THE HARMONIC OSCILLATOR

- Nearly any system near equilibrium can be approximated as a H.O.
- One of a handful of problems that can be solved exactly in quantum mechanics

examples

Classical H.O.

Hooke's Law: \[ f = -k(X - X_0) = -kx \]
(restoring force)

\[ f = ma = m \frac{d^2x}{dt^2} = -kx \implies \frac{d^2x}{dt^2} + \left(\frac{k}{m}\right)x = 0 \]
Solve diff. eq.: General solutions are\( \sin \) and \( \cos \) functions

\[
x(t) = A\sin(\omega t) + B\cos(\omega t) \quad \omega = \sqrt{\frac{k}{m}}
\]

or can also write as

\[
x(t) = C\sin(\omega t + \phi)
\]

where \( A \) and \( B \) or \( C \) and \( \phi \) are determined by the initial conditions.

e.g. \( x(0) = x_0 \) \( \quad v(0) = 0 \)
spring is stretched to position \( x_0 \) and released at time \( t = 0 \).

Then

\[
x(0) = A\sin(0) + B\cos(0) = x_0 \implies B = x_0
\]

\[
v(0) = \frac{dx}{dt}\bigg|_{x=0} = \omega \cos(0) - \omega \sin(0) = 0 \implies A = 0
\]

So

\[
x(t) = x_0 \cos(\omega t)
\]

Mass and spring oscillate with frequency: \( \omega = \sqrt{\frac{k}{m}} \)

and maximum displacement \( x_0 \) from equilibrium when \( \cos(\omega t) = \pm 1 \)

Energy of H.O.

Kinetic energy \( \equiv K \)

\[
K = \frac{1}{2}mv^2 = \frac{1}{2}m\left(\frac{dx}{dt}\right)^2 = \frac{1}{2}m[-\omega x_0 \sin(\omega t)]^2 = \frac{1}{2}kx_0^2 \sin^2(\omega t)
\]

Potential energy \( \equiv U \)

\[
f(x) = -\frac{dU}{dx} \implies U = -\int f(x)dx = \int kx dx = \frac{1}{2}kx^2 = \frac{1}{2}kx_0^2 \cos^2(\omega t)
\]
Total energy $= K + U = E$

$$E = \frac{1}{2} kx_0^2 \left[ \sin^2(\omega t) + \cos^2(\omega t) \right]$$

Most real systems near equilibrium can be approximated as H.O.

E.g. Diatomic molecular bond

$X_0$ A + B separated atoms

Equilibrium bond length
\[ U(X) = \left. U(X_0) + \frac{dU}{dX} \right|_{X=X_0} (X - X_0) + \frac{1}{2} \left. \frac{d^2U}{dX^2} \right|_{X=X_0} (X - X_0)^2 + \frac{1}{3!} \left. \frac{d^3U}{dX^3} \right|_{X=X_0} (X - X_0)^3 + \cdots \]

Redefine \( x = X - X_0 \) and \( U(X = X_0) = U(x = 0) = 0 \)

\[ U(x) = \left. \frac{dU}{dx} \right|_{x=0} x + \frac{1}{2} \left. \frac{d^2U}{dx^2} \right|_{x=0} x^2 + \frac{1}{3!} \left. \frac{d^3U}{dx^3} \right|_{x=0} x^3 + \cdots \]

At eq. \( \left. \frac{dU}{dx} \right|_{x=0} = 0 \)

For small deviations from eq. \( x^3 \ll x^2 \)

\[ \therefore \quad U(x) \approx \left. \frac{1}{2} \frac{d^2U}{dx^2} \right|_{x=0} x^2 \equiv \frac{1}{2} kx^2 \]
Total energy of molecule in 1D

\[ M = m_1 + m_2 \quad \text{total mass} \]

\[ \mu = \frac{m_1 m_2}{m_1 + m_2} \quad \text{reduced mass} \]

\[ X_{COM} = \frac{m_1 X_1 + m_2 X_2}{m_1 + m_2} \quad \text{COM position} \]

\[ x_{rel} = X_2 - X_1 \equiv x \quad \text{relative position} \]

\[ K = \frac{1}{2} m_1 \left( \frac{dX_1}{dt} \right)^2 + \frac{1}{2} m_2 \left( \frac{dX_2}{dt} \right)^2 = \frac{1}{2} M \left( \frac{dX_{COM}}{dt} \right)^2 + \frac{1}{2} \mu \left( \frac{dx}{dt} \right)^2 \]

\[ U = \frac{1}{2} kx^2 \]

\[ E = K + U = \frac{1}{2} M \left( \frac{dX_{COM}}{dt} \right)^2 + \frac{1}{2} \mu \left( \frac{dx}{dt} \right)^2 + \frac{1}{2} kx^2 \]

