2. Square Well Oscillations

Consider a particle in a symmetric 1D square well of width L:

$$\begin{aligned} V(x) &= 0, \quad |x| \leq L/2 \\ V(x) &= \infty \quad |x| > L/2 \end{aligned}$$

(a) (1 pts.) What are the energy eigenvalues and eigenstates of the first three energy levels in the well? (You do not have to derive these, you may just state them.)

(b) (2 pts.) Assume a particle is, at time t = 0, in a linear combination of the ground and first excited states of the well:

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left[|1\rangle + |2\rangle\right]$$

What is the expectation value of the position of the particle at time $t = 0$?

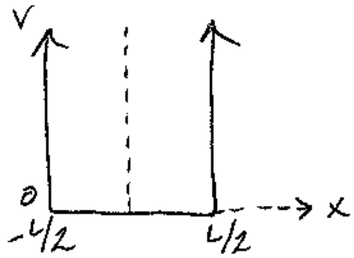
(c) (2 pts.) What is the expectation value of the momentum of the particle in the state given in (b)?

(d) (3 pts.) Starting at time $t = 0$ in the state given in (b), what are the time dependent expectation values, $\langle x\rangle(t)$ and $\langle p\rangle(t)$? Explain the relationship between these time dependent expectation values. In particular, explain the relation between the times when these expectation values are at their maximum, minimum, and are equal to zero.

(e) (2 pts.) Repeat the questions (b), (c), and (d) above for the case where the initial state of the particle is a linear combination of the ground and second excited state of the well:

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left[|1\rangle + |3\rangle\right].$$

(a)



In general, the solutions are

$$\psi(x) = A\sin(kx) + B\cos(kx),$$

where

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

We must have

$$\psi(-L/2) = \psi(L/2) = 0,$$

so

$$\psi(L/2) = A\sin\left(k\tfrac{L}{2}\right) + B\cos\left(k\tfrac{L}{2}\right) = 0$$

Let

$$\frac{kL}{2} = n\frac{\pi}{2}$$

$$k = \frac{n\pi}{L}.$$

For $n = 1, 3, 5, \ldots$ we must have $A = 0$, so

$$\psi_{odd}(x) = B\cos\left(\frac{n\pi x}{L}\right)$$

$$\psi_{odd}(x) = \sqrt{\frac{2}{L}}\cos\left(\frac{n\pi x}{L}\right)$$

For $n = 2, 4, 6, \ldots$ we must have $B = 0$, so

$$\psi_{even}(x) = A\sin\left(\frac{n\pi x}{L}\right)$$

$$\psi_{even}(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right).$$

(a), cont'd...

For the energy,

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

$$2mE = \frac{n^2\pi^2\hbar^2}{L^2}$$

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

<u>$n=1$</u>

$$\psi_1(x) = \sqrt{\frac{2}{L}}\cos\left(\frac{\pi x}{L}\right)$$

$$E_1 = \frac{\pi^2\hbar^2}{2mL^2}$$

<u>$n=2$</u>

$$\psi_2(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)$$

$$E_2 = \frac{4\pi^2\hbar^2}{2mL^2} = \frac{2\pi^2\hbar^2}{mL^2}$$

<u>$n=3$</u>

$$\psi_3(x) = \sqrt{\frac{2}{L}}\cos\left(\frac{3\pi x}{L}\right)$$

$$E_3 = \frac{9\pi^2\hbar^2}{2mL^2}$$

(b)

We know

$$\Psi(x,t=0) = \frac{1}{\sqrt{2}}\left[\sqrt{\frac{2}{L}}\cos\left(\frac{\pi x}{L}\right) + \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)\right].$$

