I. A. Sketch $\psi_5^*(x)\psi_5(x)$ vs. $x$, where $\psi_5(x)$ is the $n = 5$ wavefunction of a particle in a box. Describe, in a few words, each of the essential qualitative features of your sketch.

This is a probability density for $n = 5$ of a PIB. There are $n - 1 = 4$ nodes. The nodes are equally spaced. Each lobe between consecutive nodes is a half-cycle of $\sin\left(\frac{5\pi x}{a}\right)^2$ with maximum height of $(2/a)$. 

$$E_5 = \frac{\hbar^2}{8ma^2}(25)$$
B. Sketch $\psi_5^*(x)\psi_5(x)$ vs. $x$, where $\psi_5(x)$ is the $v = 5$ wavefunction of a harmonic oscillator. Describe, in a few words, each of the essential qualitative features of this sketch.

This is a probability density for $v = 5$ of a H.O. There are $v = 5$ nodes. One node is at $x = 0$. The 2, 3, 4 nodes are close together because the classical $p(x)$ function is largest near $x = 0$ and $\lambda = h/p$. The 1 and 5 nodes are closer to the turning points at $x_\pm = [2(h\omega 5.5)/k]^{1/2}$ than to the 2 and 4 nodes. The outer lobes have the largest maximum height and area, but cannot finish at $\psi_5^*\psi_5 = 0$ at $x_\pm[11h\omega/k]^{1/2}$, thus have exponentially decreasing tails in the classically forbidden $E < V(x)$ regions.
C. (i) Sketch $\psi_1(x)$ and $\psi_2(x)$ for a particle in a box where there is a small and thin barrier in the middle of the box, as shown on this $V(x)$:

The wavefunctions look like this:

![Wavefunctions](image)

The barrier has a negligible effect on the $n = 2$ energy and wavefunction. However, the $n = 1$ wave function tries to go to zero near $x = a/2$, but it is not allowed to actually cross zero, because that would generate an extra node. In order for $\psi_1(x)$ to approach 0 at $x = a/2$, the $E_1$ energy increases until it lies just barely below $E_2$.

(ii) Make a very approximate estimate of $E_2 - E_1$ for this PIB with a thin barrier in the middle. Specify whether $E_2 - E_1$ is smaller than or larger than $3\frac{\hbar^2}{8ma^2}$, which is the energy level spacing between the $n = 2$ and $n = 1$ energy levels of a PIB without a barrier in the middle.

$$0 < E_2 - E_1 \ll \frac{\hbar^2}{8ma^2}3 = E_2^{(0)} - E_1^{(0)}.$$  

D. Consider the half harmonic oscillator, which has $V(x) = \frac{1}{2}kx^2$ for $x < 0$ and $V(x) = \infty$ for $x \leq 0$. The energy levels of a full harmonic oscillator are

$$E(v) = \hbar\omega(v + 1/2)$$

where $\omega = \sqrt{[k/\mu]}$. Sketch the $v = 0$ and $v = 1$ $\psi_v(x)$ of the half harmonic oscillator and say as much as you can about a general energy level formula for the half harmonic oscillator. A little speculation might be a good idea.
For the half-harmonic oscillator, the $v = 0$ wave function is the left half of the $v = 1$ wave function of the full harmonic oscillator. The $v = 2$ wave function is the left half of the $v = 3$ wave function of the full HO.

<table>
<thead>
<tr>
<th>Half HO</th>
<th>Full HO</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E(v = 0) = \frac{3}{2} \hbar \omega$</td>
<td>$E(v = 0) = \frac{1}{2} \hbar \omega$</td>
</tr>
<tr>
<td>$E(v = 1) = \frac{7}{2} \hbar \omega$</td>
<td>$E(v = 1) = \frac{3}{2} \hbar \omega &gt; 1 \hbar \omega$</td>
</tr>
</tbody>
</table>

E. Give exact energy level formulas (expressed in terms of $k$ and $\mu$) for a harmonic oscillator with reduced mass, $\mu$, where

(i) $V(x) = \frac{1}{2} k x^2 + V_0$

$$E(v) = V_0 + \hbar \omega (v + \frac{1}{2})$$

(ii) $V(x) = \frac{1}{2} k (x - x_0)^2$

$$E(v) = \hbar \omega (v + \frac{1}{2})$$

(iii) $V(x) = \frac{1}{2} k' x^2$ where $k' = 4k$

$$E(v) = \hbar \left[ \frac{k'}{\mu} \right]^{1/2} (v + \frac{1}{2})$$

$$k' = 4k$$

$$E(v) = \hbar 2 \left[ \frac{k}{\mu} \right]^{1/2} (v + \frac{1}{2}) = 2 \hbar \omega (v + 1/2)$$
II. PROMISE KEPT: FREE PARTICLE

\[ \hat{H} = \frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} + V_0 \]
\[ \psi(x) = ae^{ikx} + be^{-ikx} \]