**COM coordinate describes translational motion of the molecule**

\[ E_{\text{trans}} = \frac{1}{2} M \left( \frac{dX_{COM}}{dt} \right)^2 \]

**QM description would be free particle or PIB with mass \( M \)**

We'll concentrate on relative motion (describes vibration)

\[ E_{\text{vib}} = \frac{1}{2} \mu \left( \frac{dx}{dt} \right)^2 + \frac{1}{2} kx^2 \]

and solve this problem **quantum mechanically.**
THE QUANTUM MECHANICAL HARMONIC OSCILLATOR

\[ \hat{H}\psi(x) = \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} kx^2 \right] \psi(x) = E\psi(x) \]

Note: replace \( m \) with \( \mu \) (reduced mass) if

Goal: Find eigenvalues \( E_n \) and eigenfunctions \( \psi_n(x) \)

Rewrite as:

\[ \frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} \left[ E - \frac{1}{2} kx^2 \right] \psi(x) = 0 \]

This is not a constant, as it was for P-I-B, so sin and cos functions won’t work.

TRY: \( f(x) = e^{-\alpha x^2/2} \) (gaussian function)

\[ \frac{d^2 f(x)}{dx^2} = -\alpha e^{-\alpha x^2/2} + \alpha^2 x^2 e^{-\alpha x^2/2} = -\alpha f(x) + \alpha^2 x^2 f(x) \]

or rewriting, \[ \frac{d^2 f(x)}{dx^2} + \alpha f(x) - \alpha^2 x^2 f(x) = 0 \]

which matches our original diff. eq. if

\[ \alpha = \frac{2mE}{\hbar^2} \quad \text{and} \quad \alpha^2 = \frac{mk}{\hbar^2} \]

\[ \therefore \quad E = \frac{\hbar}{2} \sqrt{\frac{k}{m}} \]
We have found one eigenvalue and eigenfunction

Recall \[ \omega = \sqrt{\frac{k}{m}} \quad \text{or} \quad \nu = \frac{1}{2\pi} \sqrt{\frac{k}{m}} \]

\[ \therefore E = \frac{1}{2} \hbar \omega = \frac{1}{2} \hbar \nu \]

This turns out to be the lowest energy: the "ground" state

For the wavefunction, we need to normalize:

\[ \psi(x) = Nf(x) = Ne^{-\alpha x^2/2} \quad \text{where } N \text{ is the normalization constant} \]

\[ \int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 1 \implies N^2 \int_{-\infty}^{\infty} e^{-\alpha x^2} = 1 \implies N = \left( \frac{\alpha}{\pi} \right)^{1/4} \frac{1}{\sqrt{\pi/\alpha}} \]

\[ \therefore \psi_0(x) = \left( \frac{\alpha}{\pi} \right)^{1/4} e^{-\alpha x^2/2} \]

\[ E_0 = \frac{1}{2} \hbar \omega = \frac{1}{2} \hbar \nu \]

Note \( \psi_0(x) \) is symmetric. It is an even function: \( \psi_0(x) = \psi_0(-x) \)

There are no nodes, & the most likely value for the oscillator displacement is 0.

So far we have just one eigenvalue and eigenstate. What about the others?
\begin{align*}
\psi_0(x) &= \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2} \\
E_0 &= \frac{1}{2} \hbar \nu \\
\psi_1(x) &= \frac{1}{\sqrt{2}} \left(\frac{\alpha}{\pi}\right)^{1/4} (2\alpha^{1/2} x) e^{-\alpha x^2/2} \\
E_1 &= \frac{3}{2} \hbar \nu \\
\psi_2(x) &= \frac{1}{\sqrt{8}} \left(\frac{\alpha}{\pi}\right)^{1/4} (4\alpha x^2 - 2) e^{-\alpha x^2/2} \\
E_2 &= \frac{5}{2} \hbar \nu \\
\psi_3(x) &= \frac{1}{\sqrt{48}} \left(\frac{\alpha}{\pi}\right)^{1/4} (8\alpha^{3/2} x^3 - 12\alpha^{1/2} x) e^{-\alpha x^2/2} \\
E_3 &= \frac{7}{2} \hbar \nu \\
\vdots & \quad \vdots \\
\text{with} \quad \alpha &= \left(\frac{km}{\hbar^2}\right)^{1/2} \\
\psi_n(x) &= \frac{1}{\left(2^n n!\right)^{1/2}} \left(\frac{\alpha}{\pi}\right)^{1/4} H_n(\alpha^{1/2} x) e^{-\alpha x^2/2} \quad n = 0, 1, 2, \ldots
\end{align*}

