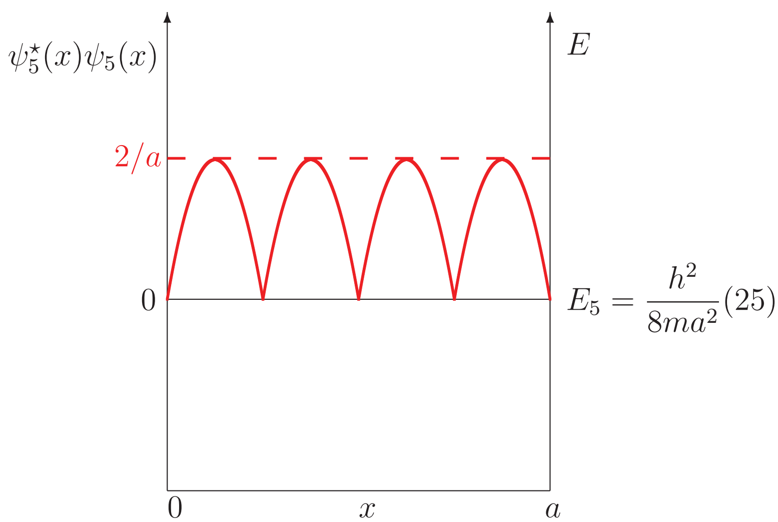
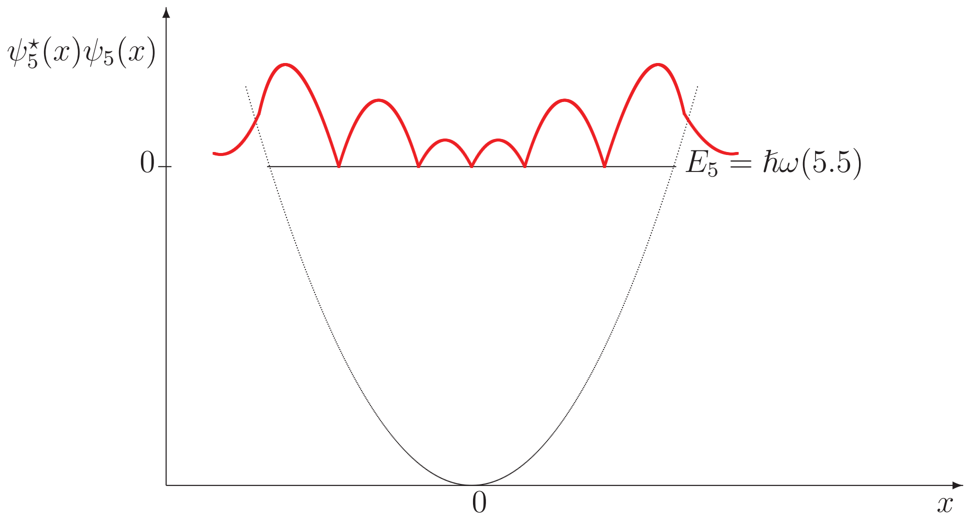
5.61 FIRST HOUR EXAM $\boxed{\text{ANSWERS}}$ Fall, 2013

I. A. Sketch $\psi_5^\star(x)\psi_5(x)$ 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 $\left[\sin\left(\frac{5\pi x}{a}\right)\right]^2$ with maximum height of $(2/a)$.

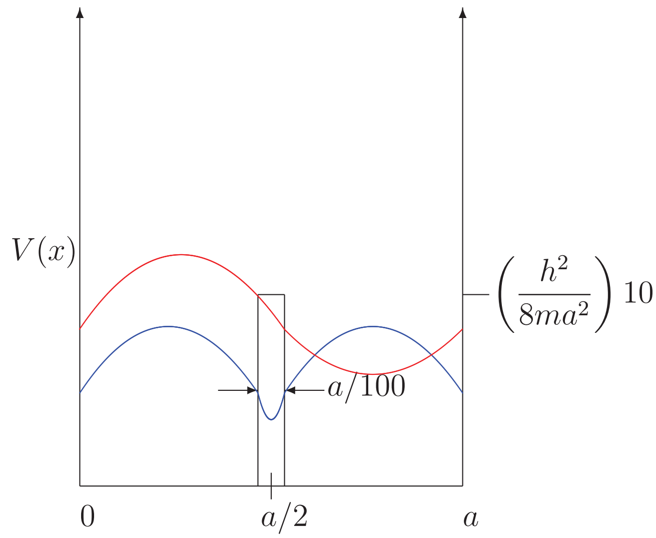
B. Sketch $\psi_5^\star(x)\psi_5(x)$ vs. x, where $\psi_5(x)$ is the $v = 5$ wavefunction of a harmonic oscillator. Describe, in a few words, each of the essential qualitative features of this sketch.