A. Is \( \psi(x) \) an eigenfunction of \( \hat{H} \)? If so, what is the eigenvalue of \( \hat{H} \), expressed in terms of \( \hbar, m, V_0, \) and \( k \)?

\[ \hat{H}\psi = -\frac{\hbar^2}{2m}[(ik)^2ae^{ikx} + (-ik)^2be^{-ikx}] \]
\[ = \frac{\hbar^2k^2}{2m}[ae^{ikx} + be^{-ikx}] \]
\( \psi \) is an eigenfunction of \( \hat{H} \) with eigenvalue \( \frac{\hbar^2k^2}{2m} \).

B. Is \( \psi(x) \) an eigenfunction of \( \hat{p} \)? Your answer must include an evaluation of \( \hat{p}\psi(x) \).

\[ \hat{p}\psi = -i\hbar[(ik)ae^{ikx} + (-ik)be^{-ikx}] \]
\[ = \hbar k[ae^{ikx} - be^{-ikx}] \]
\( \psi \) is not an eigenfunction of \( \hat{p} \).

C. Write a complete expression for the expectation value of \( \hat{p} \), without evaluating any of the integrals present in \( \langle \hat{p} \rangle \). [see answer in part D.]

D. Taking advantage of the fact that
\[ \int_{-\infty}^{\infty} dx e^{ix} = 0 \]
compute \( \langle \hat{p} \rangle \), the expectation value of \( \hat{p} \).

\[ \langle \hat{p} \rangle = \frac{\int dx \psi^* \hat{p}\psi}{\int dx \psi^* \psi} \]
\[ = \frac{\int dx \hbar k[a^*e^{-ikx} + b^*e^{ikx}][ae^{ikx} - be^{-ikx}]}{\int dx [a^*e^{-ikx} + b^*e^{ikx}][ae^{ikx} + be^{-ikx}]} \]
\[ = \frac{\hbar k}{\int dx [a^2 + |b|^2]} \]
\[ = \hbar k \frac{|a|^2 - |b|^2}{|a|^2 + |b|^2} \]
E. Suppose you perform a “click-click” experiment on this $\psi(x)$ where $a = -0.632$ and $b = 0.775$. One particle detector is located at $x = +\infty$ and another is located at $x = -\infty$. Let’s say you do 100 experiments. What would be the fraction of detection events at the $x = +\infty$ detector?

The $x = +\infty$ sees a particle at

$$f_+ = \frac{|a|^2}{|a|^2 + |b|^2} = \frac{0.40}{0.40 + 0.60} = 40\%$$

of the time.

F. What is the expectation value of $\hat{H}$?

In part A. we found that

$$\hat{H}\psi(x) = \frac{\hbar^2 k^2}{2m} \psi(x)$$

$$\langle \hat{H} \rangle = \frac{\int dx \psi^* \hat{H} \psi}{\int dx \psi^* \psi} = \frac{\hbar^2 k^2}{2m} \int dx \psi^* \psi = \frac{\hbar^2 k^2}{2m}.$$ 

If $\psi$ is an eigenstate of the measurement operator, every measurement yields the eigenvalue of $\psi$. The expectation value is the eigenvalue!
III. a and $a^\dagger$ FOR HARMONIC OSCILLATOR

$$a\psi_v = v^{1/2}\psi_{v-1}$$
$$a^\dagger\psi_v = (v+1)^{1/2}\psi_{v+1}$$
$$\hat{N}\psi_v = v\psi_v \text{ where } \hat{N} = a^\dagger a$$

A. Show that $[a^\dagger, a]$ by applying this commutator to $\psi_v$.

$$[a^\dagger, a] = a^\dagger a - aa^\dagger$$
$$[a^\dagger, a] \psi_v = a^\dagger a\psi_v - a a^\dagger \psi_v$$
$$= a^\dagger v^{1/2}\psi_{v-1} - a(v + 1)^{1/2}\psi_{v+1}$$
$$= v^{1/2} v^{1/2} \psi_v - (v + 1)^{1/2}(v + 1)^{1/2} \psi_v$$
$$= [v - (v + 1)]\psi_v = (-1)\psi_v$$
$$[a^\dagger, a] = -1$$

B. Evaluate the following expressions (it is not necessary to explicitly multiply out all of the factors of $v$).

(i) $(a^\dagger)^2(a)^5\psi_3$

$$(a^\dagger)^2(a)^5\psi_3 = 0 \text{ because } a^5\psi_3 = a^2\psi_0(3 \cdot 2 \cdot 1)^{1/2} \text{ but } a\psi_0 = 0.$$  

