Particle Moving in a Box

a)
$$\Psi(x,t) = \frac{1}{\sqrt{2}}\psi_1(x)e^{-i\frac{E_1 t}{\hbar}} + \frac{1}{\sqrt{2}}\psi_2(x)e^{-i\frac{E_2 t}{\hbar}}$$

b) See Matlab code and plots

c)
$$\langle \hat{H} \rangle = \langle \Psi | \hat{H} | \Psi \rangle$$

$$= \frac{1}{2}\left(\left(\langle \psi_1 | e^{+i\frac{E_1 t}{\hbar}} + \langle \psi_2 | e^{+i\frac{E_2 t}{\hbar}} \right) \left(E_1 e^{-iE_1 t/\hbar} | \psi_1 \rangle + E_2 e^{-iE_2 t/\hbar} | \psi_2 \rangle \right) \right)$$

$$\boxed{\langle \hat{H} \rangle = \frac{1}{2}(E_1 + E_2)} \text{ independent of time.} \quad (1)$$

We have made use of the facts that the $|\psi_n\rangle$ are orthognol and normalized.

d)
$$\langle x \rangle(t) = \langle \Psi(x,t) | \hat{x} | \Psi(x,t) \rangle$$

Now the key thing to realize here is to use the symmetry of the wavefunctions about $x = L/2$, the center of the box.

Let's recognize that

$$x = x - L/2 + L/2$$

and
$$\langle L/2 \rangle = L/2 \quad \text{b/c } \psi \text{ is normalized}$$

Now $x - L/2$ is odd about $L/2$, so examining the integrals

$$\langle \psi_1 | (x - L/2) | \psi_1 \rangle = \left(\tfrac{2}{L}\right)\int_0^L dx \, \sin\left(\tfrac{\pi x}{L}\right)(x - L/2)\sin\left(\tfrac{\pi x}{L}\right)$$

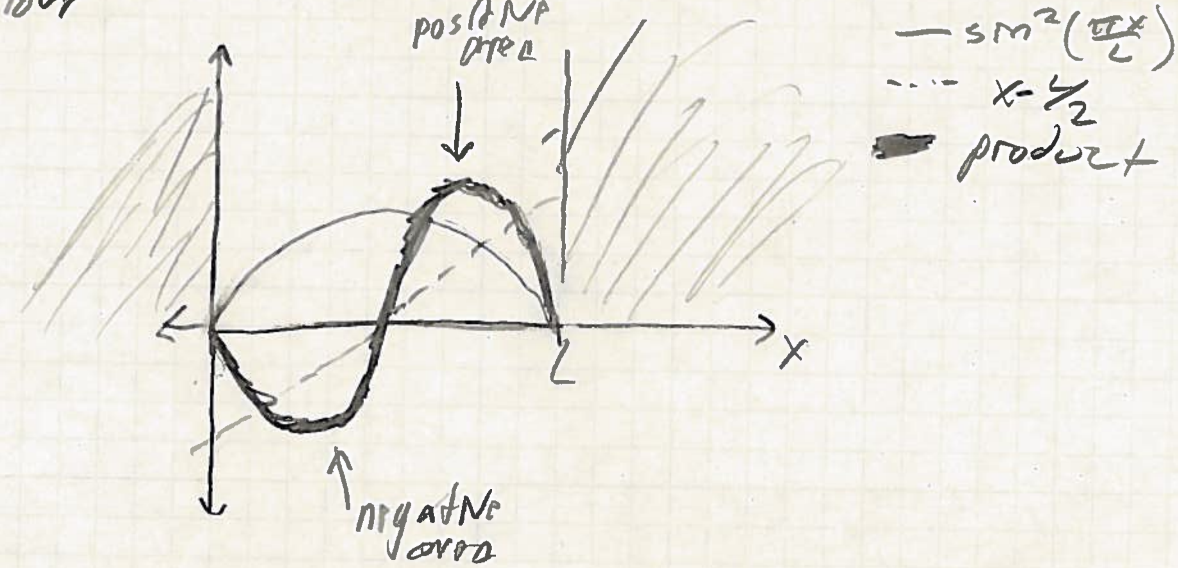
even about $L/2$

odd about $L/2$

even about $L/2$

since even x even x odd = odd

The integrand is odd about $L/2$ and the area will be zero. This is illustrated below