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 $x_\pm = [2(\hbar\omega 5.5)/k]^{1/2}$ than to the 2 and 4 nodes. The outer lobes have the largest maximum height and area, but cannot finish at $\psi_5^\star\psi_5 = 0$ at $x_\pm[11\hbar\omega/k]^{1/2}$, 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:



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.

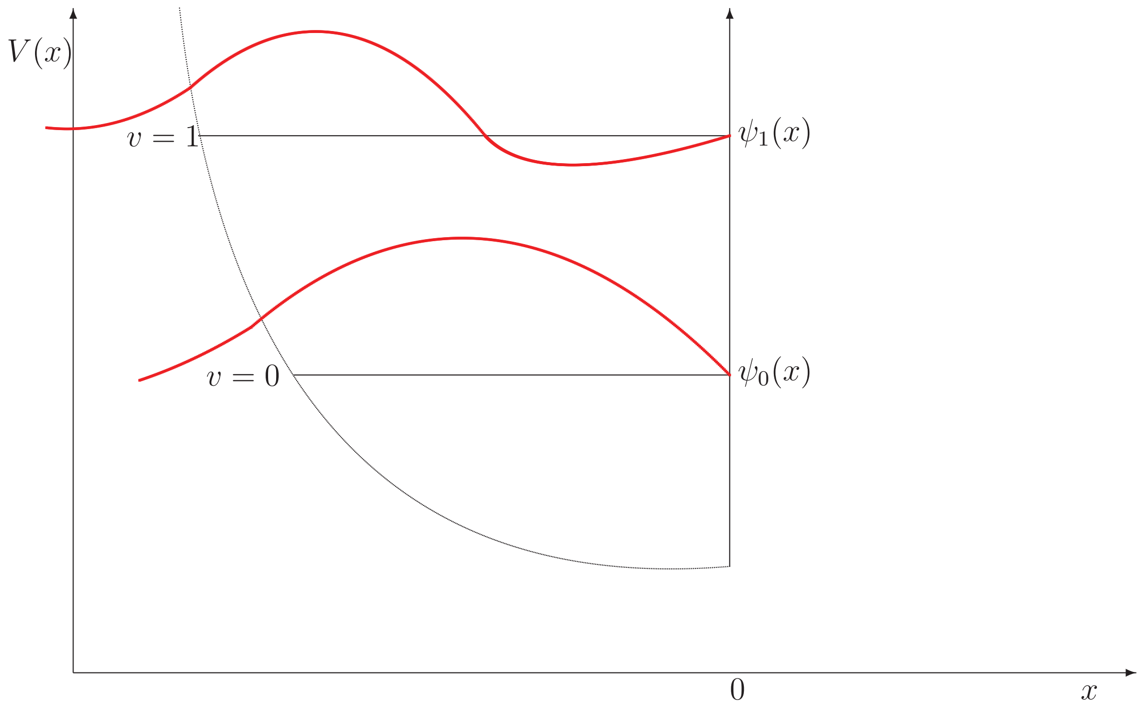
(ii) Make a very approximate estimate of $E_2 - E_1$ for this PIB with a thin barrier in the middle. Specify whether $E_2 - E_1$ is smaller than or larger than $3\frac{h^2}{8ma^2}$ which is the energy level spacing between the $n = 2$ and $n = 1$ energy levels of a PIB without a barrier in the middle.

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

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 $\omega = [k/\mu]^{1/2}$. 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.

Half HO		Full HO	
$E(v=0) = \frac{3}{2}\hbar\omega$	$2\hbar\omega$	$E(v=0) = \frac{1}{2}\hbar\omega$	$1\hbar\omega$
$E(v=1) = \frac{7}{2}\hbar\omega$		$E(v=1) = \frac{3}{2}\hbar\omega$	

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

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

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

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

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

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

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

$$k' = 4k$$

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

II. PROMISE KEPT: FREE PARTICLE

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

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

$$\begin{aligned}\widehat{H}\psi &= -\frac{\hbar^2}{2m}[(ik)^2 ae^{ikx} + (-ik)^2 be^{-ikx}] \\ &= \frac{\hbar^2 k^2}{2m}[ae^{ikx} + be^{-ikx}]\end{aligned}$$

ψ is an eigenfunction of $\widehat{H}$ with eigenvalue $\frac{\hbar^2 k^2}{2m}$.