(ii) $(a)^5(a^\dagger)^2\psi_3$

$$(a)^5(a^\dagger)^2\psi_3 = (a)^5(3 \cdot 2 \cdot 5)^{1/2}(4 \cdot 5)^{1/2} \psi_0.$$

(iii) $\int dx\psi_3(a^\dagger)^3\psi_0$

$$\int dx\psi_3(a^\dagger)^3\psi_0 = (1 \cdot 2 \cdot 3)^{1/2}.$$  

(iv) What is the selection rule for non-zero integrals of the following operator product $(a^\dagger)^2(a)^5(a^\dagger)^4$?

$$\Delta v = 2 + 4 - 5 = +1.$$  

(v) $(a + a^\dagger)^2 = a^2 + aa^\dagger + a^\dagger a + a^\dagger a^\dagger$. Simplify using $a^2 + a^\dagger a$ to yield an expression containing $a^2 + a^\dagger a$ terms that involve $\hat{N} = a^\dagger a$ and a constant.

$$ (a + a^\dagger)^2 = a^2 + a^\dagger a + a^\dagger a^\dagger \hat{N} $$

$$ aa^\dagger = [a, a^\dagger] + a^\dagger a = 1 + \hat{N} $$

$$ (a + a^\dagger)^2 = a^2 + a^\dagger a + 2\hat{N} + 1 $$
IV. TIME-DEPENDENT WAVE EQUATION AND PIB SUPERPOSITION

For the harmonic oscillator

\[ \hat{x} = \left( \frac{\hbar}{2\mu\omega} \right)^{1/2} (\hat{a}^\dagger + \hat{a}) \]
\[ \hat{p} = \left( \frac{\hbar\mu\omega}{2} \right)^{1/2} i(\hat{a}^\dagger - \hat{a}) \]
\[ \hat{N} = \hat{a}^\dagger \hat{a} \]
\[ \delta_{ij} = \int dx \psi_i^*(x) \psi_j, \text{ which means orthonormal } \{\psi_n\} \]
\[ \hat{H} \psi_n(x) = E_n \psi_n \text{ which means eigenvalues } \{E_n\} \]
\[ E_n = \hbar\omega \left( n + \frac{1}{2} \right) \]

Consider the time-dependent state

\[ \Psi(x, t) = 2^{1/2} \left[ e^{-iE_0 t/\hbar} \psi_0(x) + e^{-iE_1 t/\hbar} \psi_1(x) \right] \]
\[ = 2^{1/2} e^{-iE_0 t/\hbar} \left[ \psi_0(x) + e^{-i\hbar\omega t/\hbar} \psi_1(x) \right] \]

A. Sketch \( \Psi(x, 0) \) and \( \Psi(x, t = \pi/\omega) \)

\[ \Psi(x, 0) = \psi_0(x) + \psi_1(x) \]
\[ \Psi(x, \frac{\pi}{\omega}) = \psi_0(x) - \psi_1(x) \]
B. Compute \( \int dx \Psi^*(x,t) \hat{N} \Psi(x,t) \).

\[
\int dx \Psi^*(x,t) \hat{N} \Psi(x,t) = \frac{1}{2} \int dx (\psi_0^* + e^{i\omega t} \psi_1^*) \hat{N}(\psi_0 + e^{-i\omega t} \psi_1)
\]
\[
= \frac{1}{2} \int dx (\psi_0^* + e^{i\omega t} \psi_1^*)(0 + e^{-i\omega t} \psi_1)
\]
\[
= \frac{1}{2}
\]

because \( \hat{N} \psi_0 = 0 \psi_0 \)

C. Compute \( \langle \hat{H} \rangle = \int dx \Psi^*(x,t) \hat{H} \Psi(x,t) \) and comment on the relationship of \( \langle \hat{N} \rangle \) to \( \langle \hat{H} \rangle \).

\[
\hat{H} = \hbar \omega \left( \hat{N} + \frac{1}{2} \right)
\]
\[
\langle \hat{H} \rangle = \hbar \omega \left[ \langle \hat{N} \rangle + \langle \frac{1}{2} \rangle \right]
\]
\[
\langle \frac{1}{2} \rangle = \frac{1}{2}
\]
because \( \Psi \) is normalized to 1.

\[
\langle \hat{H} \rangle = \hbar \omega \left[ \frac{1}{2} + \frac{1}{2} \right] = \hbar \omega.
\]

