hbar \frac{d}{dx} e^{ikx} = \hbar k e^{ikx}$$

$$\langle p \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \phi^*(k') \phi(k) \hbar k \left(\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(k-k')x} \, dx \right) dk' \, dk$$

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(k-k')x} \, dx = \delta(k - k')$$

$$\langle p \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \phi^*(k') \phi(k) \hbar k \delta(k - k') \, dk' \, dk$$

$$\therefore \langle p \rangle = \int_{-\infty}^{\infty} \hbar k |\phi(k)|^2 \, dk$$

where $|\phi(k)|^2$ represents the probability density in k-space and $\hbar k$ is the momentum associated with each k.

4 Problem 4

(a) If a system is in a pure energy eigenstate, its time evolution is given by:

$$\psi(x,t) = \psi(x,0)e^{-iEt/\hbar}$$

$$\psi(x,t+T) = \psi(x,t)$$

$$\psi(x,0)e^{-iE(t+T)/\hbar} = \psi(x,0)e^{-iEt/\hbar}$$

$$\therefore e^{-iET/\hbar} = 1$$

$$\therefore \frac{ET}{\hbar} = 2\pi n, \quad n \in \mathbb{N}$$

$$T = \frac{2\pi\hbar}{E}n$$

(b)

$$E = \frac{2\pi\hbar}{T}n$$

(c) For a particle in an infinite square well

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

$$T = \frac{2\pi\hbar}{E_n}n = \frac{4m}{n\pi\hbar}L^2$$

5 Problem 5

The wave function stays undisturbed (the same) after the sudden expansion

$$\psi_0 = \sqrt{\frac{2}{L}} \cos\left(\frac{\pi}{L}x\right), \quad -\frac{L}{2} \leq x \leq \frac{L}{2}$$

The new ground state:

$$\psi_0' = \sqrt{\frac{1}{L}} \cos\left(\frac{\pi}{2L}x\right), \quad -L \leq x \leq L$$

$$\begin{aligned}
\langle \psi | \psi_0' \rangle &= \frac{\sqrt{2}}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \cos\left(\frac{\pi}{2L}x\right) \cos\left(\frac{\pi}{L}x\right) dx \\
&= \frac{\sqrt{2}}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \cos\left(\frac{\pi}{2L}x\right)\left[1 - 2\sin^2\left(\frac{\pi}{2L}x\right)\right] dx \\
&= \frac{\sqrt{2}}{L} \left[\frac{2L}{\pi} \sin\left(\frac{\pi}{2L}x\right) - \frac{4L}{3\pi} \sin^3\left(\frac{\pi}{2L}x\right)\right]_{-\frac{L}{2}}^{\frac{L}{2}} \\
&= \frac{2\sqrt{2}}{\pi} \left[\sin\left(\frac{\pi}{2L}x\right) - \frac{2}{3} \sin^3\left(\frac{\pi}{2L}x\right)\right]_{-\frac{L}{2}}^{\frac{L}{2}} \\
&= \frac{8}{3\pi}
\end{aligned}$$

$$P = |\langle \psi | \psi_0' \rangle|^2 = \left|\frac{8}{3\pi}\right|^2 = \frac{64}{9\pi^2}$$

6 Problem 6

(a)

$$V(x) = \begin{cases} 0 & \text{if } -a_0 \leq x \leq -a_0 \\ V_0 & otherwise \end{cases}$$

$$\text{where } V_0 = 20eV$$

$$m = 9.109 \times 10^{-31} kg$$

$$\hbar = 1.05457182 \times 10^{-34} m^2 kg/s$$

$$a = 2a_0, \quad a_0 = 0.529 \times 10^{-10} m$$

For bound states,

$$0 < E < V_0$$

For $-\infty \leq x \leq -a_0, \quad a_0 \leq x \leq \infty$:

Schrodinger equation:

$$\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} = -(E - V_0)\psi$$

$$\frac{\partial^2 \psi}{\partial x^2} = l^2 \psi$$

$$\text{where } l = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

$$\psi_1 = Ae^{lx} + Be^{-lx}$$

$$\psi_3 = Ee^{lx} + Fe^{-lx}$$

For $-a_0 \leq x \leq a_0$:

