5.61 Fall 2017
Problem Set #4 Solutions

1 Survival Probabilities for Wavepacket in Harmonic Well

Let $V(x) = \frac{1}{2}kx^2$, $k = \omega^2\mu$, $\omega = 10$, $\mu = 1$.

A. Consider the three term $t = 0$ wavepacket

$$\Psi(x,0) = c\psi_1 + c\psi_3 + d\psi_2.$$

Choose the constants c and d so that $\Psi(x,0)$ is both normalized and has the largest possible negative value of $\langle x \rangle$ at $t = 0$. What are the values of c and d and $\langle x \rangle_{t=0}$?

Solution:

We begin by determining $\Psi^*(x,0)\Psi(x,0)$ as follows (assuming real coefficients in the case of a harmonic oscillator)

$$\begin{aligned}
\Psi^*(x,0)\Psi(x,0) &= (c^*\psi_1^* + c^*\psi_3^* + d^*\psi_2^*)(c\psi_1 + c\psi_3 + d\psi_2) \\
&= c^2|\psi_1|^2 + c^2|\psi_3|^2 + d^2|\psi_2|^2 \\
\int \Psi^*(x,0)\Psi(x,0)dx &= c^2 + c^2 + d^2 \\
1 &= 2c^2 + d^2 \qquad (1.1)
\end{aligned}$$

Now we must compute $\langle x \rangle$ at $t = 0$ in order to determine the value of the constants at which it is most negative

$$\begin{aligned}
\int \Psi^*(x,0)x\Psi(x,0)dx = c^2 &\int \psi_1^* x\psi_1 dx + c^2 \int \psi_1^* x\psi_3 dx + cd \int \psi_1^* x\psi_2 dx \\
&+ c^2 \int \psi_3^* x\psi_1 dx + c^2 \int \psi_3^* x\psi_3 dx + cd \int \psi_3^* x\psi_2 dx \\
&+ cd \int \psi_2^* x\psi_1 dx + cd \int \psi_2^* x\psi_3 dx + d^2 \int \psi_2^* x\psi_2 dx
\end{aligned}$$

Due to the selection rules, the above equation reduces to

$$\int \Psi^*(x,0)x\Psi(x,0)dx = cd\left[\int \psi_1^* x\psi_2 dx + \int \psi_3^* x\psi_2 dx + \int \psi_2^* x\psi_1 dx + \int \psi_2^* x\psi_3 dx\right]$$

By converting x to ladder operator form, the integrals can be easily evaluated, giving the following values

$$\int \psi_1^* x \psi_2 dx = \sqrt{2}\left(\frac{\hbar}{2\mu\omega}\right)^{1/2}$$
$$\int \psi_3^* x \psi_2 dx = \sqrt{3}\left(\frac{\hbar}{2\mu\omega}\right)^{1/2}$$
$$\int \psi_2^* x \psi_1 dx = \sqrt{2}\left(\frac{\hbar}{2\mu\omega}\right)^{1/2}$$
$$\int \psi_2^* x \psi_3 dx = \sqrt{3}\left(\frac{\hbar}{2\mu\omega}\right)^{1/2}$$

As a result, we find that

$$\langle x \rangle = 2cd\left(\frac{\hbar}{2\mu\omega}\right)^{1/2}(\sqrt{2}+\sqrt{3}).$$

We can now use our relationship in Eq. (1.1) as follows:

$$1 = 2c^2 + d^2$$
$$d = \pm\sqrt{1-2c^2}$$

We choose the positive result as is the case for constants of a harmonic oscillator, and plug this into our equation for $\langle x \rangle$ as follows:

$$\langle x \rangle = 2c\sqrt{1-2c^2}\left(\frac{\hbar}{2\mu\omega}\right)^{1/2}(\sqrt{2}+\sqrt{3}).$$

We now minimize the above equation with respect to the constant c, in order to determine the extremum of x, and consequently the minimum value of x:

$$0 = \frac{d\langle x \rangle}{dc} = \left[2\sqrt{1-2c^2} + c(1-2c^2)^{-1/2}(-4c)\right]\left(\frac{\hbar}{2\mu\omega}\right)^{1/2}(\sqrt{2}+\sqrt{3})$$
$$\sqrt{1-2c^2} = \frac{2c^2}{\sqrt{1-2c^2}}$$
$$c = \pm\frac{1}{2}$$
$$d = \frac{1}{\sqrt{2}}$$

We find that if we use the $c = 1/2$,

$$\langle x \rangle = \frac{1}{\sqrt{2}}\left(\frac{\hbar}{2\mu\omega}\right)^{1/2}(\sqrt{2}+\sqrt{3})$$

and that if we use $c = -1/2$

$$\langle x \rangle = -\frac{1}{\sqrt{2}}\left(\frac{\hbar}{2\mu\omega}\right)^{1/2}(\sqrt{2}+\sqrt{3})$$

Since the question asks for the constants that give the largest possible negative value of $\langle x \rangle_{t=0}$, our final answer is

$$\begin{aligned}\langle x \rangle_{t=0} &= -\frac{1}{\sqrt{2}}\left(\frac{\hbar}{2\mu\omega}\right)^{1/2}(\sqrt{2}+\sqrt{3}) \\ c &= -\frac{1}{2} \\ d &= \frac{1}{\sqrt{2}}.\end{aligned}$$

Note that we could also hve chosen $c = \frac{1}{2}$ and $d = -\frac{1}{\sqrt{2}}$.

B. Compute and plot the time-dependences of $\langle \hat{x} \rangle$ and $\langle \hat{p} \rangle$. Do they satisfy Ehrenfest's theorem about motion of the "center" of the wavepacket?