similarly for

$$\langle \psi_2 | (x - L/2) | \psi_2 \rangle = \int \text{odd} \times \text{odd} \times \text{odd}$$

odd odd odd

$$= \int \text{odd} = \emptyset$$

Now for the cross terms

$$\langle \psi_1 | (x - L/2) | \psi_2 \rangle \neq 0$$

even odd odd

So we need to evaluate the integral

$$\langle \psi_1 | (x - L/2) | \psi_2 \rangle = \frac{2}{L}\int_0^L dx \sin\left(\frac{\pi x}{L}\right)(x - L/2)\sin\left(\frac{2\pi x}{L}\right)$$

Using the orthogonality of $\langle \psi_1 | \psi_2 \rangle = 0$ we can throw away the $-L/2$ term.

$$\frac{2}{L}\int_0^L dx \sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right) x$$

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

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

Use integration by parts

$$\int_a^b u\,dv = uv\Big|_a^b - \int_a^b v\,du$$

$u = x$ $\qquad dv = dx \sin^2\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right)$

$du = dx$

$$v = \int dv = \int dx \sin^2\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right)$$

$z = \sin\left(\frac{\pi x}{L}\right)$

$dz = \cos\left(\frac{\pi x}{L}\right)\frac{\pi}{L}dx$

$$= \frac{L}{\pi}\int dz\, z^2$$

$$= \frac{L}{\pi}\frac{z^3}{3} = \frac{L}{3\pi}\sin^3\left(\frac{\pi x}{L}\right)$$

So we want

$$\int u\,dv = \frac{L}{3\pi} \cancel{x \sin^3\left(\frac{\pi x}{L}\right)\Big|_0^L} \xrightarrow{} 0 \text{ at both bounds} - \int_0^L dx\, \frac{L}{3\pi} \sin^3\left(\frac{\pi x}{L}\right)$$

$$\sin^3\left(\frac{\pi x}{L}\right) = \sin\left(\frac{\pi x}{L}\right)\left(1 - \cos^2\left(\frac{\pi x}{L}\right)\right)$$

so now using $z = \cos\left(\frac{\pi x}{L}\right)$ $dz = -\sin\left(\frac{\pi x}{L}\right)\frac{\pi}{L}dx$

$$-\int_a^b dx\, \frac{L}{3\pi} \sin^3\left(\frac{\pi x}{L}\right) = +\frac{L}{3\pi}\frac{L}{\pi}\int_1^{-1} dz\,(1-z^2)$$

$$= \frac{-L^2}{3\pi^2}\int_{-1}^{1} dz\,(1-z^2)$$

$$= \frac{-L^2}{3\pi^2}\left(2 - \frac{2}{3}\right)$$

$$= \frac{-L^2}{3\pi^2}\frac{4}{3} = \frac{-4L^2}{9\pi^2}$$

so putting it all together, we will have

$$\langle x - L/2 \rangle = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}\langle \psi_1 | x - L/2 | \psi_2 \rangle e^{-i(E_2 - E_1)t/\hbar}$$

$$+ \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}\langle \psi_2 | (x - L/2) | \psi_1 \rangle e^{+i(E_2 - E_1)t/\hbar}$$

$$= \frac{1}{2}\frac{-4}{\cancel{L}}\left(\frac{4L^{\cancel{2}}}{9\pi^2}\right)\underbrace{\left(e^{-i\omega t} + e^{i\omega t}\right)}_{2\cos(\omega t)} \qquad \text{w/ } \omega \equiv \frac{E_2 - E_1}{\hbar}$$

$$= \frac{-16}{9\pi^2} L \cos(\omega t)$$

So

$$\langle \hat{x} \rangle(t) = \frac{L}{2} + \langle x - L/2 \rangle$$

$$= \frac{L}{2} - \frac{16}{9\pi^2} L \cos(\omega t)$$

This is also confirmed numerically in the MATLAB code.