Schrodinger equation:

$$\frac{\partial^2\psi}{\partial x^2} = -\frac{2mE}{\hbar^2}\psi$$

$$\frac{\partial^2\psi}{\partial x^2} = -k^2\psi$$

$$\text{where } k = \frac{\sqrt{2mE}}{\hbar}$$

$$\psi_2 = C\sin(kx) + D\cos(kx)$$

$$\alpha \equiv \frac{l}{k} = \sqrt{\frac{V_0}{E} - 1}, \quad \alpha > 0$$

Our ψ now is:

$$\therefore \psi(x) = \begin{cases} Ae^{lx} + Be^{-lx} & \text{if } -\infty < x < -a_0 \\ C\sin(kx) + D\cos(kx) & \text{if } -a_0 \leq x \leq a_0 \\ Ee^{lx} + Fe^{-lx} & \text{if } a_0 < x < \infty \end{cases}$$

$$\therefore \psi'(x) = \begin{cases} l(Ae^{lx} - Be^{-lx}) & \text{if } -\infty < x < -a_0 \\ k(C\cos(kx) - D\sin(kx)) & \text{if } -a_0 \leq x \leq a_0 \\ l(Ee^{lx} - Fe^{-lx}) & \text{if } a_0 < x < \infty \end{cases}$$

By applying the boundary conditions:

$$\psi(x = -\infty) = 0 \implies B = 0$$

$$\psi(x = \infty) = 0 \implies E = 0$$

$$\psi(x = -a_0) \implies Ae^{-la_0} = D\cos(ka_0) - C\sin(ka_0) \tag{1}$$

$$\psi(x = a_0) \implies Fe^{-la_0} = C\sin(ka_0) + D\cos(ka_0) \tag{2}$$

$$\psi'(x = -a_0) \implies Ae^{-la_0} = \frac{k}{l}(C\cos(ka_0) + D\sin(ka_0)) \tag{3}$$

$$\psi'(x = a_0) \implies Fe^{-la_0} = \frac{k}{l}(D\sin(ka_0) - C\cos(ka_0)) \tag{4}$$

$$\begin{pmatrix} e^{-la_0} & \sin(ka_0) & -\cos(ka_0) & 0 \\ e^{-la_0} & -\frac{k}{l}\cos(ka_0) & -\frac{k}{l}\sin(ka_0) & 0 \\ 0 & -\sin(ka_0) & -\cos(ka_0) & e^{-la_0} \\ 0 & \frac{k}{l}\cos(ka_0) & -\frac{k}{l}\sin(ka_0) & e^{-la_0} \end{pmatrix} \begin{pmatrix} A \\ C \\ D \\ F \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 & \sin(ka_0)e^{la_0} & -\cos(ka_0)e^{la_0} & 0 \\ e^{-la_0} & -\frac{k}{l}\cos(ka_0) & -\frac{k}{l}\sin(ka_0) & 0 \\ 0 & -\sin(ka_0) & -\cos(ka_0) & e^{-la_0} \\ 0 & \frac{k}{l}\cos(ka_0) & -\frac{k}{l}\sin(ka_0) & e^{-la_0} \end{pmatrix}$$

$$\begin{pmatrix} 1 & \sin(ka_0)e^{la_0} & -\cos(ka_0)e^{la_0} & 0 \\ 0 & \frac{k}{l}\cos(ka_0) & -\frac{k}{l}\sin(ka_0) & e^{-la_0} \\ 0 & \sin(ka_0) & \cos(ka_0) & -e^{-la_0} \\ 0 & \sin(ka_0) + \frac{k}{l}\cos(ka_0) & \frac{k}{l}\sin(ka_0) - \cos(ka_0) & 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 & \sin(ka_0)e^{la_0} & -\cos(ka_0)e^{la_0} & 0 \\ 0 & 1 & -\tan(ka_0) & \frac{l}{k}\frac{e^{-la_0}}{\cos(ka_0)} \\ 0 & \sin(ka_0) & \cos(ka_0) & -e^{-la_0} \\ 0 & \sin(ka_0) + \frac{k}{l}\cos(ka_0) & \frac{k}{l}\sin(ka_0) - \cos(ka_0) & 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 & \sin(ka_0)e^{la_0} & -\cos(ka_0)e^{la_0} & 0 \\ 0 & 1 & -\tan(ka_0) & \frac{l}{k}\frac{e^{-la_0}}{\cos(ka_0)} \\ 0 & 0 & 1 & -\frac{e^{-la_0}}{\cos(ka_0)}\frac{1+\frac{l}{k}\tan(ka_0)}{1+\tan^2(ka_0)} \\ 0 & \sin(ka_0) + \frac{k}{l}\cos(ka_0) & \frac{k}{l}\sin(ka_0) - \cos(ka_0) & 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 & \sin(ka_0)e^{la_0} & -\cos(ka_0)e^{la_0} & 0 \\ 0 & 1 & -\tan(ka_0) & \frac{l}{k}\frac{e^{-la_0}}{\cos(ka_0)} \\ 0 & 0 & 1 & -\frac{e^{-la_0}}{\cos(ka_0)}\frac{1+\frac{l}{k}\tan(ka_0)}{1+\tan^2(ka_0)} \\ 0 & 0 & 1 & -\frac{(\frac{l}{k}\tan(ka_0)+1)e^{-la_0}}{(\tan(ka_0)+2\frac{k}{l})\sin(ka_0)-\cos(ka_0)} \end{pmatrix}$$

