12.

**Problem 2.6** A particle in the infinite square well has as its initial wave function an even mixture of the first two stationary states:

$$\Psi(x,0) = A[\psi_1(x) + \psi_2(x)].$$

**(a)** Normalize $\Psi(x,0)$. (That is, find $A$. This is very easy if you exploit the orthonormality of $\psi_1$ and $\psi_2$. Recall that, having normalized $\Psi$ at $t=0$, you can rest assured that it *stays* normalized—if you doubt this, check it explicitly after doing part b.)

**(b)** Find $\Psi(x,t)$ and $|\Psi(x,t)|^2$. (Express the latter in terms of sinusoidal functions of time, eliminating the exponentials with the help of **Euler's formula**: $e^{i\theta} = \cos\theta + i\sin\theta$.) Let $\omega \equiv \pi^2\hbar/2ma^2$.

**(c)** Compute $\langle x\rangle$. Notice that it oscillates in time. What is the frequency of the oscillation? What is the amplitude of the oscillation? (If your amplitude is greater than $a/2$, go directly to jail.)

**(d)** Compute $\langle p\rangle$. (As Peter Lorre would say, "Do it ze *kveek* vay, Johnny!")

**(e)** Find the expectation value of $H$. How does it compare with $E_1$ and $E_2$?

**(f)** A *classical* particle in this well would bounce back and forth between the walls. If its energy is equal to the expectation value you found in (e), what is the frequency of the classical motion? How does it compare with the quantum frequency you found in (c)?

ⓐ The normalization of a wavefunction is:

$$\int_{-\infty}^{\infty} \Psi^*(x)\,\Psi(x)\,dx = \int_{-\infty}^{\infty} |\Psi(x)|^2\,dx = 1$$

$$|\Psi(x,0)|^2 = \Psi^*(x,0)\cdot\Psi(x,0) = A^*\left(\psi_1^*(x) + \psi_2^*(x)\right)\cdot A\left(\psi_1(x) + \psi_2(x)\right) =$$

$$= A^*A\cdot\left[\psi_1^*(x)\,\psi_1(x) + \psi_1^*(x)\,\psi_2(x) + \psi_2^*(x)\,\psi_1(x) + \psi_2^*(x)\,\psi_2(x)\right]$$

$$\int_{-\infty}^{\infty} |\Psi(x,0)|^2\,dx = |A|^2\left\{\int_{-\infty}^{\infty}|\psi_1(x)|^2\,dx + \int_{-\infty}^{\infty}\psi_1^*(x)\,\psi_2(x)\,dx + \int_{-\infty}^{\infty}\psi_2^*(x)\,\psi_1(x)\,dx\ +\right.$$

$$\left. + \int_{-\infty}^{\infty}|\psi_2(x)|^2\,dx\right\} = 1$$

⊛ $\int_{-\infty}^{\infty}|\psi_1(x)|^2\,dx = \int_{-\infty}^{\infty}|\psi_2(x)|^2\,dx = 1 \longrightarrow$ by the normalization condition

$\circledast$ $\int_{-\infty}^{\infty} \psi_1^*(x)\,\psi_2(x)\,dx = \int_{-\infty}^{\infty} \psi_2^*(x)\,\psi_1(x)\,dx = 0 \longrightarrow$ because $\psi_1$ and $\psi_2$ are orthogonal

So we end up with:

$$|A|^2 \{1 + 0 + 0 + 1\} = 1 \implies \boxed{A = \frac{1}{\sqrt{2}}}$$

(b) Recalling the results of a confined particle:

$$\psi_1(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}x\right) \longrightarrow E_1 = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 = \hbar\omega \quad \left(\frac{\pi^2\hbar}{2mL^2} = \omega\right)$$

$$\psi_2(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi}{L}x\right) \longrightarrow E_2 = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 4 = 4E_1 = 4\hbar\omega$$

The wavefunction in general is:

$$\psi(r,t) = \sum_i C_{E_i}\psi_{E_i}(x)\, e^{-i\frac{E_i}{\hbar}t} = \frac{1}{\cancel{\sqrt{2}}}\left[\sqrt{\frac{\cancel{2}}{L}} \sin\left(\frac{\pi}{L}x\right) e^{-i\frac{E_1}{\hbar}t} + \sqrt{\frac{\cancel{2}}{L}} \sin\left(\frac{2\pi}{L}x\right) e^{-i\frac{E_2}{\hbar}t}\right] =$$

$$\boxed{\psi(x,t) = \sqrt{\frac{1}{L}}\left[\sin\left(\frac{\pi}{L}x\right) e^{-i\frac{E_1}{\hbar}t} + \sin\left(\frac{2\pi}{L}x\right) e^{-i\frac{4E_1}{\hbar}t}\right]}$$