Solution:

Given $\langle x \rangle_{t=0}$, we know the form of $\langle x \rangle$ only has terms x_{12}, x_{32}, x_{21}, and x_{23}, where we define

$$x_{nm} = \int \psi_n^* x \psi_m dx.$$

Therefore, we can determine $\langle x \rangle$ as follows:

$$\begin{aligned}\langle x \rangle &= \int \Psi^*(x,t) x \Psi(x,t) dx \\ &= -\frac{1}{2\sqrt{2}}\left(\frac{\hbar}{2\mu\omega}\right)^{1/2}\Big[\sqrt{2}e^{-i(\overline{E}_2-\overline{E}_1)t/\hbar} + \sqrt{3}e^{i(\overline{E}_3-\overline{E}_2)t/\hbar} \\ &\quad + \sqrt{2}e^{i(E_2-E_1)t/\hbar} + \sqrt{3}e^{-i(E_3-E_2)t/\hbar}\Big]\end{aligned}$$

In the case of the HO, if we define (as per the lecture notes)

$$\omega = \frac{\Delta E}{\hbar} = \frac{E_2 - E_1}{\hbar} = \frac{E_3 - E_2}{\hbar}.$$

We find (utilizing Euler's formula)

$$\langle x \rangle = -\frac{1}{\sqrt{2}}\left(\frac{\hbar}{2\mu\omega}\right)^{1/2}(\sqrt{2}+\sqrt{3})\cos\omega t.$$

Evaluating $\hat{p}$ leads to (neglecting all zero terms as a result of selection rules)

$$\begin{aligned}\langle \hat{p} \rangle &= \int \Psi^*(x,t)\hat{p}\Psi(x,t)dx \\ &= -\frac{1}{2\sqrt{2}}\left[\int \psi_1^*\hat{p}_x\psi_2 dx e^{-i\omega t} + \int \psi_3^*\hat{p}_2\psi_2 dx e^{i\omega t}\int \psi_2^*\hat{p}_x\psi_1 dx e^{i\omega t} + \int \psi_2^*\hat{p}_x\psi_3 dx e^{-i\omega t}\right]\end{aligned}$$

To compute $\langle \hat{p} \rangle$ further, we note the ladder operator relationship

$$\hat{p} = i\left(\frac{\hbar\mu\omega}{2}\right)^{1/2}(\hat{\boldsymbol{a}}^\dagger - \hat{\boldsymbol{a}}).$$

The integrals can be evaluated as follows:

$$\begin{aligned}
\int \psi_1^* \hat{p}\psi_2 dx &= -i\sqrt{2}\left(\frac{\hbar\mu\omega}{2}\right)^{1/2} \\
\int \psi_3^* \hat{p}\psi_2 dx &= i\sqrt{3}\left(\frac{\hbar\mu\omega}{2}\right)^{1/2} \\
\int \psi_2^* \hat{p}\psi_1 dx &= i\sqrt{2}\left(\frac{\hbar\mu\omega}{2}\right)^{1/2} \\
\int \psi_2^* \hat{p}\psi_3 dx &= -i\sqrt{3}\left(\frac{\hbar\mu\omega}{2}\right)^{1/2}
\end{aligned}$$

Therefore

$$\begin{aligned}
\langle \hat{p} \rangle &= -\frac{1}{2\sqrt{2}}\left(\frac{\hbar\mu\omega}{2}\right)^{1/2}\left[i\sqrt{2}(e^{i\omega t} - e^{-i\omega t}) + i\sqrt{3}(e^{i\omega t} - e^{-i\omega t})\right] \\
&= \frac{1}{\sqrt{2}}\left(\frac{\hbar\mu\omega}{2}\right)^{1/2}(\sqrt{2}+\sqrt{3})\sin\omega t
\end{aligned}$$

Ehrenfest's theorem states

$$\frac{d\langle x \rangle}{dt} = \frac{\langle \hat{p} \rangle}{\mu}.$$

We can in fact verify this by taking the time derivative of $\langle x \rangle$ as follows:

$$\begin{aligned}
\frac{d\langle x \rangle}{dt} &= \frac{d}{dt}\left[-\frac{1}{\sqrt{2}}\left(\frac{\hbar}{2\mu\omega}\right)^{1/2}(\sqrt{2}+\sqrt{3})\cos\omega t\right] \\
&= \frac{\omega}{\sqrt{2}}\left(\frac{\hbar}{2\mu\omega}\right)^{1/2}(\sqrt{2}+\sqrt{3})\sin\omega t \\
\mu\frac{d\langle x \rangle}{dt} &= \frac{1}{\sqrt{2}}\left(\frac{\hbar\mu\omega}{2}\right)^{1/2}(\sqrt{2}+\sqrt{3})\sin\omega t) \\
&= \langle \hat{p} \rangle .
\end{aligned}$$

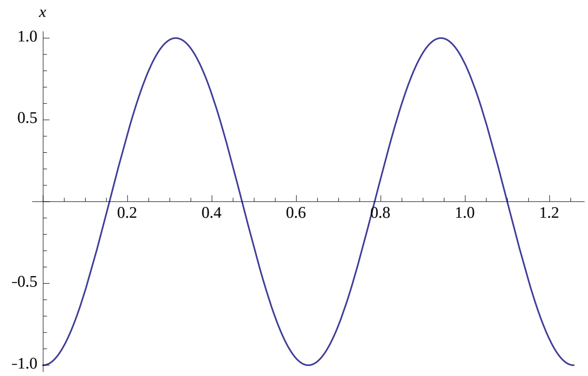
In order to plot the time-dependance of $\langle x \rangle$ and $\langle \hat{p} \rangle$, we first normalize both by the factor

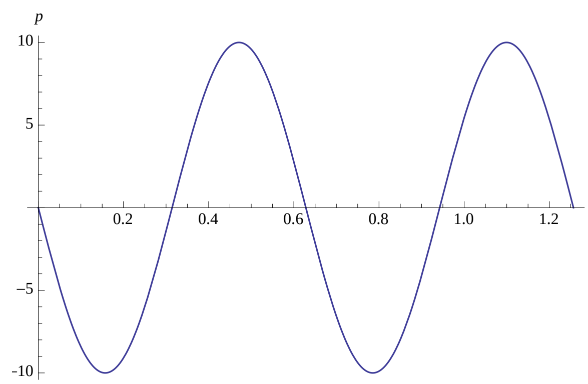
$$\frac{1}{\sqrt{2}}\left(\frac{\hbar}{2\mu\omega}\right)^{1/2}(\sqrt{2}+\sqrt{3}).$$

This gives us

$$\begin{aligned}
\bar{\bar{x}} &= -\cos\omega t = -\cos 10t \\
\bar{\bar{p}} &= \mu\omega\sin\omega t = 10\sin 10t
\end{aligned}$$

Below is a plot of Expectation Values of x and p over time:





C. Compute and plot the survival probability

$$P(t) = \left| \int dx \Psi^*(x,t)\Psi(x,0) \right|^2 .$$

Does $P(t)$ exhibit partial or full recurrences or both?