$$A + \sin(ka_0)e^{la_0}C - \cos(ka_0)e^{la_0}D = 0$$

$$C - \tan(ka_0)D + \frac{l}{k}\frac{e^{-la_0}}{\cos(ka_0)}F = 0$$

$$D - \frac{e^{-la_0}}{\cos(ka_0)}\frac{1+\frac{l}{k}\tan(ka_0)}{1+\tan^2(ka_0)}F = 0$$

$$A = (\cos(2ka_0) + \frac{l}{k}\sin(2ka_0))F$$

$$C = e^{-la_0}(\sin(ka_0) - \frac{l}{k}\cos(ka_0))F$$

$$D = e^{-la_0}(\cos(ka_0) + \frac{l}{k}\sin(ka_0))F$$

We want the last two rows to be linearly dependent in order to have more than the trivial solution.

$$-\frac{e^{-la_0}}{\cos(ka_0)}\frac{1+\frac{l}{k}\tan(ka_0)}{1+\tan^2(ka_0)} = -\frac{(\frac{l}{k}\tan(ka_0)+1)e^{-la_0}}{(\tan(ka_0)+2\frac{k}{l})\sin(ka_0)-\cos(ka_0)}$$

For this equation to hold either $1 + \frac{l}{k}\tan(ka_0) = 0$

$$\tan(ka_0) = -\frac{l}{k}$$

Or

$$1+\tan^2(ka_0) = (\tan(ka_0)+2\frac{k}{l})\tan(ka_0) - 1$$

$$\tan(ka_0) = \frac{l}{k}$$

So the general solution is

$$\tan(ka_0) = \pm\frac{l}{k}$$

$$k = \frac{\sqrt{2mE}}{\hbar}$$

$$l = \frac{\sqrt{2m(V_0-E)}}{\hbar}$$

