PROBLEM 1: Infinite Square Well

For a particle moving in an infinite square well of width $2a$, the potential energy is

$$V(x) = \begin{cases} 0 & \text{for } |x| < a, \; a > 0, \text{ and} \\ \infty & \text{for } |x| \geq a \,. \end{cases}$$

Its wave function at time $t = 0$ is

$$\psi(x, 0) = \frac{1}{\sqrt{2}} \left[u_1(x) + u_2(x) \right]$$

where $u_1(x)$ and $u_2(x)$ are the normalized ground state and first excited state wave functions respectively and they are orthogonal to each other.

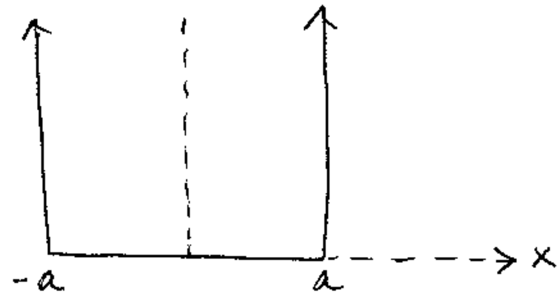
(a) Determine the energy eigenvalues E_1 and E_2 then find the wave function $\psi(x,t)$ as a function of time. *(2 points)*

(b) Find the expectation value of its kinetic energy $\langle T \rangle$ with $\psi(x,t)$. *(3 points)*

(c) What is the expectation value of its total energy ($\langle E \rangle$)? Explain the relationship between this result and what you found in Part (b). *(2 points)*

1 (d) Evaluate ΔX in this state with $\psi(x,t)$. *(3 points)*

(a)



In this case, we know

$$u_n(x) = \sqrt{\frac{1}{a}} \cos\left(\frac{n\pi x}{2a}\right) \quad , n = 1, 3, 5, \ldots$$

and

$$u_n(x) = \sqrt{\frac{1}{a}} \sin\left(\frac{n\pi x}{2a}\right) \quad , n = 2, 4, 6, \ldots$$

We know

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

and

$$k = \frac{n\pi}{2a},$$

So

$$\frac{\sqrt{2mE}}{\hbar} = \frac{n\pi}{2a}$$

$$E_n = \frac{n^2\pi^2\hbar^2}{8ma^2}.$$

Then

$$\boxed{E_1 = \frac{\pi^2\hbar^2}{8ma^2}} \text{ and } \boxed{E_2 = \frac{\pi^2\hbar^2}{2ma^2}}$$

(a), cont'd...

We know

$$\psi(x,t) = U(x,t)\,\psi(x,0),$$

where

$$U(x,t) = \sum_{n=1}^{2} |u_n\rangle\langle u_n| e^{-iE_n t/\hbar}$$
$$= |u_1\rangle\langle u_1| e^{-iE_1 t/\hbar} + |u_2\rangle\langle u_2| e^{-iE_2 t/\hbar}.$$

So

$$\psi(x,t) = \left(|u_1\rangle\langle u_1| e^{-iE_1 t/\hbar} + |u_2\rangle\langle u_2| e^{-iE_2 t/\hbar}\right)\frac{1}{\sqrt{2}}\left(|u_1\rangle + |u_2\rangle\right)$$
$$= \frac{1}{\sqrt{2}}|u_1\rangle e^{-iE_1 t/\hbar} + \frac{1}{\sqrt{2}}|u_2\rangle e^{-iE_2 t/\hbar}$$

$$\boxed{\psi(x,t) = \frac{1}{\sqrt{2}}\left[e^{-i\frac{\pi^2\hbar}{8ma^2}t}|u_1\rangle + e^{-i\frac{\pi^2\hbar}{2ma^2}t}|u_2\rangle\right]}$$

where

$$|u_1\rangle = u_1(x) = \sqrt{\frac{1}{a}}\cos\left(\frac{\pi x}{2a}\right)$$
$$|u_2\rangle = u_2(x) = \sqrt{\frac{1}{a}}\sin\left(\frac{\pi x}{a}\right).$$

(b)

The expectation value of the kinetic energy is given by

$$\langle T\rangle = \langle \psi(x,t)|T|\psi(x,t)\rangle = \int_{-a}^{a}\psi(x,t)^*\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\psi(x,t)\,dx.$$

We know

$$\psi(x,t) = \frac{1}{\sqrt{2a}}\left[\cos\left(\frac{\pi x}{2a}\right)e^{-i\frac{\pi^2\hbar}{8ma^2}t} + \sin\left(\frac{\pi x}{a}\right)e^{-i\frac{\pi^2\hbar}{2ma^2}t}\right].$$