<u>Solution:</u>

$$\Psi^*(x,t) = c\Psi_1^*(x,t)e^{iE_1t/\hbar} + c\Psi_3^*(x,t)e^{iE_3t/\hbar} + c\Psi_2^*(x,t)e^{iE_2t/\hbar}$$
$$\Psi(x,t) = c\Psi_1(x,t)e^{-iE_1t/\hbar} + c\Psi_3(x,t)e^{-iE_3t/\hbar} + c\Psi_2(x,t)e^{-iE_2t/\hbar}$$
$$\int \Psi^*(x,t)\Psi(x,0)dx = |c|^2 e^{iE_1t/\hbar} + |c|^2 e^{iE_2t/\hbar} + |d|^2 e^{iE_2t/\hbar}$$
$$\left|\int \Psi^*(x,t)\psi(x,0)dx\right|^2 = \frac{1}{16} + \frac{1}{16}e^{i\omega_{31}t} + \frac{1}{8}e^{i\omega_{21}t} + \frac{1}{16}e^{-i\omega_{31}t} + \frac{1}{16}$$
$$+ \frac{1}{8}e^{-i\omega_{32}t} + \frac{1}{8}e^{-i\omega_{21}t} + \frac{1}{8}e^{i\omega_{32}t} + \frac{1}{4}$$
$$= \frac{3}{8} + \frac{1}{8}\cos 2\omega t + \frac{1}{2}\cos\omega t.$$

Where we define (in the case of a Hamiltonian Operator)

$$\omega = \omega_{21} = \omega_{32} = \frac{\omega_{31}}{2} = \frac{\Delta E}{\hbar}$$

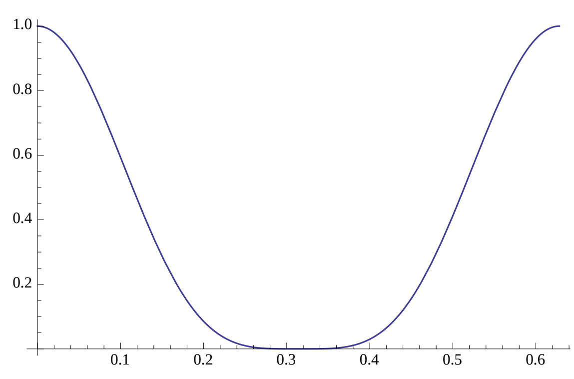
It is clear that the survival probability exhibits both partial and full recurrences, with full recurrence defined as

$$\omega t_{\text{full rec}} = 2\pi$$
$$t_{\text{full rec}} = \frac{2\pi}{\omega} = \frac{\pi}{5}.$$

Partial recurrence is defined as:

$$2\omega t_{\text{par rec}} = 2\pi$$
$$t_{\text{par rec}} = \frac{\pi}{\omega} = \frac{\pi}{10}.$$

The survival probability is plotted below.



D.

Plot $\Psi^*(x, t_{1/2})\Psi(x, t_{1/2})$ at the time $t_{1/2}$, defined as one-half the time between $t = 0$ and the first full recurrence. How does this snapshot of the wavepacket look relative to the $\Psi * (x, 0)\Psi(x, 0)$ snapshot? Should you be surprised?

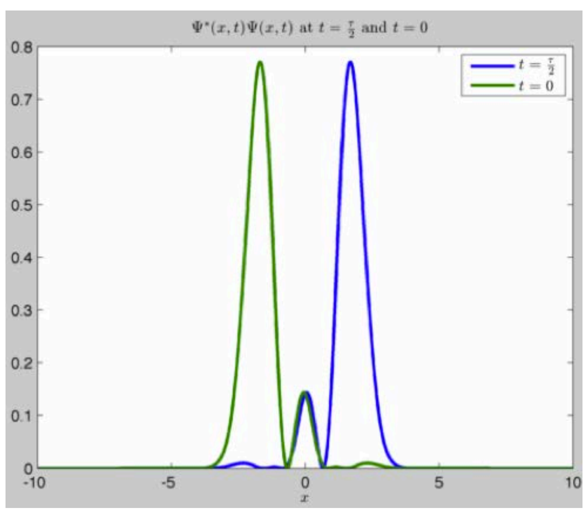
Solution:

$$\Psi^*(x,t)\Psi(x,t) = \frac{1}{4}\psi_1^2 + \frac{1}{4}\psi_3^2 + \frac{1}{2}\psi_2^2 + \frac{1}{2}\psi_1\psi_3(\cos 2\omega t) - \frac{1}{\sqrt{2}}\psi_1\psi_2(\cos\omega t) - \frac{1}{\sqrt{2}}\psi_1\psi_3(\cos\omega t)$$

We can determine $\Psi^*(x, t_{1/2})\Psi(x, t_{1/2})$ and $\Psi^*(x, 0)\Psi(x, 0)$ where $t_{1/2} = \frac{\pi}{10}$.

$$\Psi^*(x,t_{1/2})\Psi(x,t_{1/2}) = \frac{1}{4}\psi_1^2 + \frac{1}{4}\psi_3^2 + \frac{1}{2}\psi_2^2 + \frac{1}{2}\psi_1\psi_3 + \frac{1}{\sqrt{2}}\psi_1\psi_2 + \frac{1}{\sqrt{2}}\psi_2\psi_3$$
$$\Psi^*(x,0)\Psi(x,0) = \frac{1}{4}\psi_1^2 + \frac{1}{4}\psi_3^2 + \frac{1}{2}\psi_2^2 + \frac{1}{2}\psi_1\psi_3 - \frac{1}{\sqrt{2}}\psi_1\psi_2 - \frac{1}{\sqrt{2}}\psi_2\psi_3$$

We can plot both $\Psi^*(x, t_{1/2})\Psi(x, t_{1/2})$ and $\Psi^*(x, 0)\Psi(x, 0)$ assuming for convenience that $\alpha = 1$. We see that the wavepacket has moved from one side of the well to the other side in half the oscillation time, as shown below.