Table of Contents


```
%ParticleMovingInBox
%
%This script makes plots of a superposition of two states in a box.
%
%Tom Allison 8/8/2013

set(0,'DefaultLineLineWidth',2);
```

Preliminaries

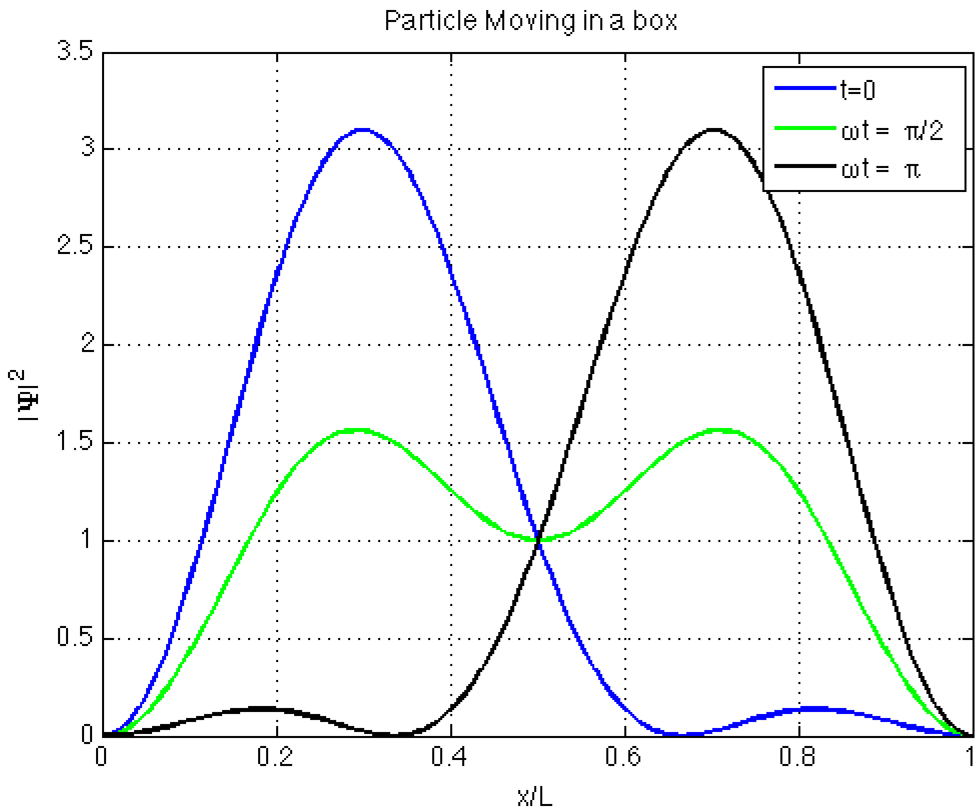
```
L = 1; %Define length of box
x = linspace(0,L); % make linearly spaced array for x-axis
psi1 = sqrt(2/L)*sin(pi*x/L); %first stationary state.
psi2 = sqrt(2/L)*sin(2*pi*x/L); %second stationary state.
```

Add stationary states with appropriate relative phase.

The thing to realize here is that all that matters is the relative phase between the stationary states, because an overal phase of the wavefunction does not matter in quantum mechanics.

```
psi_t0 = 1/sqrt(2)*psi1 + 1/sqrt(2)*psi2; % no phase factors at t=0;
psi_t1 = 1/sqrt(2)*psi1 + 1/sqrt(2)*psi2*exp(-i*pi/2); % DeltaE*t/hbar = pi/2
psi_t2 = 1/sqrt(2)*psi1 + 1/sqrt(2)*psi2*exp(-i*pi); % % DeltaE*t/hbar = pi

figure(1);
h0 = plot(x,psi_t0.*conj(psi_t0),'b');
hold on
h1 = plot(x,psi_t1.*conj(psi_t1),'g');
h2 = plot(x,psi_t2.*conj(psi_t2),'k');
hold off
xlabel('x/L');
ylabel('|\Psi|^2');
grid on
legend([h0,h1,h2],'t=0','\omegat = \pi/2','\omegat = \pi');
title('Particle Moving in a box');
setfigfont(1,14);
```



Check integral from part d)

```
dx = x(2)-x(1); % construct dx from difference of first two points.
xbar0 = dx*trapz(conj(psi_t0).*x.*psi_t0) %perform trapezoidal integration.

%compare to the analytical result
xbar0_analytical = L/2 - 16/(9*pi^2)*L*cos(0)
```

```
xbar0 =

    0.3199


xbar0_analytical =

    0.3199
```

Published with MATLAB® 8.0