# HOMEWORK 3

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

$\Rightarrow \Psi(0,t)=0$ & $\Psi(a,t)=0$ for infinite square well.

$\Rightarrow V(x) = \begin{cases} 0 & \text{for } 0\leq x\leq a \\ \infty & \text{otherwise} \end{cases}$

Assuming that the wave equation $\Psi(x,t)$ has the solution of $\Psi(x)\phi(t)$.

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

$$\Leftrightarrow i\hbar\, \Psi(x)\phi'(t) = \frac{\hbar^2}{2m}\Psi''(x)\phi(t) + V(x)\Psi(x)\phi(t)$$

For infinite square well: $\begin{cases} \Psi(0,t)=0 \Rightarrow \Psi(0)\phi(t)=0 \Rightarrow \Psi(0)=0 \\ \Psi(a,t)=0 \Rightarrow \Psi(a)\phi(t)=0 \Rightarrow \Psi(a)=0 \end{cases}$

Separating both the values of $t$ & $x$ and set equal to NRGE:

$$i\hbar \frac{\phi'(t)}{\phi(t)} = -\frac{\hbar^2}{2m}\frac{\Psi''(x)}{\Psi(x)} + V(x) = E$$

$$\Rightarrow i\hbar\frac{\phi'(t)}{\phi(t)} = E \ (1) \ \& \ -\frac{\hbar^2}{2m}\frac{\Psi''(x)}{\Psi(x)} + V(x) = E \ (2)$$

Since (2) is a time indep. Schrödinger equation:

$$\Rightarrow \frac{d^2\Psi}{dx^2} = \frac{2m}{\hbar^2}[V(x)-E]\Psi \Rightarrow \begin{cases} \frac{d^2\Psi}{dx^2} = -\frac{2mE}{\hbar^2}\Psi & \text{for } 0\leq x\leq a \\ \frac{d^2\Psi}{dx^2} = -\frac{2m\infty}{\hbar^2}\Psi & \text{otherwise} \end{cases}$$

$\Rightarrow$ Only $\frac{d^2\Psi}{dx^2} = -\frac{2mE}{\hbar^2}\Psi$ valid for $0\leq x\leq a$.

$\Rightarrow \Psi(x) = C_1 \sin\left(\frac{\sqrt{2mE}}{\hbar}x\right) + C_2 \cos\left(\frac{\sqrt{2mE}}{\hbar}x\right)$

For $\Psi(0) \Rightarrow C_2 = 0$. $\Psi(a) \Rightarrow C_1 \sin\left(\frac{\sqrt{2mE}}{\hbar}a\right) + C_2 \cos\left(\frac{\sqrt{2mE}}{\hbar}a\right) = 0$

$\Rightarrow C_1 \sin\left(\frac{\sqrt{2mE}}{\hbar}a\right) = 0$, Assuming $C_1 \neq 0 \Rightarrow \sin\left(\frac{\sqrt{2mE}}{\hbar}a\right) = 0$

$\Rightarrow \frac{\sqrt{2mE}}{\hbar}a = n\pi$ (for $n = 0, 1, 2 \ldots$) $\Rightarrow E = \frac{\hbar^2\pi^2n^2}{2ma^2} \Rightarrow \Psi(x) = A \sin \frac{n\pi x}{a}$

Find A thru normallization: $\int_0^a |\Psi(x)|^2 dx = 1 \Rightarrow \int_0^a A^2 \sin^2 \frac{n\pi x}{a} dx = 1 \Rightarrow A = \sqrt{\frac{2}{a}}$

Replaced E in (1):

$\Rightarrow i\hbar \frac{\phi'(t)}{dt)} = \frac{\hbar^2\pi^2n^2}{2ma^2} \Rightarrow \frac{\phi'(t)}{\phi(t)} = -i\frac{\hbar\pi^2n^2}{2ma^2} \Leftrightarrow \frac{d}{dt}\ln\phi(t) = -i\frac{\hbar\pi^2n^2}{2ma^2}$

$\Rightarrow \int \frac{d}{dt}\ln\phi(t)\,dt = \int -\frac{i\hbar\pi^2n^2}{2ma^2}dt = \ln\phi(t) = -\frac{i\hbar\pi^2n^2}{2ma^2}t + C$

$\Rightarrow \phi(t) = e^{-i\hbar\pi^2n^2t/2ma^2} e^C \Rightarrow \phi(t) = e^{(-i\hbar\pi^2n^2t/2ma^2)}$

Now for $0$: $\frac{d^2\Psi}{dx^2} = 0 \Rightarrow \Psi(x) = C_3x + C_4 \Rightarrow \begin{cases} \Psi(0) = C_4 = 0 \\ \Psi(a) = C_3a + C_4 = 0 \Rightarrow C_3 = 0 \end{cases}$

$\Rightarrow 0$ is not an eigenvalue.