This is not surprising because the average \( E \) in \( \Psi(x,t) \) is

\[
\frac{E_{v=0} + E_{v=1}}{2} = \hbar \omega
\]

and \( E \) is conserved.
D. Compute $\langle \hat{x} \rangle = \int dx \Psi^*(x, t) \hat{x} \Psi(x, t)$.

\[
\hat{x} = \left( \frac{\hbar}{2\mu \omega} \right)^{1/2} (\hat{a}^\dagger + \hat{a})
\]
\[
\hat{x} \Psi(x, t) = 2^{-1/2} e^{-iE_0 t / \hbar} \left( \frac{\hbar}{2\mu \omega} \right)^{1/2} (\hat{a}^\dagger + \hat{a})(\psi_0 + e^{-i\omega t} \psi_1)
\]
\[
= 2^{-1/2} e^{-i\omega t / 2} \left( \frac{\hbar}{2\mu \omega} \right)^{1/2} (\psi_1 + 2^{1/2} e^{-i\omega t} \psi_2 + e^{-i\omega t} \psi_0)
\]
\[
\Psi^* \hat{x} \Psi = \frac{1}{2} \left( \frac{\hbar}{2\mu \omega} \right)^{1/2} (\psi_0^* + e^{i\omega t} \psi_1^*)(e^{-i\omega t} \psi_0 + \psi_1 + 2^{1/2} e^{-i\omega t} \psi_2)
\]
\[
\langle \hat{x} \rangle \int dx \Psi^* \hat{x} \Psi = \frac{1}{2} \left( \frac{\hbar}{2\mu \omega} \right)^{1/2} (e^{-i\omega t} + e^{i\omega t} + 0)
\]
\[
= \frac{1}{2} \left( \frac{\hbar}{2\mu \omega} \right)^{1/2} 2 \cos\omega t.
\]

This reveals a phase ambiguity. The picture of $\Psi^*(x, 0)\Psi(x, 0)$ in Part IV.A. suggests that $\langle \hat{x} \rangle_t$ starts negative and oscillates cosinusoidally. But the calculation using $\hat{a}, \hat{a}^\dagger$ shows that $\langle \hat{x} \rangle_t$ starts positive at $t = 0$. This means that the implicit phase convention for $\psi_v(x)$ is outermost lobe positive not innermost lobe positive as assumed in part A.

E. Compute $\langle \hat{x}^2 \rangle$.

The selection rule for $\hat{x}^2$ is $\Delta v = \pm 2, 0$.

Since $\Psi(x, t)$ contains only $\psi_0$ and $\psi_1$, there will be no $\Delta v = \pm 2$ integrals. We only need the $\Delta v = 0$ part of $\hat{x}^2$.

\[
\hat{x}^2 = \left( \frac{\hbar}{2\mu \omega} \right) (\hat{a} + \hat{a}^\dagger)^2
\]
\[
= \left( \frac{\hbar}{2\mu \omega} \right) (\hat{a}^2 + \hat{a}^\dagger^2 + 2\hat{N} + 1)
\]

So we want $\frac{\hbar}{2\mu \omega} \langle 2\hat{N} + 1 \rangle$.

\[
\langle 2\hat{N} + 1 \rangle = 2 \langle \hat{\mathcal{H}} \rangle / \hbar \omega
\]
\[
\langle \hat{x}^2 \rangle = \left( \frac{\hbar}{2\mu \omega} \right) (2) = 2 \frac{\hbar}{2\mu \omega}.
\]
**F.** Based on your answer to part E, evaluate \( \langle \hat{V}(x) \rangle \).

\[
\hat{V} = \frac{1}{2} k \langle \dot{x}^2 \rangle \\
= \frac{1}{2} k \frac{\hbar}{\mu \omega} = \frac{1}{2} \hbar \omega \\
because \omega = (k/\mu)^{1/2}.
\]

**G.** Based on your answer to parts C and F, evaluate \( \langle \hat{T} \rangle \).

From part C. \( \langle \hat{H} \rangle = \hbar \omega \).

From part F. \( \langle \hat{V} \rangle = \hbar \omega / 2 \).

\[
\hat{T} = \hat{H} - \hat{V} \\
\langle \hat{T} \rangle = \langle \hat{H} \rangle - \langle \hat{V} \rangle = \hbar \omega - \frac{\hbar \omega}{2} = \frac{\hbar \omega}{2}.
\]

Why are \( \langle \hat{T} \rangle \) and \( \langle \hat{V} \rangle \) independent of \( t \)? Because \( \Psi(x, t) \) contains only \( \psi_0 \) and \( \psi_1 \) and the motion of \( \langle \dot{x}^2 \rangle \) or \( \langle \dot{p}^2 \rangle \) requires \( \psi_v \) in \( \Psi(x, t) \) differing in \( v \) by \( \pm 2 \).