So

$$\frac{d^2\psi(x,t)}{dx^2} = \frac{1}{\sqrt{2a}}\left[-\frac{\pi^2}{4a^2}\cos\left(\frac{\pi x}{2a}\right)e^{-i\frac{\pi^2\hbar}{8ma^2}t} - \frac{\pi^2}{a^2}\sin\left(\frac{\pi x}{a}\right)e^{-i\frac{\pi^2\hbar}{2ma^2}t}\right]$$

and

$$\langle T\rangle = \left(\frac{\hbar^2}{2m}\right)\left(\frac{1}{2a}\right)\int_{-a}^{a}\left[\frac{\pi^2}{4a^2}\cos\left(\frac{\pi x}{2a}\right)e^{-i\frac{\pi^2\hbar}{8ma^2}t} + \frac{\pi^2}{a^2}\sin\left(\frac{\pi x}{a}\right)e^{-i\frac{\pi^2\hbar}{2ma^2}t}\right] \cdot \left[\cos\left(\frac{\pi x}{2a}\right)e^{+i\frac{\pi^2\hbar}{8ma^2}t} + \sin\left(\frac{\pi x}{a}\right)e^{+i\frac{\pi^2\hbar}{2ma^2}t}\right]dx$$

$$= \frac{\hbar^2}{4ma}\int_{-a}^{a}\left[\frac{\pi^2}{4a^2}\cos^2\left(\frac{\pi x}{2a}\right) + \frac{\pi^2}{a^2}\sin^2\left(\frac{\pi x}{a}\right) + \frac{\pi^2}{4a^2}\sin\left(\frac{\pi x}{a}\right)\cos\left(\frac{\pi x}{2a}\right)e^{i\frac{3\pi^2\hbar}{8ma^2}t} + \frac{\pi^2}{a^2}\sin\left(\frac{\pi x}{a}\right)\cos\left(\frac{\pi x}{2a}\right)e^{-i\frac{3\pi^2\hbar}{8ma^2}t}\right]dx$$

$$= \frac{\hbar^2}{4ma}\int_{-a}^{a}\left[\frac{\pi^2}{8a^2}\left(1+\cos\left(\frac{\pi x}{a}\right)\right) + \frac{\pi^2}{2a^2}\left(1-\cos\left(\frac{2\pi x}{a}\right)\right) + \frac{\pi^2}{8a^2}e^{i\frac{3\pi^2\hbar}{8ma^2}t}\left(\sin\left(\frac{3\pi x}{2a}\right)+\sin\left(\frac{\pi x}{2a}\right)\right) + \frac{\pi^2}{2a^2}e^{-i\frac{3\pi^2\hbar}{8ma^2}t}\left(\sin\left(\frac{3\pi x}{2a}\right)+\sin\left(\frac{\pi x}{2a}\right)\right)\right]dx$$

$$= \frac{\hbar^2}{4ma}\int_{-a}^{a}\left[\frac{\pi^2}{8a^2} + \frac{\pi^2}{8a^2}\cos\left(\frac{\pi x}{a}\right) + \frac{\pi^2}{2a^2} - \frac{\pi^2}{2a^2}\cos\left(\frac{2\pi x}{a}\right) + \frac{\pi^2}{8a^2}e^{i\frac{3\pi^2\hbar}{8ma^2}t}\sin\left(\frac{3\pi x}{2a}\right) + \frac{\pi^2}{8a^2}e^{i\frac{3\pi^2\hbar}{8ma^2}t}\sin\left(\frac{\pi x}{2a}\right) + \frac{\pi^2}{2a^2}e^{-i\frac{3\pi^2\hbar}{8ma^2}t}\sin\left(\frac{3\pi x}{2a}\right) + \frac{\pi^2}{2a^2}e^{-i\frac{3\pi^2\hbar}{8ma^2}t}\sin\left(\frac{\pi x}{2a}\right)\right]dx$$

$$= \frac{\hbar^2}{4ma}\left[\frac{\pi^2}{8a^2}x + \frac{\pi^2}{2a^2}x + \frac{\pi}{8a}\sin\left(\frac{\pi x}{a}\right) - \frac{\pi}{a}\sin\left(\frac{2\pi x}{a}\right) - \frac{\pi}{12a}\cos\left(\frac{3\pi x}{2a}\right)e^{i\frac{3\pi^2\hbar}{8ma^2}t} - \frac{\pi}{4a}\cos\left(\frac{\pi x}{2a}\right)e^{i\frac{3\pi^2\hbar}{8ma^2}t} - \frac{\pi}{3a}\sin\left(\frac{3\pi x}{2a}\right)e^{-i\frac{3\pi^2\hbar}{8ma^2}t} - \frac{\pi}{a}\cos\left(\frac{\pi x}{2a}\right)e^{-i\frac{3\pi^2\hbar}{8ma^2}t}\right]\Bigg|_{-a}^{a}$$