Now for negative eigenvalue $E = -\theta^2 \Rightarrow \frac{d^2\Psi}{dx^2} = \frac{2m\theta^2}{\hbar^2}\Psi$

$\Rightarrow \Psi(x) = C_5 \sinh\left(\frac{\sqrt{2m}\theta}{\hbar}x\right) + C_6 \cosh\left(\frac{\sqrt{2m}\theta}{\hbar}x\right)$

$\Rightarrow \begin{cases} \Psi(0) = C_6 = 0 \\ \Psi(a) = C_5 \sinh\left(\frac{\sqrt{2m}\theta}{\hbar}a\right) + C_6 \cosh\left(\frac{\sqrt{2m}\theta}{\hbar}a\right) = 0 \Rightarrow C_5 = 0 \end{cases}$

(No value for $\cosh = 0$)

$\Rightarrow$ The only solution would be: $\Psi(x,t) = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} B_n e^{-i\hbar\pi^2n^2t/2ma^2} \sin\frac{n\pi x}{a}$

2.4. For infinite square well: $V(x)=\begin{cases}0 & \text{for } 0\le x\le a\\ \infty & \text{otherwise}\end{cases}$

According to 2.3:

$$\psi(x,t)=\sqrt{\frac{2}{a}}\,e^{-i\hbar\pi^2n^2t/2ma^2}\sin\frac{n\pi x}{a} \quad \text{for } 0\le x\le a$$

• $$\langle x\rangle=\int_{-\infty}^{\infty}\psi^*(x,t)\,x\,\psi(x,t)\,dx=\frac{2}{a}\int_0^a \sin^2\frac{n\pi x}{a}\,x\,dx$$

$$=\frac{2}{a}\int_0^a \frac{x}{2}\left(1-\cos\frac{2n\pi x}{a}\right)dx=\frac{1}{a}\left(\int_0^a x\,dx-\int_0^a x\cos\frac{2n\pi x}{a}\,dx\right)$$

$$=\frac{1}{a}\left(\frac{a^2}{2}-\frac{2\pi an\overbrace{\sin(2\pi an)}^{0}+\overbrace{\cos(2\pi an)}^{1}-1}{4\pi^2n^2}\right)=\frac{a}{2}$$

• $$\langle x^2\rangle=\frac{2}{a}\int_0^a x^2\sin^2\frac{n\pi x}{a}\,dx=\frac{1}{a}\left(\frac{a^3}{3}-\frac{(2\pi^2a^3n^2-a^3)\overbrace{\sin(2\pi n)}^{0}+2\pi a^3n\overbrace{\cos(2\pi n)}^{1}}{4\pi^3n^3}\right)=\frac{1}{a}\left(\frac{a^3}{3}-\frac{a^3}{2\pi^2n^2}\right)=\frac{a^2}{3}-\frac{a^2}{2\pi^2n^2}$$

• $$\langle \sigma_x\rangle=\sqrt{\langle x^2\rangle-\langle x\rangle^2}=\sqrt{\frac{a^2}{3}-\frac{a^2}{2\pi^2n^2}-\frac{a^2}{4}}=\sqrt{\frac{a^2}{12}-\frac{a^2}{2n^2\pi^2}}=\frac{a}{2}\sqrt{\frac{1}{3}-\frac{2}{n^2\pi^2}}$$

$$=\frac{a}{2}\sqrt{\frac{n^2\pi^2-6}{3n^2\pi^2}}=\frac{a}{2n\pi}\sqrt{\frac{n^2\pi^2-6}{3}}$$

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

$$=-i\hbar\int_0^a\left(\sqrt{\frac{2}{a}}\,e^{+i\hbar\pi^2n^2t/2ma^2}\sin\frac{n\pi x}{a}\right)\frac{\partial}{\partial x}\left(\sqrt{\frac{2}{a}}\,e^{-i\hbar\pi^2n^2t/2ma^2}\sin\frac{n\pi x}{a}\right)dx$$

$$=-i\hbar\frac{2}{a}\int_0^a\left(\sin\frac{n\pi x}{a}\cdot\frac{n\pi}{a}\cos\frac{n\pi x}{a}\right)dx=\frac{-2i\hbar\,n\pi}{a^2}\int_0^a \sin\frac{n\pi x}{a}\cos\frac{n\pi x}{a}\,dx$$