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

$$\begin{aligned}\hat{p}\psi &= -i\hbar[(ik)ae^{ikx} + (-ik)be^{-ikx}] \\ &= \hbar k[ae^{ikx} - be^{-ikx}]\end{aligned}$$

ψ 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

$$\int_{-\infty}^{\infty} dx e^{icx} = 0$$

compute $\langle\hat{p}\rangle$, the expectation value of $\hat{p}$.

$$\begin{aligned}\langle\hat{p}\rangle &= \frac{\int dx \psi^\star \hat{p}\psi}{\int dx \psi^\star \psi} \\ &= \frac{\int dx \hbar k[a^\star e^{-ikx} + b^\star e^{ikx}][ae^{ikx} - be^{-ikx}]}{\int dx [a^\star e^{-ikx} + b^\star e^{ikx}][ae^{ikx} + be^{-ikx}]} \\ \langle\hat{p}\rangle &= \frac{\hbar k \int dx[|a|^2 - |b|^2]}{\int dx[|a|^2 + |b|^2]} \\ &= \hbar k \frac{|a|^2 - |b|^2}{|a|^2 + |b|^2}\end{aligned}$$

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

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

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

In part **A.** we found that

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

$$\left\langle \widehat{H} \right\rangle = \frac{\int dx \psi^\star \widehat{H}\psi}{\int dx \psi^\star \psi} = \frac{\frac{\hbar^2 k^2}{2m}\int dx \psi^\star \psi}{\int dx \psi^\star \psi} = \frac{\hbar^2 k^2}{2m}.$$

If ψ is an eigenstate of the measurement operator, every measurement yields the eigenvalue of ψ. The expectation value is the eigenvalue!

III. $\hat{\mathbf{a}}$ AND $\hat{\mathbf{a}}^\dagger$ FOR HARMONIC OSCILLATOR

$$\begin{aligned}
\hat{\mathbf{a}}\psi_v &= v^{1/2}\psi_{v-1} \\
\hat{\mathbf{a}}^\dagger\psi_v &= (v+1)^{1/2}\psi_{v+1} \\
\widehat{N}\psi_v &= v\psi_v \quad \text{where} \quad \widehat{N} = \hat{\mathbf{a}}^\dagger\hat{\mathbf{a}}
\end{aligned}$$

A. Show that $[\hat{\mathbf{a}}^\dagger, \hat{\mathbf{a}}]$ by applying this commutator to ψ_v.

$$\begin{aligned}
[\hat{\mathbf{a}}^\dagger, \hat{\mathbf{a}}] &= \hat{\mathbf{a}}^\dagger\hat{\mathbf{a}} - \hat{\mathbf{a}}\hat{\mathbf{a}}^\dagger \\
[\hat{\mathbf{a}}^\dagger, \hat{\mathbf{a}}]\psi_v &= \hat{\mathbf{a}}^\dagger\hat{\mathbf{a}}\psi_v - \hat{\mathbf{a}}\hat{\mathbf{a}}^\dagger\psi_v \\
&= \hat{\mathbf{a}}^\dagger v^{1/2}\psi_{v-1} - \hat{\mathbf{a}}(v+1)^{1/2}\psi_{v+1} \\
&= v^{1/2}v^{1/2}\psi_v - (v+1)^{1/2}(v+1)^{1/2}\psi_v \\
&= [v-(v+1)]\psi_v = (-1)\psi_v \\
[\hat{\mathbf{a}}^\dagger, \hat{\mathbf{a}}] &= -1
\end{aligned}$$

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

(i) $(\hat{\mathbf{a}}^\dagger)^2(\hat{\mathbf{a}})^5\psi_3$

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

(ii) $(\hat{\mathbf{a}})^5(\hat{\mathbf{a}}^\dagger)^2\psi_3$

$(\hat{\mathbf{a}})^5(\hat{\mathbf{a}}^\dagger)^2$ has selection rule $\Delta v = -3$ $(\hat{\mathbf{a}})^5(\hat{\mathbf{a}}^\dagger)^2\psi_3 = (1\cdot 2\cdot 3\cdot 4\cdot 5)^{1/2}(4\cdot 5)^{1/2}\psi_0$.