$$\frac{l}{k} = \sqrt{\frac{V_0}{E}-1}$$

$$\tan(\frac{\sqrt{2mE}}{\hbar}a_0) = \pm\sqrt{\frac{V_0}{E}-1}$$

$$\text{let,} \quad z = \frac{\sqrt{2mE}}{\hbar}a_0$$

$$E = \frac{\hbar^2}{2ma_0^2} z^2$$

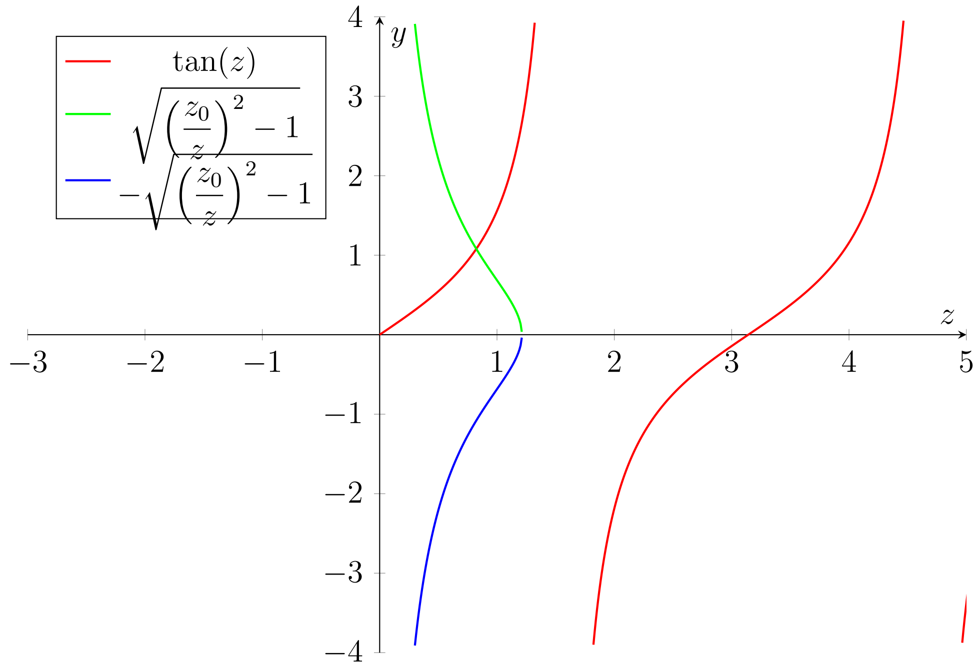
$$z_0 = \frac{\sqrt{2mV_0} a_0}{\hbar}$$

$$= \frac{\sqrt{2 \times 9.1093837 \times 10^{-31} kg \times 20 \times 1.60218 \times 10^{-19} kg \cdot m^2 \cdot s^{-2}} \times 0.529 \times 10^{-10} m}{1.05457182 \times 10^{-34} \frac{m^2 kg}{s}}$$

$$= 1.2120196376$$

$$\tan(z) = \pm\sqrt{(\frac{z_0}{z})^2 - 1}$$

Plot of $\tan(z)$ and $\pm\sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$



$$z \approx 0.82364$$

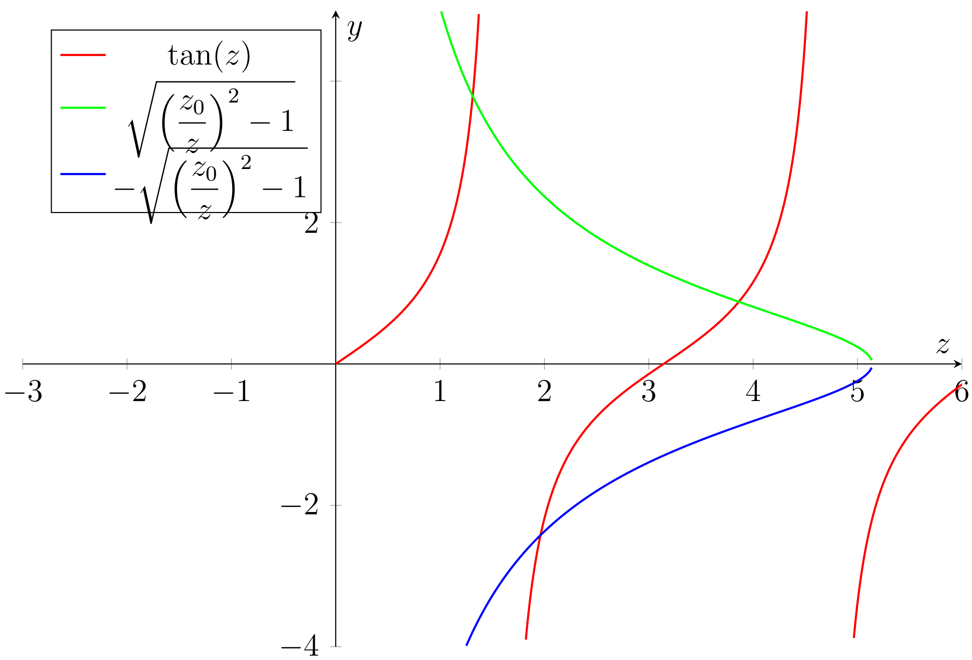
$$E \approx \frac{\hbar^2}{2ma_0^2}(0.82364)^2 = 13.6eV$$

$$l = 3.677188792 \times 10^{17}$$

$$k = 5.3603776075 \times 10^{17}$$

Plot of $\tan(z)$ and $\pm\sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$

(b)



$$z \approx 1.31266, 3.86258, 1.96234$$

References

[1] M.H. El-Deeb. PEU-323 Assignments.