$$=\frac{-i\hbar n\pi}{a^2}\int_0^a \sin\frac{2n\pi x}{a}\,dx=\frac{-i\hbar n\pi}{a^2}\left(\frac{-a}{2n\pi}\cos\frac{2n\pi x}{a}\right)_0^a$$

$$=\frac{-i\hbar n\pi}{a}\left[\frac{-a}{2n\pi}\left(\overbrace{\cos 2\pi n-\cos 0}^{0}\right)\right]=0$$

$$\cdot \langle p^2\rangle = \int_{-\infty}^{\infty} \psi^*(x,t)\left(-i\hbar\frac{\partial}{\partial x}\right)^2 \psi(x,t)\,dx = -\hbar^2\int_0^a \left(\sqrt{\frac{2}{a}}e\sin\frac{n\pi x}{a}\right)\left(-\sqrt{\frac{2}{a}}\frac{n^2\pi^2}{a^2}e\sin\frac{n\pi x}{a}\right)dx$$

$$= \frac{2\hbar^2n^2\pi^2}{a^3}\int_0^a \sin^2\frac{n\pi x}{a}\,dx = \frac{2\hbar^2n^2\pi^2}{a^3}\int_0^a \frac{1}{2}\left(1-\cos\frac{2n\pi x}{a}\right)dx$$

$$= \frac{\hbar^2n^2\pi^2}{a^3}\left(x-\frac{a}{2n\pi}\sin\frac{2n\pi x}{a}\right)\Big|_0^a = \frac{\hbar^2n^2\pi^2}{a^3}a = \frac{\hbar^2n^2\pi^2}{a^2}$$

$$\cdot \langle \sigma_p\rangle = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \sqrt{\frac{\hbar^2n^2\pi^2}{a^2}} = \frac{\hbar n\pi}{a}$$

$\Rightarrow \sigma_x\sigma_p = \frac{a}{2n\pi}\sqrt{\frac{n^2\pi^2-6}{3}}\,\frac{\hbar n\pi}{a} = \frac{\hbar}{2}\sqrt{\frac{n^2\pi^2-6}{3}} \geq \frac{\hbar}{2}$ $\Rightarrow$ consistent with Heisenberg uncertainty principal.

$\Rightarrow$ The ground state $(n=1)$ will come closer to this uncertainty limit.

2.5. $\Psi(x,0) = A[\psi_1(x)+\psi_2(x)] = A\left(\sqrt{\frac{2}{a}}\sin\frac{\pi x}{a} + \sqrt{\frac{2}{a}}\sin\frac{2\pi x}{a}\right)$ for infinite square well.

a) $$\int_{-\infty}^{\infty}|\Psi^*(x,t)|^2dx = 1 = \frac{2A^2}{a^2}\int_0^a\left(\sin^2\frac{\pi x}{a} + \sin^2\frac{2\pi x}{a} + 2\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a}\right)dx$$

$$= \frac{2A^2}{a^2}\left\{\int_0^a\frac{1}{2}\left(1-\cos\frac{2\pi x}{a}\right)dx + \int_0^a\frac{1}{2}\left(1-\cos\frac{4\pi x}{a}\right)dx + 2\int_0^a\frac{1}{2}\left[\cos\left(\frac{\pi x}{a}-\frac{2\pi x}{a}\right) - \cos\left(\frac{\pi x}{a}+\frac{2\pi x}{a}\right)\right]dx\right\}$$

$$= \frac{A^2}{a}\left[\int_0^a\left(1-\cos\frac{2\pi x}{a}\right)dx + \int_0^a\left(1-\cos\frac{4\pi x}{a}\right)dx + 2\int_0^a\left(\cos\frac{\pi x}{a}-\cos\frac{3\pi x}{a}\right)dx\right]$$

$$= \frac{A^2}{a}\left[\left(x-\frac{a}{2\pi}\sin\frac{2\pi x}{a}\right)\Big|_0^a + \left(x-\frac{a}{4\pi}\sin\left(\frac{4\pi x}{a}\right)\right)\Big|_0^a + 2\left(\frac{a}{\pi}\sin\frac{\pi x}{a} - \frac{a}{3\pi}\sin\frac{3\pi x}{a}\right)\Big|_0^a\right]$$

$$= \frac{A^2}{a}(a+2.0+a) = 2A^2 = 1 \Rightarrow A = \frac{1}{\sqrt{2}}$$

b) For infinite square well: $\Psi(x,t) = \sqrt{\frac{2}{a}}\sum_{n=1}^{\infty} B_n e^{-i\hbar\pi^2n^2t/2ma^2}\sin\frac{n\pi x}{a}$ for $0\leq x\leq a$