Blue curve is $t = t_{1/2}$
Green curve is $t = t = 0$

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2 Vibrational Transitions

The intensity of a transition between the initial vibrational level, v_i, and the final vibrational level, v_f, is given by

$$I_{v_f,v_i} = \left| \int \psi^*_{v_f}(x)\hat{\mu}(x)\psi_{v_i}(x)dx \right|^2,$$

where $\mu(x)$ is the "electric dipole transition moment function"

$$\begin{aligned}\hat{\mu}(x) &= \mu_0 + \left.\frac{d\mu}{dx}\right|_{x=0}\hat{x} + \left.\frac{d^2\mu}{dx^2}\right|_{x=0}\frac{\hat{x}^2}{2} + \text{ higher-order terms} \\ &= \mu_0 + \mu_1\hat{x} + \mu_2\hat{x}^2\big/2 + \mu_3\hat{x}^3\big/6 + \dots\end{aligned}$$

Consider only μ_0, μ_1, and μ_2 to be non-zero constants and note that all $\psi_v(x)$ are real. You will need some definitions from Lecture Notes #9:

$$\begin{aligned}\hat{x} &= \left(\frac{2\mu\omega}{\hbar}\right)^{-1/2}(\hat{\boldsymbol{a}} + \mathbf{a}^\dagger) \\ \hat{\boldsymbol{a}}\psi_v &= v^{1/2}\psi_{v-1} \\ \hat{\boldsymbol{a}}^\dagger\psi_v &= (v+1)^{1/2}\psi_{v+1} \\ [\hat{\boldsymbol{a}}, \hat{\boldsymbol{a}}^\dagger] &= +1.\end{aligned}$$

A. Derive a formula for all $v+1 \leftarrow v$ vibrational transition intensities. The $v = 1 \leftarrow v = 0$ transition is called the "fundamental".

Solution:

We can derive the formula for the $\nu + 1 \leftarrow \nu$ as follows:

$$\begin{aligned}I_{\nu+1,\nu} &= \left| \int \psi^*_{\nu+1}\hat{\mu}\psi_\nu dx \right|^2 \\ &= \left| \mu_0 \int \psi^*_{\nu+1}\psi_\nu dx + \mu_1 \int \psi^*_{\nu+1}x\psi_\nu dx + \frac{\mu_2}{2}\int \psi^*_{\nu+1}x^2\psi_\nu dx \right|^2 \\ &= \left| \mu_1 \left(\frac{\hbar}{2\mu\omega}\right)^2 \sqrt{\nu+1} \right|^2\end{aligned}$$

We see that the 1st and 3rd terms go to zero as a result of our selection rules, and the above epxression simplifies to

$$I_{\nu+1,\nu} = \mu_1^2\left(\frac{\hbar}{2\mu\omega}\right)(v+1)$$

B. What is the expected ratio of intensities for the $v = 11 \leftarrow v = 10$ band ($I_{11,10}$) and the $v = 1 \leftarrow v = 0$ band ($I_{1,0}$)?

Solution:

The ratio of intensities can be calculated as follows:

$$I_{11,10} = \mu_1^2 \left(\frac{\hbar}{2\mu\omega} \right) (11)$$
$$I_{1,0} = \mu_1^2 \left(\frac{\hbar}{2\mu\omega} \right) (1)$$
$$\frac{I_{11,10}}{I_{1,0}} = 11$$

C. Derive a formula for all $v + 2 \leftarrow v$ vibrational transition intensities. The $v = 2 \leftarrow v = 0$ transition is called the "first overtone".

Solution:

$$\begin{aligned}
I_{\nu+2,\nu} &= \left| \int \psi_{\nu+2}^* \hat{\mu} \psi_\nu dx \right|^2 \\
&= \left| \mu_0 \int \psi_{\nu+2}^* \psi_\nu dx + \mu_1 \int \psi_{\nu+2}^* x \psi_\nu dx + \frac{\mu_2}{2} \int \psi_{\nu+2}^* x^2 \psi_\nu dx \right|^2 \\
&= \left| \frac{\mu_2}{2} \left(\frac{\hbar}{2\mu\omega} \right) \sqrt{\nu+1}\sqrt{\nu+2} \right|^2 \\
&= \frac{\mu_2^2}{4} \left(\frac{\hbar}{2\mu\omega} \right)^2 (v+1)(v+2)
\end{aligned}$$

D. Typically $\left(\frac{2\mu\omega}{\hbar} \right)^{-1/2} = 1/10$ and $\mu_2/\mu_1 = 1/10$ (do not worry about the units). Estimate the ratio $I_{2,0}/I_{1,0}$.

Solution:

$$I_{2,0} = \frac{\mu_2^2}{2}\left(\frac{\hbar}{2\mu\omega}\right)^2$$
$$I_{1,0} = \mu_1^2\left(\frac{\hbar}{2\mu\omega}\right)$$
$$\frac{I_{2,0}}{I_{1,0}} = \frac{1}{2}\left(\frac{\mu_2}{\mu_1}\right)^2\left(\frac{\hbar}{2\mu\omega}\right)$$
$$= \frac{1}{2}\left(\frac{1}{10}\right)(10)^2$$
$$= \frac{1}{2}.$$

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3 More Wavepacket for Harmonic Oscillator

$$\sigma_x \equiv \left[\left\langle \hat{x}^2\right\rangle - \langle x\rangle^2\right]^{1/2}$$
$$\sigma_{p_x} \equiv \left[\left\langle \hat{p}^2\right\rangle - \langle \hat{p}\rangle^2\right]^{1/2}$$
$$\Psi_{1,2}(x,t) = 2^{-1/2}\left[e^{-i\omega t}\psi_1 + e^{-2i\omega t}\psi_2\right]$$
$$\Psi_{1,3}(x,t) = 2^{-1/2}\left[e^{-i\omega t}\psi_1 + e^{-3i\omega t}\psi_3\right]$$

A. Compute $\sigma_x\sigma_{p_x}$ for $\Psi_{1,2}(x,t)$.

Solution:

The first step to compute $\Delta x\Delta p$ is to compute four quantites: $\langle x\rangle$, $\left\langle x^2\right\rangle$, $\langle p\rangle$, and finally $\left\langle p^2\right\rangle$. The first thing to remember is how to write these integrals in terms of the ladder operators.

$$\hat{x} = \left(\frac{\hbar}{2\mu\omega}\right)^2\left(\hat{\boldsymbol{a}} + \hat{\boldsymbol{a}}^\dagger\right)$$
$$\hat{x}^2 = \left(\frac{\hbar}{2\mu\omega}\right)(\hat{\boldsymbol{a}} + \hat{\boldsymbol{a}}^\dagger)^2 = \left(\frac{\hbar}{2\mu\omega}\right)\left(\hat{\boldsymbol{a}}^2 + 2\widehat{N} + 1 + \hat{\boldsymbol{a}}^{\dagger 2}\right)$$
$$\hat{p} = i(\hbar\mu\omega/2)^{1/2}(\hat{\boldsymbol{a}}^\dagger - \hat{\boldsymbol{a}})$$
$$\hat{p}^2 = -\frac{\hbar\mu\omega}{2}(\hat{\boldsymbol{a}}^\dagger + \hat{\boldsymbol{a}})^2 = -\frac{\hbar\mu\omega}{2}\left(\hat{\boldsymbol{a}}^2 + 2\widehat{N} - 1 + \hat{\boldsymbol{a}}^{\dagger 2}\right)$$