(iii) $\int dx\psi_3(\hat{\mathbf{a}}^\dagger)^3\psi_0$

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

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

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

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

$$\begin{aligned}
(\hat{\mathbf{a}}+\hat{\mathbf{a}}^\dagger)^2 &= \hat{\mathbf{a}}^2+\hat{\mathbf{a}}^{\dagger 2}+\hat{\mathbf{a}}\hat{\mathbf{a}}^\dagger+\overbrace{\hat{\mathbf{a}}^\dagger\hat{\mathbf{a}}}^{\widehat{N}} \\
\hat{\mathbf{a}}\hat{\mathbf{a}}^\dagger &= [\hat{\mathbf{a}}, \hat{\mathbf{a}}^\dagger]+\hat{\mathbf{a}}^\dagger\hat{\mathbf{a}} = 1+\widehat{N} \\
(\hat{\mathbf{a}}+\hat{\mathbf{a}}^\dagger)^2 &= \hat{\mathbf{a}}^2+\hat{\mathbf{a}}^{\dagger 2}+2\widehat{N}+1
\end{aligned}$$

IV. TIME-DEPENDENT WAVE EQUATION AND PIB SUPERPOSITION

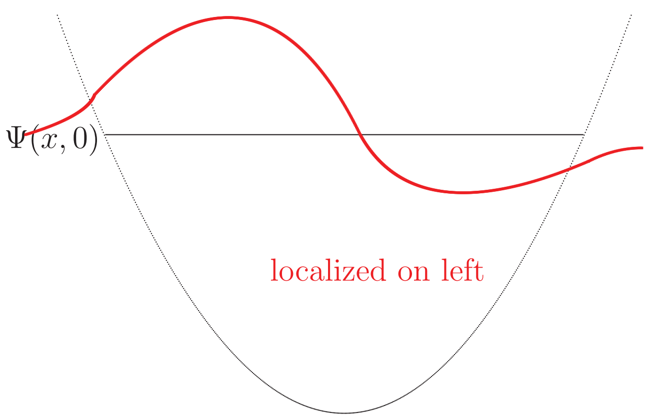
For the harmonic oscillator

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

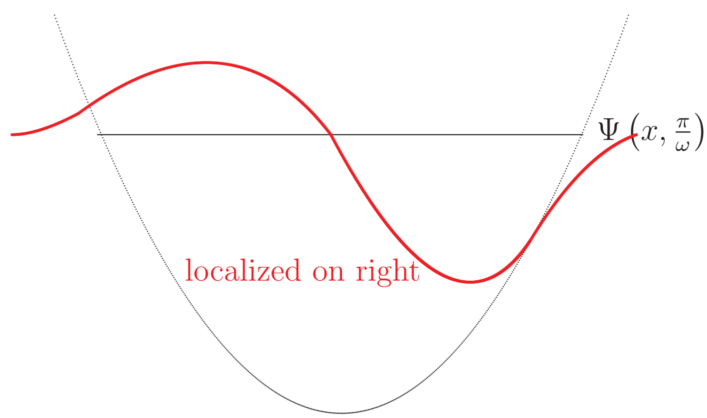
Consider the time-dependent state

$$\begin{aligned}\Psi(x,t) &= 2^{1/2}\left[e^{-iE_0t/\hbar}\psi_0(x) + e^{-iE_1t/\hbar}\psi_1(x)\right] \\ &= 2^{1/2}e^{-iE_0t/\hbar}\left[\psi_0(x) + e^{-i\hbar\omega t/\hbar}\psi_1\right]\end{aligned}$$

A. Sketch $\Psi(x,0)$ and $\Psi(x,t=\frac{\pi}{\omega})$



$\Psi(x,0) = \psi_0(x) + \psi_1(x)$



$\Psi(x,\frac{\pi}{\omega}) = \psi_0(x) - \psi_1(x)$

B. Compute $\int dx \Psi^\star(x,t)\widehat{N}\Psi(x,t)$.

$$\begin{aligned}
\int dx \Psi^\star(x,t)\widehat{N}\Psi(x,t) &= \frac{1}{2}\int dx(\psi_0^\star + e^{i\omega t}\psi_1^\star)\widehat{N}(\psi_0 + e^{-i\omega\hbar}\psi_1) \\
&= \frac{1}{2}\int dx(\psi_0^\star + e^{i\omega t}\psi_1^\star)(0 + e^{-i\omega t}\psi_1) \\
&\qquad\qquad\qquad\qquad\qquad \text{because } \widehat{N}\psi_0 = 0\psi_0 \\
&= \frac{1}{2}
\end{aligned}$$

C. Compute $\left\langle \widehat{H} \right\rangle = \int dx \Psi^\star(x,t)\widehat{H}\Psi(x,t)$ and comment on the relationship of $\left\langle \widehat{N} \right\rangle$ to $\left\langle \widehat{H} \right\rangle$.

$$\widehat{H} = \hbar\omega\left(\widehat{N} + \frac{1}{2}\right)$$

$$\left\langle \widehat{H} \right\rangle = \hbar\omega\left[\left\langle \widehat{N} \right\rangle + \left\langle \frac{1}{2} \right\rangle\right]$$

$$\left\langle \frac{1}{2} \right\rangle = \frac{1}{2} \text{ because } \Psi \text{ is normalized to 1.}$$