To get $|\psi(x,t)|^2$ we do these first calculations:

$\circledast$ $\sin\left(\frac{\pi}{L}x\right) e^{+i\frac{E_1}{\hbar}t} \cdot \sin\left(\frac{\pi}{L}x\right) e^{-i\frac{E_1}{\hbar}t} = \sin^2\left(\frac{\pi}{L}x\right)$

$\circledast$ $\sin\left(\frac{\pi}{L}x\right) e^{+i\frac{E_1}{\hbar}t} \cdot \sin\left(\frac{2\pi}{L}x\right) \cdot e^{-i\frac{4E_1}{\hbar}t} = \sin\left(\frac{\pi}{L}x\right) \sin\left(\frac{2\pi}{L}x\right) e^{-i\frac{3E_1}{\hbar}t} =$

$= \sin\left(\frac{\pi}{L}x\right) \sin\left(\frac{2\pi}{L}x\right)\left[\cos(3\omega t) - i\sin(3\omega t)\right]$

$\circledast$ $\sin\left(\frac{\pi}{L}x\right) e^{-i\frac{E_1}{\hbar}t} \sin\left(\frac{2\pi}{L}x\right) e^{+i\frac{4E_1}{\hbar}t} = \sin\left(\frac{\pi}{L}x\right) \sin\left(\frac{2\pi}{L}x\right) e^{+i\frac{3E_1}{\hbar}t} =$

$= \sin\left(\frac{\pi}{L}x\right) \sin\left(\frac{2\pi}{L}x\right)\left[\cos(3\omega t) + i\sin(3\omega t)\right]$

$\circledast$ $\sin\left(\frac{2\pi}{L}x\right) e^{+i\frac{4E_1}{\hbar}t} \cdot \sin\left(\frac{2\pi}{L}x\right) e^{-i\frac{4E_1}{\hbar}t} = \sin^2\left(\frac{2\pi}{L}x\right)$

Adding everything:

$$\boxed{|\Psi_{(x,t)}|^2 = \frac{1}{L}\left[\sin^2\left(\frac{\pi}{L}x\right) + \sin^2\left(\frac{2\pi}{L}x\right) + 2\sin\left(\frac{\pi}{L}x\right)\sin\left(\frac{2\pi}{L}x\right)\cos(3\omega t)\right]}$$

## Ⓒ Computing $\langle x \rangle$

For an observable in general: $\langle \hat{O}(t) \rangle = \int \Psi^*_{(\vec{r},t)}\, \hat{O}\, \Psi_{(\vec{r},t)}\, d\vec{r}$

$$\langle x \rangle = \int_{-\infty}^{\infty} \Psi^*_{(x,t)} \, x \, \Psi_{(x,t)}\, dx = \int_0^L \Psi^*_{(x,t)} \, x \, \Psi_{(x,t)}\, dx = \frac{1}{L}\int_0^L x\, |\Psi_{(x,t)}|^2\, dx =$$

$$= \frac{1}{L}\left[\underbrace{\int_0^L x \sin^2\left(\frac{\pi}{L}x\right) dx}_{1} + \underbrace{\int_0^L x \sin^2\left(\frac{2\pi}{L}x\right) dx}_{2} + \cos(3\omega t)\underbrace{\int_0^L 2x \sin\left(\frac{\pi}{L}x\right)\sin\left(\frac{2\pi x}{L}\right) dx}_{3}\right.$$

① $$\int_0^L x \cdot \left[\frac{1}{2} - \frac{1}{2}\cos\left(\frac{2\pi}{L}x\right)\right] = \int_0^L \frac{x}{2} - \cancelto{0}{\int_0^L \frac{1}{2} x \cos\left(\frac{2\pi}{L}x\right) dx} = \left[\frac{x^2}{4}\right]_0^L = \frac{L^2}{4}$$

The period of $\cos(ax)$ is $T = \frac{2\pi}{a}$ so $\Rightarrow T = \frac{2\pi}{\frac{2\pi}{L}} = L$. Also $x$ is an odd function and $\cos\left(\frac{2\pi}{L}x\right)$ is an even function $\Rightarrow x\cos\left(\frac{2\pi}{L}x\right)$ is an odd function. Integrating this from 0 to L makes the integral equal to zero

② $$\int_0^L x \sin^2\left(\frac{2\pi}{L}x\right) dx = \int_0^L \frac{x}{2} dx - \cancelto{0}{\int_0^L \frac{1}{2} x \cos\left(\frac{4\pi}{L}x\right) dx} = \frac{L^2}{4}$$

We use the same argument here but instead of being one period of cosine there are 2.