We can now compute the expectation values for these quantities.

$$\langle x\rangle = \frac{1}{2}\int(\psi_1 e^{i\omega t} + \psi_2 e^{2i\omega t})\left(\frac{\hbar}{2\mu\omega}\right)^{1/2}(\hat{\boldsymbol{a}} + \hat{\boldsymbol{a}}^\dagger)(\psi_1 e^{-i\omega t} + \psi_2 e^{2i\omega t})dx$$
$$\langle x\rangle = \frac{1}{2}\left(\frac{\hbar}{2\mu\omega}\right)^{1/2}\sqrt{2}(e^{i\omega t} + e^{-i\omega t}) = \left(\frac{\hbar}{\mu\omega}\right)^{1/2}\cos(\omega t)$$

Computing $\langle x^2 \rangle$ is easier because the time-dependence cancels out.

$$\langle x^2 \rangle = \frac{1}{2}\left(\frac{\hbar}{2\mu\omega}\right)(2(1)+1+2(2)+1) = \frac{2\hbar}{\mu\omega}.$$

By Ehrenfest's theorem, we can calculate the expectation value of p

$$\mu\frac{d\langle x \rangle}{dt} = -(\hbar\mu\omega)^{1/2}\sin(\omega t) = \langle p \rangle\,.$$

We can compute the value of p^2 as well to be

$$\langle p^2 \rangle = 2\hbar\mu\omega.$$

Now we can compute Δx

$$\Delta x = \left(\langle x^2 \rangle - \langle x \rangle^2\right)^{1/2} = \left(\frac{\hbar}{\mu\omega}\right)^{1/2}\left(2-\cos^2(\omega t)\right)^{1/2}.$$

Similarly, Δp is

$$\Delta p = (\hbar\mu\omega)^{1/2}(2-\sin^2(\omega t))^{1/2}.$$

Therefore,

$$\Delta x\Delta p = \hbar(2+1/4\sin^2(2\omega t))^{1/2}.$$

B. Compute $\sigma_x\sigma_{p_x}$ for $\Psi_{1,3}(x,t)$.

Solution:

For this case, we can first compute the expectation values of x and p.

$$\langle x \rangle = \frac{1}{2}\int(\psi_1 e^{i\omega t}+\psi_3 e^{3i\omega t})\left(\frac{\hbar}{2\mu\omega}\right)^{1/2}(\hat{\boldsymbol{a}}+\hat{\boldsymbol{a}}^\dagger)(\psi_1 e^{-i\omega t}+\psi_3 e^{-3i\omega t})dx.$$

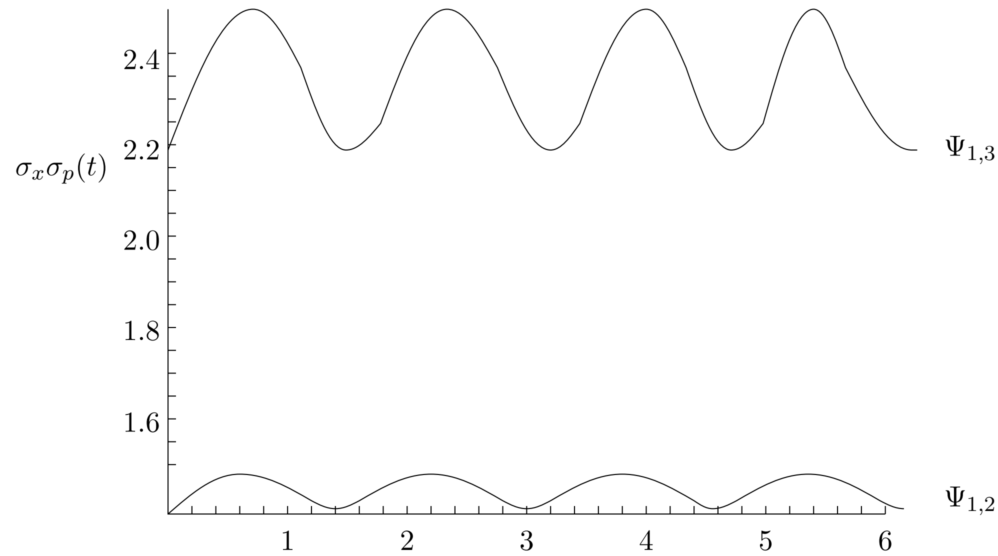
In this case, operating with x will result in terms of eigenfunctions ψ_0, ψ_2, and ψ_4. These are orthogonal to ψ_1 and ψ_3, resulting in

$$\langle x \rangle = 0$$

Similarly, we know that

$$\langle p \rangle = 0$$

We can compute the expectation value of x^2.



$$\langle x\rangle = \frac{1}{2}\int (\psi_1 e^{i\omega t} + \psi_3 e^{3i\omega t})\left(\frac{\hbar}{2\mu\omega}\right)(\hat{\boldsymbol{a}} + \hat{\boldsymbol{a}}^\dagger)^2(\psi_1 e^{-i\omega t} + \psi_3 e^{-3i\omega t})dx$$

First, let's consider the time-independent terms. These are the terms of the form $\psi_v(2N+1)\psi_v$. Adding up these two terms from ψ_1 and ψ_3 gives $\frac{1}{2}\frac{\hbar}{2\mu\omega}(2(1)+1+2(3)+1) = \frac{5\hbar}{2\mu\omega}$. Now we can consider the cross terms that would result in motion. There are two terms that would be nonzero, $\psi_1\hat{\boldsymbol{a}}^2\psi_3$ and $\psi_3\hat{\boldsymbol{a}}^{\dagger 2}\psi_1$. Computing this gives us

$$\frac{1}{2}\frac{\hbar}{2\mu\omega}\sqrt{6}(e^{2i\omega t} + e^{-2i\omega t}) = \frac{\sqrt{6}\hbar}{2\mu\omega}\cos(2\omega t).$$

Therefore

$$\left\langle x^2\right\rangle = \frac{\hbar}{\mu\omega}\left(\frac{5}{2} + \frac{\sqrt{6}}{2}\cos(2\omega t)\right).$$

