Test 1 (17 April 2014)
ZCT 205 Quantum Mechanics

Name:

Matrix Number:

1. Solve the time independent Schroedinger equation

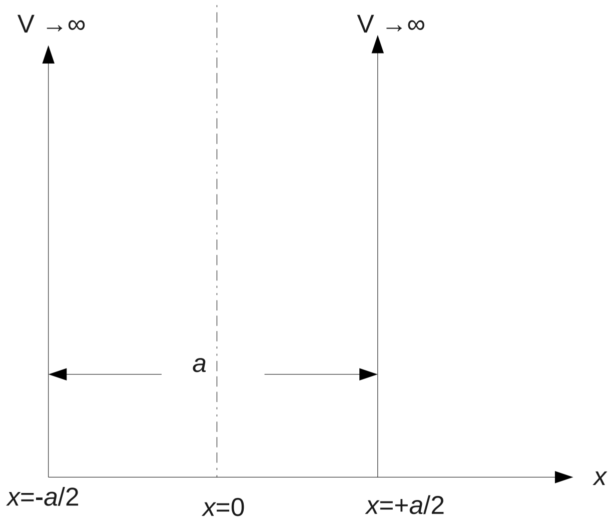
$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t)$$

for an infinite quantum well of the form

$$V(x) = \begin{cases} 0, & \text{if } -a/2 \le x \le a/2 \\ \infty, & \text{otherwise} \end{cases}$$

where initial profile of the wavefunction is

$$\Psi(x,0) = A(x-a/2)(x+a/2).$$



2. Create a table to compare the essential commonalities and differences between the TISE solutions of an infinite quantum well and that in a harmonic potential.

Solution for Q1

Total Solution $\Psi(x,t) = \sum_n C_n \psi_n(x) e^{-iE_n t/\hbar}$.

Need to know: ① $\psi_n(x)$; ② E_n; ③ C_n.

First, solve for $\psi_n(x)$, using TISE:

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

For $-\frac{a}{2} \leq x \leq \frac{a}{2}$, $V(x) = 0 \longrightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$

or $\frac{d^2\psi(x)}{dx^2} = -k^2\psi(x)$ — Eq(1)

where $k^2 = \frac{2mE}{\hbar^2}$, real & positive.

Solution to Eq(1) is $\psi(x) = G\cos kx + D\sin kx$

Boundary condition at $x = -a/2$: $\psi(-\frac{a}{2}) = 0$

$G\cos k(-a/2) + D\sin k(-\frac{a}{2}) = 0$

$G\cos\frac{ka}{2} - D\sin\frac{ka}{2} = 0$ — Eq(2)

note: $\cos(-x) = \cos x$, $\sin(-x) = -\sin x$

Boundary condition at $x = a/2$, $\psi(\frac{a}{2}) = 0$

$G\cos\frac{ka}{2} + D\sin\frac{ka}{2} = 0$ — Eq(3).

Eq(3) - Eq(2): $2D\sin\frac{ka}{2} = 0$

$D \neq 0$, $\frac{ka}{2} = \pi, 2\pi, 3\pi, 4\pi \ldots$

$k = \frac{2\pi}{a}, \frac{4\pi}{a}, \frac{6\pi}{a}, \ldots$

or $k_n = n\pi/a$; $n = 2, 4, 6 \ldots$ (even)

Eq(2) + Eq(3):

$2G\cos\frac{ka}{2} = 0$

$G \neq 0$, $\frac{ka}{2} = \frac{\pi}{2}, 3(\frac{\pi}{2}), 5(\frac{\pi}{2}), 7(\frac{\pi}{2}), \ldots$

or $k_n = n\pi/a$; $n = 1, 3, 5, 7, \ldots$ (odd)

$\therefore$ Solution to T.I.S.E is

$$\psi_n(x) = \begin{cases} \cancel{D \sin} \\ D \sin k_n x & ; k_n = \frac{n\pi}{a} ; n = 2, 4, 6 \ldots \text{(even)} \\ C \cos k_n x & ; k_n = \frac{n\pi}{a} ; n = 1, 3, 5, 7, \ldots \text{(odd)}. \end{cases}$$