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

$$= \sqrt{\frac{2}{a}}B_1\sin\frac{\pi x}{a} + \sqrt{\frac{2}{a}}B_2\frac{2\pi x}{a} + \sqrt{\frac{2}{a}}B_3\sin\frac{3\pi x}{a} + \ldots$$

$\Rightarrow \sqrt{\frac{2}{a}}B_1 = \sqrt{\frac{2}{a}}B_2 = \frac{1}{\sqrt{a}} \Rightarrow B_1 = B_2 = \frac{1}{\sqrt{2}}$, $B_3 \to B_n = 0$.

$$\Rightarrow \Psi(x,t) = \sqrt{\frac{2}{a}}\, b_1 e^{\frac{-i\hbar\pi^2 t}{2ma^2}} \sin\frac{\pi x}{a} + \sqrt{\frac{2}{a}}\, B_2 e^{\frac{-i\hbar\pi^2 4t}{2ma^2}} \sin\frac{2\pi x}{a}$$

$$= \frac{1}{\sqrt{a}} e^{\frac{-i\hbar\pi^2 t}{2ma^2}} \sin\frac{\pi x}{a} + \frac{1}{\sqrt{a}} e^{\frac{-i\hbar\pi^2 4t}{2ma^2}} \sin\frac{2\pi x}{a}$$

For $\omega = \pi^2\hbar/2ma^2$

$$\Rightarrow \Psi(x,t) = \frac{1}{\sqrt{a}} e^{-i\omega t} \sin\frac{\pi x}{a} + \frac{1}{\sqrt{a}} e^{-4i\omega t} \sin\frac{2\pi x}{a}$$

$$\Rightarrow |\Psi(x,t)|^2 = \left(\frac{1}{\sqrt{a}} e^{i\omega t} \sin\frac{\pi x}{a} + \frac{1}{\sqrt{a}} e^{4i\omega t} \sin\frac{2\pi x}{a}\right)\left(\frac{1}{\sqrt{a}} e^{-i\omega t} \sin\frac{\pi x}{a} + \frac{1}{\sqrt{a}} e^{-4i\omega t} \sin\frac{2\pi x}{a}\right)$$

$$= \frac{1}{a}\sin^2\frac{\pi x}{a} + \frac{1}{a} e^{3i\omega t} \sin\frac{2\pi x}{a} + \frac{1}{a} e^{-3i\omega t} \sin\frac{2\pi x}{a} + \frac{1}{a}\sin^2\frac{2\pi x}{a}$$

$$= \frac{1}{a}\left[\sin^2\frac{\pi x}{a} + (e^{3i\omega t} + e^{-3i\omega t}) \sin\frac{\pi x}{a} \sin\frac{2\pi x}{a} + \sin^2\frac{2\pi x}{a}\right]$$

$$= \frac{1}{a}\left(\sin^2\frac{\pi x}{a} + 2\cos 3\omega t \sin\frac{\pi x}{a} \sin\frac{2\pi x}{a} + \sin^2\frac{2\pi x}{a}\right)$$

$\Rightarrow$ Sinusoidal function of time:

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = \frac{1}{a}\underbrace{\int_0^a \sin^2\frac{\pi x}{a} dx}_{a/2} + 2\cos 3\omega t \overbrace{\int_0^a \sin\frac{\pi x}{a} \sin\frac{2\pi x}{a} dx}^{0} + \underbrace{\int_0^a \sin^2\frac{2\pi x}{a} dx}_{a/2} = 1$$

c) $\langle x \rangle = \int_{-\infty}^{\infty} |\Psi(x,t)|^2 x\, dx$

$$= \frac{1}{a}\int_0^a x\left(\sin^2\frac{\pi x}{a} + 2\cos 3\omega t \sin\frac{\pi x}{a} \sin\frac{2\pi x}{a} + \sin^2\frac{2\pi x}{a}\right) dx$$

$$= \frac{1}{2a}\left[\int_0^a x\,dx - \int_0^a x\cos\frac{2\pi x}{a} dx + 2\cos 3\omega t\left(\int_0^a x\cos\frac{\pi x}{a} dx - \int_0^a x\cos\frac{3\pi x}{a} dx\right) + \int_0^a x\,dx - \int_0^a x\cos\frac{4\pi x}{a} dx\right]$$

$$= \frac{1}{2a}\left[\frac{a^2}{2} - 0 + 2\cos 3\omega t\left(-\frac{2a^2}{\pi^2} + \frac{2a^2}{9\pi^2}\right) + \frac{a^2}{2} - 0\right]$$

$$= \frac{1}{2a}\left(a^2 - \frac{32a^2}{9\pi^2}\cos 3\omega t\right) = \frac{a}{2} - \frac{16a}{9\pi^2}\cos 3\omega t$$