These have the general form

\begin{align*}
\psi_n(x) &= \frac{1}{\left(2^n n!\right)^{1/2}} \left(\frac{\alpha}{\pi}\right)^{1/4} H_n(\alpha^{1/2} x) e^{-\alpha x^2/2} \\
&\quad \text{Normalization} \quad \text{Gaussian} \\
&\quad \text{Hermite polynomial (pronounced “air-MEET”)}
\end{align*}

\begin{align*}
H_0(y) &= 1 & \text{even} \quad (n = 0) \\
H_1(y) &= 2y & \text{odd} \quad (n = 1) \\
H_2(y) &= 4y^2 - 2 & \text{even} \quad (n = 2) \\
H_3(y) &= 8y^3 - 12y & \text{odd} \quad (n = 3) \\
H_4(y) &= 16y^4 - 48y^2 + 12 & \text{even} \quad (n = 4) \\
\vdots & \quad \vdots
\end{align*}
Energies are

\[ E_n = \left( n + \frac{1}{2} \right) \hbar \nu \]

Note \( E \) increases linearly with \( n \).

\[ \Rightarrow \text{ Energy levels are evenly spaced} \]

\[ E_{n+1} - E_n = \left( (n+1) + \frac{1}{2} \right) \hbar \nu - \left( n + \frac{1}{2} \right) \hbar \nu = \hbar \nu \quad \text{regardless of } n \]

There is a “zero-point” energy

\[ E_0 = \frac{1}{2} \hbar \nu \]

\( E = 0 \) is not allowed by the Heisenberg Uncertainty Principle.
Symmetry properties of $\psi$'s

$\psi_{0,2,4,6,\ldots}$ are even functions
$\psi(x) = \psi(-x)$

$\psi_{1,3,5,7,\ldots}$ are odd functions
$\psi(x) = -\psi(-x)$

Useful properties:

- (even) · (even) = even
- (odd) · (odd) = even
- (odd) · (even) = odd

\[
\frac{d}{dx}(\text{odd}) = (\text{even}) \quad \frac{d}{dx}(\text{even}) = (\text{odd})
\]

\[
\int_{-\infty}^{\infty} (\text{odd}) \, dx = 0 \quad \int_{-\infty}^{\infty} (\text{even}) \, dx = 2 \int_{0}^{\infty} (\text{even}) \, dx
\]

Just from symmetry:

\[
\langle x \rangle_n = \int_{-\infty}^{\infty} \psi_n^*(x) x \psi_n(x) \, dx = 0 \quad \langle p \rangle_n = \int_{-\infty}^{\infty} \psi_n^* \left( -i\hbar \frac{d}{dx} \right) \psi_n(x) \, dx = 0
\]

Odd
Odd

Average displacement & average momentum = 0

IR spectroscopy $\Rightarrow$ H.O. selection rules

Intensity of vibrational absorption features

Vibrational transition

$\delta^+$

$\delta^-$

$n' = 1$

$n = 0$

$\hbar \nu$
Intensity \( I_{nn'} \propto \left| \frac{d\mu}{dx} \int_{-\infty}^{\infty} \psi^*_n x \psi_n \, dx \right|^2 \)

1) Dipole moment of molecule must change as molecule vibrates \( \Rightarrow \)
HCl can absorb IR radiation, but N\(_2\), O\(_2\), H\(_2\) cannot.

2) Only transitions with \( n' = n \pm 1 \) allowed (selection rule).
(Prove for homework.)

**QUANTUM MECHANICAL HARMONIC OSCILLATOR & TUNNELING**

Classical turning points

Classical H.O.: Total energy \( E_T = \frac{1}{2} kx_0^2 \)
oscillates between \( K \) and \( U \).

Maximum displacement \( x_0 \) occurs when all the energy is potential.

\[ x_0 = \sqrt{\frac{2 E_T}{k}} \] is the “classical turning point”

The classical oscillator with energy \( E_T \) can never exceed this displacement, since if it did it would have more potential energy than the total energy.
**Quantum Mechanical Harmonic Oscillator.**

At high n, probability density begins to look classical, peaking at turning points.

Non-zero probability at \( x > x_0! \)

Prob. of \((x > x_0, x < -x_0):\)

\[
2 \int_{-\infty}^{\infty} |\psi_0^2(x)| dx = 2 \left( \frac{\alpha}{\pi} \right)^{1/2} \int_{-\infty}^{\infty} e^{-\alpha x^2} dx
\]

\[
= \frac{2}{\pi^{1/2}} \int_{1}^{\infty} e^{-y^2} dy = \text{erfc}(1)
\]

"Complementary error function" tabulated or calculated numerically

Prob. of \((x > x_0, x < -x_0) = \text{erfc}(1) = 0.16\)

Significant probability!
The oscillator is "tunneling" into the classically forbidden region. This is a purely QM phenomenon!