(b), cont'd...

$$\langle T \rangle = \frac{\hbar^2}{4ma}\left[\frac{\pi^2}{4a} + \frac{\pi^2}{a} + 0 + 0 + 0 + 0 - \frac{\pi}{3a} e^{-i\frac{3\pi^2\hbar}{8ma^2}t}(-1-1)\right]$$

$$= \frac{\hbar^2}{4ma}\left[\frac{5\pi^2}{4a} + \frac{2\pi}{3a} e^{-i\frac{3\pi^2\hbar}{8ma^2}t}\right]$$

$$= \frac{5\pi^2\hbar^2}{16ma^2} + \frac{\pi\hbar^2}{6ma^2} e^{-i\frac{3\pi^2\hbar}{8ma^2}t}$$

(c)

Since $V=0$ in the infinite well between $-a < x < a$, we know that the result for $\langle E \rangle$ is equivalent to the result for $\langle T \rangle$.

As $t \to \infty$, we get the average of $E_1 + E_2$, which is

$$\frac{1}{2}(E_1 + E_2) = \frac{5\pi^2\hbar^2}{16ma^2}.$$

(d)

We know

$$\Delta X = \sqrt{\langle X^2\rangle - \langle X\rangle^2},$$

so we must determine $\langle X^2\rangle$ and $\langle X\rangle$. We have

$$\begin{aligned}\langle X\rangle &= \int_{-a}^{a} \psi^*(x,t)\, x\, \psi(x,t)\, dx \\ &= \frac{1}{2a}\int_{-a}^{a} x\left[\cos^2\left(\frac{\pi x}{2a}\right) + \sin^2\left(\frac{\pi x}{a}\right) + \sin\left(\frac{\pi x}{a}\right)\cos\left(\frac{\pi x}{2a}\right)e^{i\frac{3\pi^2\hbar}{8ma^2}t} \right.\\ &\qquad \left. + \sin\left(\frac{\pi x}{a}\right)\cos\left(\frac{\pi x}{2a}\right)e^{-i\frac{3\pi^2\hbar}{8ma^2}t}\right]dx \\ &= \frac{1}{2a}\left[0 + 0 + \frac{32a^2}{9\pi^2}e^{i\frac{3\pi^2\hbar}{8ma^2}t} + \frac{32a^2}{9\pi^2}e^{-i\frac{3\pi^2\hbar}{8ma^2}t}\right] \\ &= \frac{32a}{9\pi^2}\left(e^{i\frac{3\pi^2\hbar}{8ma^2}t} + e^{-i\frac{3\pi^2\hbar}{8ma^2}t}\right) \\ &= \frac{64a}{9\pi^2}\cos\left(\frac{3\pi^2\hbar}{8ma^2}t\right)\end{aligned}$$

and

$$\langle X\rangle^2 = \left(\frac{64}{9}\right)^2 \frac{a^2}{\pi^4}\cos^2\left(\frac{3\pi^2\hbar}{8ma^2}t\right).$$

We also have

$$\begin{aligned}\langle X^2\rangle &= \int_{-a}^{a} \psi^*(x,t)\, x^2\, \psi(x,t)\, dx \\ &= \frac{1}{2a}\left[\frac{(\pi^2-6)a^3}{3\pi^2} + \frac{(2\pi^2-3)a^3}{6\pi^2} + 0 + 0\right] \\ &= \frac{1}{2a}\left(\frac{2\pi^2a^3 - 12a^3 + 2\pi^2a^3 - 3a^3}{6\pi^2}\right) \\ &= \frac{4\pi^2a^2 - 15a^2}{12\pi^2}\end{aligned}$$

(d), cont'd...

Then

$$\Delta X = \sqrt{\frac{4\pi^2 a^2 - 15a^2}{12\pi^2} - \left(\frac{64}{9}\right)^2 \frac{a^2}{\pi^4} \cos^2\left(\frac{3\pi^2 \hbar}{8ma^2} t\right)}$$

(There doesn't seem to be a great way to simplify this...)