Computing $\left\langle p^2\right\rangle$ by the fact that $\left\langle \widehat{H}\right\rangle = \langle T\rangle + \langle V\rangle$ is the simplest route. Since $\langle V\rangle = 1/2\mu\omega^2\left\langle x^2\right\rangle$, we know that $\langle V\rangle = \frac{\hbar\omega}{2}\left(\frac{5}{2} + \frac{\sqrt{6}}{2}\cos(2\omega t)\right)$. We calculate $\left\langle \widehat{H}\right\rangle = \frac{E_1+E_3}{2} = \frac{5}{2}\hbar\omega$. A little algebra gives us that $\langle T\rangle = \frac{\hbar\omega}{2}\left(\frac{5}{2} + \frac{\sqrt{6}}{2}\cos(2\omega t)\right) = \frac{\left\langle p^2\right\rangle}{2m}$. Therefore

$$\left\langle p^2\right\rangle = \hbar\mu\omega\left(\frac{5}{2} - \frac{\sqrt{6}}{2}\cos(2\omega t)\right)$$

Now we can compute the uncertainty relationship very quickly

$$\begin{aligned}\Delta x\Delta p &= \hbar\left[\left(\frac{5}{6} + \frac{\sqrt{6}}{2}\cos(2\omega t)\right)\left(\frac{5}{6} - \frac{\sqrt{6}}{2}\cos(2\omega t)\right)\right]^{1/2} \\ &= \frac{\hbar}{2}[25 - 6\cos^2(2\omega t)]^{1/2}.\end{aligned}$$

C. The uncertainty principle is

$$\sigma_x \sigma_{p_x} \geq \hbar/2.$$

The $\Psi_{1,2}(x,t)$ wavepacket is moving and the $\Psi_{1,3}(x,t)$ wavepacket is "breathing". Discuss the time-dependence of $\sigma_x \sigma_{p_x}$ for these two classes of wavepackets.

Solution:

Let's look at plots of the uncertainties, as computing in parts **A** and **B**. From these plots, we see that both uncertainties oscillate, although the wavepacket with a lower average energy (from part **A**) has lower average uncertainty than the wavepacket from part **B**. Both oscillate with the same frequency but with different amplitudes. The uncertainties don't necessarily reflect the movement of the wavepacket directly. The wavepacket from part **A** will dephase and move from side-to-side. The wavepacket from part **B** (the breathing wavepacket) will dephase and rephase, while the average value of x will remain 0.

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4 Two-Level Problem

A. Algebraic Approach

$$\int \psi_1^* \widehat{H} \psi_1 d\tau = H_{11} = E_1$$
$$\int \psi_2^* \widehat{H} \psi_2 d\tau = H_{22} = E_2$$
$$\int \psi_2^* \widehat{H} \psi_1 d\tau = H_{12} = V$$

Find eigenfunctions:

$$\begin{aligned} \psi_+ &= a\psi_1 + b\psi_2 \qquad &&\text{(must be normalized, } \psi_1, \psi_2 \text{ are orthonormal)} \\ \widehat{H}\psi_+ &= E_+ \psi_+ \\ \psi_- &= c\psi_1 + d\psi_2 \qquad &&\text{(must be normalized, and orthonormal to } \psi_+\text{)} \\ \widehat{H}\psi_- &= E_- \psi_- \end{aligned}$$

Use any brute force algebraic method (but not matrix diagonalization) to solve for E_+, E_-, a, b, c and d.

Solution:

We are given

$$H_{11} = E_1$$
$$H_{22} = E_2$$
$$H_{12} = V$$

We want eigenfunctions:

$$\widehat{H}\psi_+ = E_+\psi_+ \qquad \text{where } \psi_+ = a\psi_1 + b\psi_2$$
$$\widehat{H}\psi_- = E_-\psi_- \qquad \text{where } \psi_- = c\psi_1 + d\psi_3$$

$$\widehat{H}\psi_* = \widehat{H}(a\psi_1 + b\psi_2) = E_+(a\psi_1 + b\psi_2) = E_+\psi_+$$

left multiplied by ψ_1^* integrate with respect to τ →
$$\int_{-\infty}^{\infty} \psi_1 = \overline{H}(a\psi_1 + b\psi_2)d\tau = E_+ \int_{-\infty}^{\infty} \psi_1^+(a\psi_1 + b\psi_2)d\tau$$

$$a(H_{11}) + b(V) = E_+(a + 0b)$$
$$c(H_{11}) + d(V) = E_-(c + 0d)$$
$$a(H_{11} - E_+) + bV = 0 \tag{4.1}$$
$$c(H_{11} - E_-) + dV = 0 \tag{4.2}$$

Now repeat the process, but for left multiply by ψ_2^*:

$$\int_{-\infty}^{\infty} \psi^2 H(a\psi_1 + b\psi_2)d\tau = E_+ \int_{-\infty}^{\infty} \psi_2^+(a\psi_1 + b\psi_2)$$

$$aV + b(H_{22} - E_+) = 0 \tag{4.3}$$
$$cV + d(H_{22} - E_-) = 0 \tag{4.4}$$

Rearrange Eq. (4.1) and Eq. (4.3), then set equal

$$\frac{a}{b} = \frac{V}{H_{11} - E_+} = \frac{H_{22} - E_+}{V} \tag{4.5}$$

same for Eqs. (4.2) and (4.4)

$$\frac{c}{d} = \frac{V}{H_{11} - E_-} = \frac{H_{22} - E_-}{V} \tag{4.6}$$

Cross-multiply Eqs. (4.5) & (4.6) and rearrange

$$V^2 = (H_{11} - E_\pm)(H_{22} - E_\pm) = H_{11}H_{22} - H_{11}E_\pm - E_\pm H_{22} + E_\pm^2.$$

Quadratic function of $E_\pm \Rightarrow E_\pm^2 - (H_{11} + H_{22})E_\pm + H_{11}H_{22} - V^2 = 0$.