We want to determine $\langle x \rangle$. So

$$\langle x \rangle = \int_{-L/2}^{L/2} x\frac{1}{L}\left[\cos^2\left(\frac{\pi x}{L}\right) + \sin^2\left(\frac{2\pi x}{L}\right) + 2\sin\left(\frac{2\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right)\right]dx$$

$$= \frac{2}{L}\int_{-L/2}^{L/2} x\sin\left(\frac{2\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right)dx$$

$$\boxed{\langle x \rangle = \frac{16L}{9\pi^2}}$$

(c)

We have

$$\langle p \rangle = -i\hbar\int_{-L/2}^{L/2}\left[\sqrt{\frac{1}{L}}\cos\left(\frac{\pi x}{L}\right) + \sqrt{\frac{1}{L}}\sin\left(\frac{2\pi x}{L}\right)\right]\frac{d}{dx}\left[\sqrt{\frac{1}{L}}\cos\left(\frac{\pi x}{L}\right) + \sqrt{\frac{1}{L}}\sin\left(\frac{2\pi x}{L}\right)\right]dx$$

$$= \frac{-i\hbar}{L}\int_{-L/2}^{L/2}\left[\cos\left(\frac{\pi x}{L}\right) + \sin\left(\frac{2\pi x}{L}\right)\right]\left[-\frac{\pi}{L}\sin\left(\frac{\pi x}{L}\right) + \frac{2\pi}{L}\cos\left(\frac{2\pi x}{L}\right)\right]dx$$

$$= -\frac{i\hbar}{L}\int_{-L/2}^{L/2}\Big[-\frac{\pi}{L}\sin\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right) + \frac{2\pi}{L}\cos\left(\frac{\pi x}{L}\right)\cos\left(\frac{2\pi x}{L}\right)$$
$$-\frac{\pi}{L}\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right) + \frac{2\pi}{L}\sin\left(\frac{2\pi x}{L}\right)\cos\left(\frac{2\pi x}{L}\right)\Big]dx$$

$$= -\frac{i\hbar}{L}\left[0 + \frac{4}{3} - \frac{4}{3} + 0\right]$$

$$\boxed{\langle p \rangle = 0}$$

(d)

We know

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

where

$$U(x,t=0) = \sum_n |n\rangle\langle n| e^{-iE_n t/\hbar}.$$

So

$$\psi(x,t) = \left[|1\rangle\langle 1| e^{-iE_1 t/\hbar} + |2\rangle\langle 2| e^{-iE_2 t/\hbar}\right]\frac{1}{\sqrt{2}}\left[|1\rangle + |2\rangle\right]$$
$$= \frac{1}{\sqrt{2}}\left[|1\rangle e^{-iE_1 t/\hbar} + |2\rangle e^{-iE_2 t/\hbar}\right]$$
$$= \frac{1}{\sqrt{L}}\left[\cos\left(\frac{\pi x}{L}\right)e^{-iE_1 t/\hbar} + \sin\left(\frac{2\pi x}{L}\right)e^{-iE_2 t/\hbar}\right].$$

Then

$$\langle x\rangle(t) = \int_{-L/2}^{L/2} \psi^*(x,t)\, x\, \psi(x,t)\, dx$$
$$= \int_{-L/2}^{L/2} \frac{x}{L}\left[\cos\left(\frac{\pi x}{L}\right)e^{iE_1 t/\hbar} + \sin\left(\frac{2\pi x}{L}\right)e^{iE_2 t/\hbar}\right]\left[\cos\left(\frac{\pi x}{L}\right)e^{-iE_1 t/\hbar} + \sin\left(\frac{2\pi x}{L}\right)e^{-\frac{iE_2 t}{\hbar}}\right]dx$$
$$= \frac{1}{L}\int_{-L/2}^{L/2} x\left[\cos^2\left(\frac{\pi x}{L}\right) + \cos\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right)e^{\frac{i(E_1-E_2)t}{\hbar}} + \cos\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right)e^{\frac{i(E_2-E_1)t}{\hbar}} + \sin^2\left(\frac{2\pi x}{L}\right)\right]dx$$
$$= \frac{1}{L}\left[\frac{8L^2}{9\pi^2}e^{i(E_1-E_2)t/\hbar} + \frac{8L^2}{9\pi^2}e^{i(E_2-E_1)t/\hbar}\right]$$
$$= \frac{8L}{9\pi^2}\left[e^{i(E_1-E_2)t/\hbar} + e^{-i(E_1-E_2)t/\hbar}\right]$$

$$\boxed{\langle x\rangle(t) = \frac{16L}{9\pi^2}\cos\left(\frac{(E_1-E_2)t}{\hbar}\right)}$$