$\Rightarrow$ Amplitude $= \frac{16}{9\pi^2} a \approx 0.18a < 0.5a$ (Thanks god I'm not going to fail)

$\Rightarrow$ Oscillation: $3\omega = \frac{3\hbar\pi^2}{2ma^2}$

d) $\langle p \rangle = m\frac{d\langle x \rangle}{dt} = m\frac{d}{dt}\left(\frac{a}{2} - \frac{16a}{9\pi^2}\cos 3\omega t\right) = \frac{16ma\omega}{3\pi^2}\sin 3\omega t$

e) $\Psi(x,t) = \frac{1}{\sqrt{a}} e^{-i\omega t} \sin\frac{\pi x}{a} + \frac{1}{\sqrt{a}} e^{-4i\omega t} \sin\frac{2\pi x}{a}$

$$= \frac{1}{\sqrt{2}}\Big(\underbrace{\sqrt{\frac{2}{a}} \sin\frac{\pi x}{a}}_{\psi_1(x)}\Big) e^{-i\omega t} + \frac{1}{\sqrt{2}}\Big(\underbrace{\sqrt{\frac{2}{a}} \sin\frac{2\pi x}{a}}_{\psi_2(x)}\Big) e^{-4i\omega t}$$

$\Rightarrow E_1 = \frac{\hbar^2\pi^2}{2ma^2}$, $E_2 = \frac{2\hbar^2\pi^2}{ma^2}$ $\Rightarrow P(E_1) = P(E_2) = \left|\frac{1}{\sqrt{2}}\right|^2 = \frac{1}{2}$

$\Rightarrow \langle H \rangle = P(E_1)E_1 + P(E_2)E_2 = \frac{1}{2}\frac{\hbar^2\pi^2}{2ma^2} + \frac{1}{2}\frac{2\hbar^2\pi^2}{ma^2} = \frac{5\hbar^2\pi^2}{4ma^2}$

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

$\Rightarrow \int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx = \int_0^{a/2} A^2 dx + \int_{a/2}^{a} 0^2 dx = A^2 \frac{a}{2} = 1 \Rightarrow A = \sqrt{\frac{2}{a}}$

$\Rightarrow \Psi(x,0) = \begin{cases} \sqrt{\frac{2}{a}} & 0 \le x \le a/2 \\ 0, & a/2 \le x \le a \end{cases} \Rightarrow \Psi(x,0) = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} B_n \sin \frac{n\pi x}{a}$

Multiply both sides by $\frac{m\pi x}{a}$ to solve for $B_n$

$\Rightarrow \Psi(x,0) \sin \frac{m\pi x}{a} = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} B_n \sin \frac{n\pi x}{a} \sin \frac{m\pi x}{a}$

$\Rightarrow \int_0^a \Psi(x,0) \sin \frac{m\pi x}{a} dx = \int_0^a \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} \overset{(*)}{B_n \sin \frac{n\pi x}{a} \sin \frac{m\pi x}{a}} dx$

For $m \neq n \Rightarrow (*) = 0$. Therefore, $m = n$ is the only term left.

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

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

$= \sqrt{\frac{2}{a}} \left( \int_0^{a/2} \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} dx + \int_{a/2}^{a} 0 \sin \frac{n\pi x}{a} dx \right)$

$= \frac{2}{a} \int_0^{a/2} \sin \frac{n\pi x}{a} dx = \frac{2}{a} \left( -\frac{a}{n\pi} \cos \frac{n\pi x}{a} \right)\Big|_0^{a/2} = \frac{2}{a} \left( -\frac{a}{n\pi} \cos \frac{n\pi}{2} + \frac{a}{n\pi} \right)$

$= \frac{2}{n\pi} \left( 1 - \cos \frac{n\pi}{2} \right)$

$\Rightarrow \Psi(x,t) = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} \frac{2}{n\pi} \left( 1 - \cos \frac{n\pi}{2} \right) e^{\frac{-i\hbar\pi^2 n^2 t}{2ma^2}} \boxed{\sin \frac{\pi n x}{a}} \rightarrow \Psi_n(x)$

$E_n = \frac{\hbar^2\pi^2 n^2}{2ma^2} \Rightarrow P(E_n) = \left| \frac{2}{n\pi} \left( 1 - \cos \frac{n\pi}{2} \right) \right|^2 = \frac{4}{n^2\pi^2} \left( 1 - \cos \frac{n\pi}{2} \right)^2$

$\Rightarrow P(E_1) = \frac{4}{\pi^2} \approx .405.$