$2\sin a \cdot \sin b = \cos(a-b) - \cos(a+b)$

③ $$\int_0^L 2x \sin\left(\frac{\pi}{L}x\right)\sin\left(\frac{2\pi}{L}x\right) dx = \int_0^L x\cos\left(\frac{\pi}{L}x\right) dx - \int_0^L x \cos\left(\frac{3\pi}{L}x\right) dx = \begin{matrix}\text{D-I} \\ \text{method}\end{matrix}$$

| | D | I |
|---|---|---|
| + | $x$ | $\cos(\alpha x)$ |
| − | $1$ | $\frac{1}{\alpha}\sin(\alpha x)$ |
| + | $0$ | $-\frac{1}{\alpha^2}\cos(\alpha x)$ |

$$= \left[\frac{L}{\pi} x \sin\left(\frac{\pi}{L}x\right) + \frac{L^2}{\pi^2}\cos\left(\frac{\pi}{L}x\right)\right]_0^L$$

$$- \left[\frac{L}{3\pi} x \sin\left(\frac{3\pi}{L}x\right) + \frac{L^2}{9\pi^2}\cos\left(\frac{3\pi}{L}x\right)\right]_0^L =$$

$$= \left[0 + (-1)\frac{L^2}{\pi^2} - \left(0 + \frac{L^2}{\pi^2}(1)\right)\right] - \left[\left(0 + (-1)\cdot\frac{L^2}{9\pi^2} - \left(0 + \frac{L^2}{9\pi^2}\right)\right)\right] =$$

$$= -2\frac{L^2}{\pi^2} + \frac{2}{9}\frac{L^2}{\pi^2} = -\frac{16}{9}\frac{L^2}{\pi^2}$$

Adding all the elements:

$$\langle x\rangle = \frac{1}{\cancel{L}}\cdot\left[\frac{L^{\cancel{2}}}{4} + \frac{L^{\cancel{2}}}{4} - \frac{16L^{\cancel{2}}}{9\pi^2}\cos(3\omega t)\right] \Rightarrow \boxed{\langle x\rangle = \frac{L}{2}\left[1 - \frac{32}{9\pi^2}\cos(3\omega t)\right]}$$

$$\boxed{\begin{aligned}&\text{Amplitude} = \frac{16L}{9\pi^2} \simeq 0{,}36\,\frac{L}{2}\\ &\text{Frequency} = 3\omega\end{aligned}}$$

(d) Compute $\langle p\rangle$

$$\hat{p} = -i\hbar\frac{d}{dx} \longrightarrow \langle p\rangle = \int_0^L \psi^*_{(x,t)}\,\hat{p}\,\psi_{(x,t)}\,dx$$

$$\hat{p}\,\psi_{(x,t)} = -i\hbar\sqrt{\frac{1}{L}}\;\frac{d}{dx}\left[\sin\left(\frac{\pi}{L}x\right)e^{-i\omega t} + \sin\left(\frac{2\pi}{L}x\right)e^{-i4\omega t}\right] =$$

$$= +i\hbar\sqrt{\frac{1}{L}}\cdot\frac{L}{\pi}\left[\cos\left(\frac{\pi}{L}x\right)e^{-i\omega t} + \frac{1}{2}\cos\left(\frac{2\pi}{L}x\right)e^{-i4\omega t}\right]$$

$$\psi^*_{(x,t)}\,\hat{p}\,\psi_{(x,t)} = \cancel{\sqrt{\frac{1}{L}}}\left[\sin\left(\frac{\pi}{L}x\right)e^{+i\omega t} + \sin\left(\frac{2\pi}{L}x\right)e^{+i4\omega t}\right]\cdot$$

$$\cdot\; i\hbar\cancel{\sqrt{\frac{1}{L}}}\cdot\frac{\cancel{L}}{\pi}\left[\cos\left(\frac{\pi}{L}x\right)e^{-i\omega t} + \frac{1}{2}\cos\left(\frac{2\pi}{L}x\right)e^{-i4\omega t}\right] =$$