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

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 $\langle \hat{x} \rangle = \int dx \Psi^\star(x,t)\hat{x}\Psi(x,t)$.

$$\hat{x} = \left(\frac{\hbar}{2\mu\omega}\right)^{1/2} (\mathbf{\hat{a}}^\dagger + \mathbf{\hat{a}})$$

$$\begin{aligned}
\hat{x}\Psi(x,t) &= 2^{-1/2} e^{-iE_0 t/\hbar} \left(\frac{\hbar}{2\mu\omega}\right)^{1/2} (\mathbf{\hat{a}}^\dagger + \mathbf{\hat{a}})(\psi_0 + e^{-i\omega t}\psi_1) \\
&= 2^{-1/2} e^{-i\omega t/2} \left(\frac{\hbar}{2\mu\omega}\right)^{1/2} (\psi_1 + 2^{1/2} e^{-i\omega t}\psi_2 + e^{-i\omega t}\psi_0) \\
\Psi^\star \hat{x}\Psi &= \frac{1}{2}\left(\frac{\hbar}{2\mu\omega}\right)^{1/2} (\psi_0^\star + e^{i\omega t}\psi_1^\star)(e^{-i\omega t}\psi_0 + \psi_1 + 2^{1/2} e^{-i\omega t}\psi_2) \\
\langle \hat{x} \rangle \int dx \Psi^\star \hat{x}\Psi &= \frac{1}{2}\left(\frac{\hbar}{2\mu\omega}\right)^{1/2} (e^{-i\omega t} + e^{i\omega t} + 0) \\
&= \frac{1}{2}\left(\frac{\hbar}{2\mu\omega}\right)^{1/2} 2\cos\omega t.
\end{aligned}$$

This reveals a phase ambiguity. The picture of $\Psi^\star(x,0)\Psi(x,0)$ in Part **IV.A.** suggests that $\langle x \rangle_t$ starts negative and oscillates cosinusoidally. But the calculation using $\mathbf{\hat{a}}, \mathbf{\hat{a}}^\dagger$ shows that $\langle x \rangle_t$ 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 ψ_0 and ψ_1, there will be no $\Delta v = \pm 2$ integrals. We only need the $\Delta v = 0$ part of $\hat{x}^2$.

$$\begin{aligned}
\hat{x}^2 &= \left(\frac{\hbar}{2\mu\omega}\right) (\mathbf{\hat{a}} + \mathbf{\hat{a}}^\dagger)^2 \\
&= \left(\frac{\hbar}{2\mu\omega}\right) (\mathbf{\hat{a}}^2 + \mathbf{\hat{a}}^{\dagger 2} + 2\widehat{N} + 1)
\end{aligned}$$

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

$$\begin{aligned}
\left\langle 2\widehat{N} + 1 \right\rangle &= 2\left\langle \widehat{H} \right\rangle / \hbar\omega \\
\left\langle \hat{x}^2 \right\rangle &= \left(\frac{\hbar}{2\mu\omega}\right)(2) = 2\frac{\hbar}{2\mu\omega}.
\end{aligned}$$

F. Based on your answer to part **E**, evaluate $\left\langle \widehat{V}(x) \right\rangle$.

$$\begin{aligned} \widehat{V} &= \frac{1}{2} k \left\langle \hat{x}^2 \right\rangle \\ &= \frac{1}{2} k \frac{\hbar}{\mu\omega} = \frac{1}{2}\hbar\omega \end{aligned}$$

because $\omega = (k/\mu)^{1/2}$.

G. Based on your answer to parts **C** and **F**, evaluate $\left\langle \widehat{T} \right\rangle$.

From part **C.** $\left\langle \widehat{H} \right\rangle = \hbar\omega$.

From part **F.** $\left\langle \widehat{V} \right\rangle = \hbar\omega/2$.

$$\widehat{T} = \widehat{H} - \widehat{V}$$

$$\left\langle \widehat{T} \right\rangle = \left\langle \widehat{H} \right\rangle - \left\langle \widehat{V} \right\rangle = \hbar\omega - \frac{\hbar\omega}{2} = \frac{\hbar\omega}{2}.$$

Why are $\left\langle \widehat{T} \right\rangle$ and $\left\langle \widehat{V} \right\rangle$ independent of t? Because $\Psi(x,t)$ contains only ψ_0 and ψ_1 and the motion of $\langle \hat{x}^2 \rangle$ or $\langle \hat{p}^2 \rangle$ requires ψ_v in $\Psi(x,t)$ differing in v by ± 2.