Normalisation : $\displaystyle\int_{-a/2}^{a/2} \psi_n^2(x)\, dx = 1$

$$D^2 \int_{-a/2}^{a/2} \sin^2 k_n x = C^2 \int_{-a/2}^{a/2} \cos^2 k_n x = 1$$

$$(\sin^2 k_n x + \cos^2 k_n x) = 1$$

$$\int_{-a/2}^{a/2} \sin^2 k_n x\, dx + \int_{-a/2}^{a/2} \cos^2 k_n a\, dx = \int_{-a/2}^{a/2} 1 . dx = a$$

$$\therefore \int_{-a/2}^{a/2} \sin^2 k_n x\, dx = \int_{-a/2}^{a/2} \cos^2 k_n x\, dx = \frac{a}{2}$$

$$\Rightarrow D^2\left(\frac{a}{2}\right) = C^2\left(\frac{a}{2}\right) = 1$$

$$\Rightarrow D = C = \sqrt{\frac{2}{a}}$$

$$\therefore \psi_n(x) = \begin{cases} \sqrt{\frac{2}{a}} \sin \frac{k_n \pi}{2} & ; k_n = \frac{n\pi}{a} ; n = 2, 4, 6 \ldots \\ \sqrt{\frac{2}{a}} \cos \frac{k_n \pi}{2} & ; k_n = \frac{n\pi}{a} ; n = 1, 3, 5, 7 \ldots \end{cases}$$

$$\because k^2 = \frac{2mE}{\hbar^2} \Rightarrow E_n = \frac{k_n^2 \hbar^2}{2m} \; ; k_n = \frac{n\pi}{a} ; n = 1, 2, 3, 4 \ldots$$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \; ; n = 1, 2, 3, 4 \ldots$$

Solution for Q1 (cont.2)

Now, solve for C_n as in

$$\Psi(x,t) = \sum_n C_n \psi_n(x) e^{-iE_n t/\hbar}$$

set $t=0$,

$$\Psi(x,0) = \sum_n C_n \psi_n(x) = A(x-a/2)(x+a/2)$$

$$= A\left(x^2 - \frac{a^2}{4}\right)$$

Normalization $\int_{-a/2}^{a/2} |\Psi(x,0)|^2 dx = 1$

$$\therefore A^2 \int_{-a/2}^{a/2} \left(x^2 - \frac{a^2}{4}\right)^2 dx = 1$$

Solution for Q1 (cont.3)

$$A^2 \int_{-a/2}^{a/2} \left(x^2 - \frac{a^2}{4}\right)^2 dx = 1$$

$$A^2 \int_{-a/2}^{a/2} \left(x^4 - \frac{a^2x^2}{2} + \frac{a^4}{16}\right) dx = A^2 \left[\frac{x^5}{5} - \frac{a^2x^3}{6} + \frac{a^4}{16}x\right]_{-a/2}^{+a/2}$$

$$= \cancel{A^2 \left\{ -\frac{2a^5}{5.32} + 2\frac{a^2 a^3}{6.8} + \frac{2.a^4}{16}\left(\frac{a}{2}\right) \right.}$$

$$= -A^2 \left[\frac{-a^5}{5.32} + \frac{a^2}{6}\frac{a^3}{8} + \frac{a^4}{16}\cdot\left(\frac{-a}{2}\right) - \frac{a^5}{5.32} + \frac{a^2 a^3}{6.8} - \frac{a^4}{16}\left(\frac{a}{2}\right)\right]$$

$$= -A^2 \left[-\frac{a^5}{80} + \frac{a^5}{24} - \frac{a^5}{16} \right] = A^2 a^5 \left[+\frac{1}{30}\right] = \frac{A^2 a^5}{30} = 1$$

$$\Rightarrow \quad A = \sqrt{\frac{30}{a^5}}$$

Solution for Q1 (cont. 4)