$$= \frac{i\hbar}{\pi}\left[\underset{①}{\sin\left(\frac{\pi}{L}x\right)\cos\left(\frac{\pi}{L}x\right)} + \underset{②}{\frac{1}{2}\sin\left(\frac{\pi}{L}x\right)\cos\left(\frac{2\pi}{L}x\right)e^{-i3\omega t}} + \underset{③}{\sin\left(\frac{2\pi}{2}x\right)\cos\left(\frac{\pi}{L}x\right)e^{+i3\omega t}} +\right.$$

$$\left. + \underset{④}{\frac{1}{2}\sin\left(\frac{2\pi}{L}x\right)\cos\left(\frac{2\pi}{L}x\right)}\right]$$

We now split in several integrals:

(1) $\rightarrow \displaystyle\int_0^L \sin\left(\frac{\pi}{L}x\right)\cos\left(\frac{\pi}{L}x\right)dx = \frac{1}{2}\int_0^L \sin\left(\frac{2\pi}{L}x\right)dx = 0$

$2\sin(a)\cos(b) = \sin(a+b) + \sin(a-b)$

Here we have again an odd function in a period $T = \frac{2\pi}{\frac{2\pi}{L}} = L$

To simplify we do: $\alpha = \frac{1}{2}e^{-i3\omega t}$ $\quad\beta = e^{+i3\omega t}$

(2) $\rightarrow \displaystyle\alpha\int_0^L \sin\left(\frac{\pi}{L}x\right)\cos\left(\frac{2\pi}{L}x\right)dx = \frac{\alpha}{2}\left[\int_0^L \sin\left(\frac{3\pi}{L}x\right) - \int_0^L \sin\left(\frac{\pi}{L}x\right)dx\right] =$

$$= \frac{\alpha}{2}\left(-\frac{L}{3\pi}\left[\cos\left(\frac{3\pi}{L}x\right)\right]_0^L + \frac{L}{\pi}\left[\cos\left(\frac{\pi}{L}x\right)\right]_0^L\right) = \frac{\alpha}{2}\left(\frac{2L}{3\pi} - \frac{2L}{\pi}\right) = -\frac{2\alpha L}{3\pi} =$$

$$= -\frac{L}{3\pi}e^{-i3\omega t}$$

(3) $\rightarrow \displaystyle\beta\int_0^L \sin\left(\frac{2\pi}{L}x\right)\cos\left(\frac{\pi}{L}x\right)dx = \frac{\beta}{2}\left[\int_0^L \sin\left(\frac{3\pi}{L}x\right)dx + \int_0^L \sin\left(\frac{\pi}{L}x\right)dx\right] =$

$$\frac{\beta}{2}\left(\frac{2L}{3\pi} + \frac{2L}{\pi}\right) = \frac{4\beta L}{3\pi} = \frac{4L}{3\pi}e^{+i3\omega t}$$

(4) $\rightarrow \displaystyle\frac{1}{2}\int_0^L \sin\left(\frac{2\pi}{L}x\right)\cos\left(\frac{2\pi}{L}x\right)dx = \frac{1}{4}\int_0^L \sin\left(\frac{4\pi}{L}x\right)dx = 0$ Two periods of the function from 0 to L

Adding everything:

$$\langle p\rangle = \frac{i\hbar}{\pi}\left[0 - \frac{L}{3\pi}e^{-i3\omega t} + \frac{4L}{3\pi}e^{+i3\omega t} + 0\right] = \frac{\hbar L}{\pi^2}e^{+i\pi/2}\left(e^{-i3\omega t} + e^{i3\omega t}\right) =$$

$$= 2\frac{\hbar L}{\pi^2}\cos\left(3\omega t + \frac{\pi}{2}\right) = -\frac{2\hbar L}{\pi^2}\cancel{\sin(3\omega t)}$$

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**13.**

For the asymmetric quantum well worked out in class ($E$=4.85 µeV, $V_1$= 5 µeV and a = 1 µm):

a. compute the electron wavevector k inside the well
b. compute the electron wavevector $k_1$ inside the left barrier
c. compute the shift $\delta$ and the probability densities C and $B_1$
d. write the specific form of the eigenfunctions (i) inside the well and (ii) inside the left barrier
e. compute the probability of finding the electron in the "whole" region [0,-d] on the left of the well
f. compute and plot the probability of finding the electron at a "specific" distance $-d_0$ to the left of the well, as $d_0$ varies from 0 to 5 µm.