Solve using the quadratic formula

$$\boxed{E_+ = \frac{1}{2}\left[(H_{11} + H_{22}) \pm \left[(H_{11} + H_{22})^2 - 4(H_{11}H_{22} - V^2)\right]^{1/2}\right]}$$

We want a simpler expression for $E_\pm$.

$$\text{Let } \overline{E} = \frac{H_{11} + H_{22}}{2}$$
$$\Delta = \frac{H_{11} - H_{22}}{2}$$

$$\boxed{E_{\pm} = \overline{E} \pm [\Delta^2 + V^2]^{1/2}}$$

We want normalized wavefunctions:

$$1 = a^2 + b^2 = c^2 + d^2$$
$$a = \sqrt{1 - b^2}$$
$$c = \sqrt{1 - d^2}$$

Rewriting Eq. (4.5)

$$\frac{\sqrt{1-b^2}}{b^2} = \frac{V}{H_{11} - E_+} = \frac{V}{H_{11} - \overline{E} - [\Delta^2 + V^2]^{1/2}} = \frac{V}{\Delta - [\Delta^2 + V^2]^{1/2}}$$

Let $\Delta^2 + V^2 = x$

$$\frac{\sqrt{1-b^2}}{b^2} = \frac{\sqrt{x - \Delta^2}}{\Delta - \sqrt{x}}$$
$$\frac{\sqrt{1-b^2}}{b^2} = \frac{\sqrt{x - \Delta^2}}{\Delta^2 - 2\Delta\sqrt{x} + x} = \frac{(\sqrt{x} - \Delta)(\sqrt{x} + \Delta)}{+(\sqrt{x} - \Delta)(\sqrt{x} - \Delta)}$$
$$\frac{1-b^2}{b^2} = \frac{\sqrt{x} + \Delta}{\sqrt{x} - \Delta}$$
$$1 = b^2\left(1 + \frac{\sqrt{x} + \Delta}{\sqrt{x} - \Delta}\right) = b^2\left(\frac{2\sqrt{x}}{\sqrt{x} - \Delta}\right)$$
$$b^2 = \frac{\sqrt{x} - \Delta}{2\sqrt{x}} = \frac{1}{2}\left(1 - \frac{\Delta}{\sqrt{x}}\right)$$

$$b = \sqrt{\frac{1}{2}\left(1 - \frac{\Delta}{\sqrt{x}}\right)}$$

$$a = \sqrt{\frac{1}{2}\left(1 + \frac{\Delta}{\sqrt{x}}\right)}$$ ← plug b into $a = \sqrt{1 - b^2}$

$$c = \sqrt{\frac{1}{2}\left(1 - \frac{\Delta}{\sqrt{x}}\right)}$$

$$d = -\sqrt{\frac{1}{2}\left(1 + \frac{\Delta}{\sqrt{x}}\right)}$$

← use same procedure to find these values (c and d)

B. Matrix Approach

$$\mathbf{H} = \begin{pmatrix} E_1 & V \\ V^* & E_2 \end{pmatrix} = \begin{pmatrix} \overline{E} & 0 \\ 0 & \overline{E} \end{pmatrix} + \begin{pmatrix} \Delta & V \\ V^* & \Delta \end{pmatrix}$$
$$\overline{E} = \frac{E_1 + E_2}{2}$$
$$\Delta = \frac{E_1 - E_2}{2} < 0 \qquad \text{(assume } E_1 < E_2\text{)}$$

(i) Find the eigenvalues of **H** by solving the determinantal secular equation

$$0 = \begin{vmatrix} \Delta - E & V \\ V^* & -\Delta - E \end{vmatrix}$$
$$0 = -\Delta^2 + E^2 - |V|^2$$

<u>Solution:</u>

$$\widehat{H} = \begin{pmatrix} E_1 & V \\ V^* & E_2 \end{pmatrix} = \begin{pmatrix} \overline{E} + \Delta & V \\ V^* & \overline{E} - \Delta \end{pmatrix}$$
$$\widehat{H}\vec{C} = E\vec{C} \Rightarrow (\widehat{H} - EI)\vec{C} = 0$$
$$0 = \begin{pmatrix} \overline{E} + \Delta - E & V \\ V^* & \overline{E} - \Delta - E \end{pmatrix} \vec{C}$$

Let $E' = -\overline{E} + E$

$$0 = \begin{pmatrix} \Delta - E' & V \\ V^* & -\Delta - E' \end{pmatrix} \begin{pmatrix} V_{11} \\ V_{12} \end{pmatrix}$$

$$\det \begin{vmatrix} \Delta - E' & V \\ V^* & -\Delta - E' \end{vmatrix} = -1(\Delta^2 - E'^2) - |V|^2 = 0$$

$$0 = -\Delta^2 + E'^2 - |V|^2$$
$$E' = \pm\sqrt{\Delta^2 + |V|^2}$$

$$\boxed{E_\pm = \overline{E} \pm \sqrt{\Delta^2 + |V|^2}}$$

(ii) *If you dare*, find the eigenfunctions (eigenvectors) of **H**. Do these eigenvectors depend on the value of $\overline{E}$?

Solution:

$$\begin{pmatrix} \Delta - \sqrt{\Delta^2 + |V|^2} & V \\ V^* & -\Delta - \sqrt{\Delta^2 + |V|^2} \end{pmatrix} \begin{pmatrix} V_{11} \\ V_{12} \end{pmatrix} = 0$$

$$(\Delta - \sqrt{\Delta^2 + V^2})V_{11} + VV_{12} = 0$$

$$V_{11} = \frac{+V}{\sqrt{\Delta^2 + V^2} - \Delta} V_{12}$$

$$V_{11} = \frac{\sqrt{x - \Delta^2}}{\sqrt{x} - \Delta} V_{12} = \frac{\sqrt{(\sqrt{x} + \Delta)(\sqrt{x} - \Delta)}}{\sqrt{x} - \Delta} V_{12} = \sqrt{\frac{(\sqrt{x} + \Delta)(\sqrt{x} - \Delta)}{(\sqrt{x} - \Delta)(\sqrt{x} - \Delta)}} V_{12}$$

$$V_{11} = \sqrt{\frac{\sqrt{x} + \Delta}{\sqrt{x} - \Delta}} V_{12}$$

$$\begin{pmatrix} \Delta + \sqrt{\Delta^2 + |V|^2} & V \\ V^* & -\Delta + \sqrt{\Delta^2 + |V|^2} \end{pmatrix} \begin{pmatrix} V_{21} \\ V_{22} \end{pmatrix} = 0$$

$$V_{21} = \frac{V}{\sqrt{\Delta^2 + |V|^2 + \Delta V_{22}}} = \frac{\sqrt{x - \Delta^2}}{\sqrt{x} + \Delta} V_{22}$$

$$\boxed{\vec{V}_2 = \begin{pmatrix} \sqrt{\frac{\sqrt{x} - \Delta}{\sqrt{x} + \Delta}} \\ 1 \end{pmatrix} \frac{1}{\sqrt{1 + \frac{\sqrt{x} - \Delta}{\sqrt{x} + \Delta}}}}$$

Eigenvectors do not depend on $\overline{E}$.