(d), cont'd...

We have

$$\langle P\rangle(t) = \int_{-L/2}^{L/2} \psi^*(x,t)\left(-i\hbar\frac{d}{dx}\right)\psi(x,t)\,dx$$

$$= \frac{-i\hbar}{L}\int_{-L/2}^{L/2}\left[\cos\left(\frac{\pi x}{L}\right)e^{iE_1t/\hbar} + \sin\left(\frac{2\pi x}{L}\right)e^{iE_2t/\hbar}\right]\left[-\frac{\pi}{L}\sin\left(\frac{\pi x}{L}\right)e^{-iE_1t/\hbar} + \frac{2\pi}{L}\cos\left(\frac{2\pi x}{L}\right)e^{-iE_2t/\hbar}\right]dx$$

$$= \frac{-i\hbar}{L}\int_{-L/2}^{L/2}\left[-\frac{\pi}{L}\cos\left(\frac{\pi x}{L}\right)\sin\left(\frac{\pi x}{L}\right) + \frac{2\pi}{L}\cos\left(\frac{\pi x}{L}\right)\cos\left(\frac{2\pi x}{L}\right)e^{\frac{i(E_1-E_2)t}{\hbar}} - \frac{\pi}{L}\sin\left(\frac{2\pi x}{L}\right)\sin\left(\frac{\pi x}{L}\right)e^{\frac{i(E_2-E_1)t}{\hbar}} + \frac{2\pi}{L}\cos\left(\frac{2\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right)\right]dx$$

$$= \frac{-i\hbar}{L}\left(0 + \frac{2\pi}{L}\left(\frac{2L}{3\pi}\right)e^{i(E_1-E_2)t/\hbar} - \frac{\pi}{L}\left(\frac{4L}{3\pi}\right)e^{-i(E_1-E_2)t/\hbar} + 0\right)$$

$$= \frac{-i\hbar}{L}\left(\frac{4}{3}e^{i(E_1-E_2)t/\hbar} - \frac{4}{3}e^{-i(E_1-E_2)t/\hbar}\right)$$

$$= -i\hbar\frac{4}{3L}\left(2i\sin\left(\frac{(E_1-E_2)t}{\hbar}\right)\right)$$

$$\boxed{\langle P\rangle(t) = \frac{8\hbar}{3L}\sin\left(\frac{(E_1-E_2)t}{\hbar}\right)}$$

At $t=0$, we have $\langle x\rangle(t=0) = 16L/9\pi^2$ and $\langle P\rangle(t=0)=0$, as expected from parts (b) and (c).

We will have $\langle P\rangle(t)$ at a maximum when $\frac{(E_1-E_2)t}{\hbar} = c\frac{\pi}{2}$ or $t = c\frac{\pi\hbar}{2(E_1-E_2)}$ where $c = 1,5,9,\ldots$ This is where $\langle x\rangle(t)$ will be zero, which will also occur for $c = 3,7,11,\ldots$ (odd c). At these values, $\langle P\rangle(t)$ is at a minimum.

We will have $\langle x\rangle(t)$ at a maximum when $c = 0,4,8,\ldots$ and $\langle x\rangle(t)$ at a minimum when $c = 2,6,10,\ldots$ At even values of c, $\langle P\rangle(t)$ is zero.

This makes sense due to the uncertainty principle.