(4)

$$\int_{-a/2}^{a/2} \varphi_m^*(x)\,\psi(x,0)\,dx = \int_{-\frac{a}{2}}^{\frac{a}{2}} \varphi_m^*(x)\,.\,\sum_n c_n \varphi_n(x)\,dx$$

$$= \sum_n c_n \overbrace{\int_{-a/2}^{a/2} \varphi_m^*(x)\varphi_n(x)\,dx}^{\text{orthonormality}} = \sum_n c_n \delta_{m,n} = c_m$$

$$\therefore\; c_m = \int_{-\frac{a}{2}}^{a/2} \varphi_m^*(x)\,\psi(x,0)\,dx$$

$$= \int_{-\frac{a}{2}}^{a/2} \varphi_m^*(x)\,.\,A\left(x^2-\frac{a^2}{4}\right)dx = A\int_{-\frac{a}{2}}^{a/2} \varphi_m^*(x)\left(x^2-\frac{a^2}{4}\right)dx$$

m odd, $c_m = A\int_{-\frac{a}{2}}^{a/2} \sqrt{\frac{2}{a}} \cos \frac{k_n x}{2}\,.\left(x^2-\frac{a^2}{4}\right)$; $k_n = 1,3,5\ldots$

m even, $c_m = A\int_{-\frac{a}{2}}^{a/2} \sqrt{\frac{2}{a}} \sin \frac{k_n x}{2}\left(x^2-\frac{a^2}{4}\right)$; $k_n = 2,4,6\ldots$

Look at m odd:

$$c_m = A\,.\left[\sqrt{\frac{2}{a}}\left(\int_{-\frac{a}{2}}^{a/2} x^2 \cos\frac{k_n x}{a}dx - \frac{a^2}{4}\int_{-\frac{a}{2}}^{a/2} \cos\frac{k_n x}{a}dx\right)\right]$$; ~~$k_n = 1,3,5,7,\ldots$~~ ; $k_n = \frac{n\pi}{a}$; $n=1,3,5,\ldots$

$\int_{-\frac{a}{2}}^{a/2} \cos\frac{n x\pi}{a}dx = \frac{2a}{\pi}\left(\frac{1}{n}\right)$; $n=1,3,5\ldots$ (even function)	
$\int_{-\frac{a}{2}}^{a/2} \sin\frac{n\pi x}{a}dx = 0$ (odd function)	
$\int_{-\frac{a}{2}}^{a/2} x^2 \cos\frac{n\pi x}{a}dx = \frac{a^3(-8+n\pi^2)}{2n^3\pi^3}$ (even function).	$\int_{-\frac{a}{2}}^{a/2} x^2 \sin\frac{n\pi x}{a}dx = 0$ (odd function)

$$\therefore\; c_{m,\,\text{odd}} = A\,.\sqrt{\frac{2}{a}}\,.\left[\frac{a^3(-8+n\pi^2)}{2n^3\pi^3} - \frac{a^2}{4}\left(\frac{2a}{\pi n}\right)\right]$$; $n=1,3,5,7\ldots$

$c_{m,\,\text{meven}} = A\sqrt{\frac{2}{a}}\,[\,0\,] = 0$; $A = \sqrt{\frac{30}{a^5}}$.

Suggested solutions to Q2: Infinite Quantum Well (IQW) vs. Harmonic Potential Well (HPW)

Similarity

1. Energy are quantised
2. Solutions are divided into odd and even parts
3. Total solutions are made up of the linear superposition of stationary solutions
4. The solutions vanish at $x \rightarrow \pm\infty$
5. The solutions are normalised
6. The stationary solutions are orthonormal
7. The stationary solutions are complete.
8. Allowed energies are positive
9. Infinite energy levels are allowed.
10 ...

Dissimilarity

1. stationary solutions in harmonic well display tunnelling effect
2. Forms of stationary solutions are different: for IQW, they are made up of sinusoidal functions; for HPW, it is made up of Hermit polynomials.
3. The allowed energies are different in form.
4. Lowest energy level in HPW is n=0; whereas it is n=1 for IQW.
5. ...