(iii) Show that

$$E_+ + E_- = 2\overline{E} \text{ (trace of } \mathbf{H})$$

$$(E_+)(E_-) = \begin{vmatrix} \Delta & V \\ V^* & -\Delta \end{vmatrix} \qquad \text{(determinant of } \mathbf{H})$$

Solution:

SAME

$$E_+ + E_- = \overline{E} + \sqrt{\Delta^2 + |V|^2} + \overline{E} - \sqrt{\Delta^2 + |V|^2} = 2\overline{E}$$
$$Tr(\widehat{H}) = E_1 + E_2 = \overline{E} + \sqrt{\Delta^2 + |V|^2} + \overline{E} - \sqrt{\Delta^2 + |V|^2} = 2\overline{E}$$
$$(E_+)(E_0) = (\overline{E} + \sqrt{\Delta^2 + |V|^2})(\overline{E} - \sqrt{\Delta^2 + |V|^2}) = \overline{E}^{\,2} - \Delta^2 - |V|^2 = \det(\widehat{H})$$
$$\det(\widehat{H}) = \begin{vmatrix} \Delta + \overline{E} & V \\ V^* & \overline{E} - \Delta \end{vmatrix} = \overline{E}^2 - \Delta^2 - |V|^2$$

(iv) This is the most important part of the problem: If $|V| \ll \Delta$, show that $E_\pm = \overline{E} \pm \frac{|V|^2}{(E_2 - E_1)}$ by doing a power series expansion of $[\Delta^2 + |V|^2]^{1/2}]$. Also show that

$$\psi_+ \approx \alpha\psi_2 + \frac{|V|}{(E_2 - E_1)}\psi_1$$

where

$$\alpha = \left[1 - \left(\frac{|V|}{(E_2 - E_1)}\right)^2\right]^{1/2} \approx 1.$$

It is always a good strategy to show that ψ_+ belongs to E_+ (not E_-). This minimizes sign and algebraic errors.

Solution:

No answer given

C. You have derived the basic formulas of non-degenerate perturbation theory. Use this formalism to solve for the energies of the three-level problem:

$$\mathbf{H} = \begin{pmatrix} E_1^{(0)} & V_{12} & V_{13} \\ V_{12}^* & E_2^{(0)} & V_{23} \\ V_{13}^* & V_{23}^* & E_3^{(0)} \end{pmatrix}$$

$$\begin{aligned} \text{Let } E_1^{(0)} &= -10 \\ E_2^{(0)} &= 0 \\ E_3^{(0)} &= +20 \\ V_{12} &= 1 \\ V_{13} &= 2 \\ V_{23} &= 1 \end{aligned}$$

Solution:

$$\widehat{H} = \begin{pmatrix} -10 & 1 & 2 \\ 1 & 0 & 1 \\ 2 & 1 & 20 \end{pmatrix}$$

$$\widehat{H}\psi = E\psi$$
$$\mathbf{H}\vec{c} = E\vec{c}$$

$$(\mathbf{H} - E\mathbf{I})\vec{c} = 0$$

Solution for E obtained from:

$$\begin{aligned}
0 &= \det(\mathbf{H} - E\mathbf{I}) \\
&= \det\begin{vmatrix} -10-E & 1 & 2 \\ 1 & -E & 1 \\ 2 & 1 & 20-E \end{vmatrix} \\
&= (-10-E)[E^2 - 20E - 1) + 1(2 - 20 + E + 2(1 + 2E) \\
&= -E^3 + 20E^2 + E - 10E^2 + 200E + 10 - 18 + E + 2 + 4E \\
&= -E^3 + 10E^2 + 206E - 6
\end{aligned}$$

Solve this numerically:

$$\begin{aligned}
E_1 &= -10.218 \\
E_2 &= 0.029085 \\
E_3 &= 20.189
\end{aligned}$$

D. The formulas of non-degenerate perturbation theory enable a solution for the three approximate eigenvectors of $\mathbf{H}$ as shown below. Show that $\mathbf{H}$ is *approximately diagonalized* when you use ψ_1' below to evaluate $\mathbf{H}$:

$$\begin{aligned}
\psi_1' &= \psi_1 + \frac{V_{12}}{E_1 - E_2}\psi_2 + \frac{V_{13}}{E_1 - E_3}\psi_3 \\
\psi_2' &= \psi_2 + \frac{V_{12}}{E_2 - E_1}\psi_1 + \frac{V_{13}}{E_2 - E_3}\psi_3 \\
\psi_3' &= \psi_3 + \frac{V_{13}}{E_3 - E_1}\psi_1 + \frac{V_{23}}{E_3 - E_2}\psi_2
\end{aligned}$$

This problem is less burdensome when you use numerical values rather than symbolic values for the elements of $\mathbf{H}$.

Solution:

Given the appropriate solution vectors, we want to test that they "nearly" diagonalized **H**. Writing ψ_1', ψ_2' and ψ_3' is the ψ_1, ψ_2, ψ_3 basis.

$$\psi_1' \qquad \psi_1' = \begin{pmatrix} 1 \\ \frac{1}{-10-0} \\ \frac{2}{-10-20} \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{-1}{10} \\ \frac{-1}{15} \end{pmatrix}$$

$$\psi_2' \qquad \psi_2' = \begin{pmatrix} \frac{1}{0+10} \\ 1 \\ \frac{1}{0-20} \end{pmatrix} = \begin{pmatrix} \frac{1}{10} \\ 1 \\ \frac{-1}{20} \end{pmatrix}$$

$$\psi_3' \qquad \psi_3' = \begin{pmatrix} \frac{2}{20+10} \\ \frac{1}{20-0} \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{15} \\ \frac{1}{20} \\ 1 \end{pmatrix}$$

The transformation into this new approximate eigenbasis is

$$\mathbf{U} = \begin{pmatrix} \psi_1' & \psi_2' & \psi_2' \end{pmatrix}$$

$$\mathbf{U} = \begin{pmatrix} 1 & \frac{1}{10} & \frac{1}{15} \\ \frac{-1}{10} & 1 & \frac{1}{20} \\ \frac{-1}{15} & \frac{-1}{20} & 1 \end{pmatrix}$$

Then

$$\mathbf{U}^{-1}\mathbf{H}U = \mathbf{H}'$$

which should be approximately diagonal:

$$H' = \begin{pmatrix} -10.218 & -0.116 & 0.031 \\ -0.066 & 0.029 & 0.060 \\ -1.125 & 0.190 & 20.189 \end{pmatrix}$$

which is nearly diagonal with eigenvalues very similar to those calculated exactly in part **C**.