Tunneling is a general feature of QM systems, especially those with very low mass like e- and H.

Even though the energy is less than the barrier height, the wavefunction is nonzero within the barrier! So a particle on the left may escape or "tunnel" into the right hand side.

Inside barrier: $$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_0 \right] \psi(x) = E \psi(x)$$

or $$\frac{d^2 \psi(x)}{dx^2} = \left[ \frac{2m(V_0 - E)}{\hbar^2} \right] \psi(x) \equiv \gamma^2 \psi(x)$$

Solutions are of the form $$\psi(x) = Be^{-\gamma x}$$ with $$\gamma = \left[ \frac{2m(V_0 - E)}{\hbar^2} \right]^{1/2}$$

Note $$\gamma \propto (V_0 - E)^{1/2}$$ and $$\gamma \propto m^{1/2}$$

If barrier is not too much higher then the energy and if the mass is light, then tunneling is significant.
Important for protons (e.g. H-bond fluctuations, tautomerization)
Important for electrons (e.g. scanning tunneling microscopy)

**Nonstationary states of the QM H.O.**

System may be in a state other than an eigenstate, e.g.

\[ \psi = c_0 \psi_0 + c_1 \psi_1 \quad \text{with} \quad |c_0|^2 + |c_1|^2 = 1 \quad \text{(normalization), e.g.} \quad |c_0| = |c_1| = \frac{1}{\sqrt{2}} \]

Full time-dependent eigenstates can be written as

\[ \Psi_0(x,t) = \psi_0(x) e^{-i\omega_0 t} \quad \Psi_1(x,t) = \psi_1(x) e^{-i\omega_1 t} \]

where

\[ \hbar \omega_0 = E_0 = \frac{1}{2} \hbar \omega_{\text{vib}} \Rightarrow \omega_0 = \frac{1}{2} \omega_{\text{vib}} \quad \hbar \omega_1 = E_1 = \frac{3}{2} \hbar \omega_{\text{vib}} \Rightarrow \omega_1 = \frac{3}{2} \omega_{\text{vib}} \]

System is then time-dependent:

\[ \Psi(x,t) = \frac{1}{\sqrt{2}} e^{-i\omega_0 t} \psi_0(x) + \frac{1}{\sqrt{2}} e^{-i\omega_1 t} \psi_1(x) = c_0(t) \psi_0(x) + c_1(t) \psi_1(x) \]

where \[ c_0(t) = \frac{1}{\sqrt{2}} e^{-i\omega_0 t} \quad c_1(t) = \frac{1}{\sqrt{2}} e^{-i\omega_1 t} \]

What is probability density?

\[ \Psi^* (x,t) \Psi(x,t) = \frac{1}{2} \left[ \psi_0^* (x) e^{i\omega_0 t} + \psi_1^* (x) e^{i\omega_1 t} \right] \left[ \psi_0(x) e^{-i\omega_0 t} + \psi_1(x) e^{-i\omega_1 t} \right] \]

\[ = \frac{1}{2} \left[ \psi_0^* \psi_0 + \psi_1^* \psi_1 + \psi_1^* \psi_0 e^{i(\omega_1 - \omega_0) t} + \psi_0^* \psi_1 e^{-i(\omega_1 - \omega_0) t} \right] \]

\[ = \frac{1}{2} \left[ \psi_0^2 + \psi_1^2 + 2 \psi_0 \psi_1 \cos(\omega_{\text{vib}} t) \right] \]

Probability density oscillates at the vibrational frequency!
What happens to the expectation value $\langle x \rangle$?
\[ \langle x \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t) \hat{x} \Psi(x,t) \, dx \]

\[ = \frac{1}{2} \int_{-\infty}^{\infty} \left[ \psi^*_0(x) e^{i\omega_0 t} + \psi^*_1(x) e^{i\omega_1 t} \right] x \left[ \psi_0(x) e^{-i\omega_0 t} + \psi_1(x) e^{-i\omega_1 t} \right] \, dx \]

\[ = \frac{1}{2} \left[ \int_{-\infty}^{\infty} \psi^*_0(x) x \psi_0(x) \, dx + \int_{-\infty}^{\infty} \psi^*_1(x) x \psi_1(x) \, dx + \int_{-\infty}^{\infty} \psi^*_1(x) \psi_0(x) e^{i(\omega_1 - \omega_0) t} \, dx + \int_{-\infty}^{\infty} \psi^*_0(x) \psi_1(x) e^{-i(\omega_1 - \omega_0) t} \, dx \right] \]

\[ <x>_0 = 0 \quad <x>_1 = 0 \quad = \cos(\omega_{vib} t) \int_{-\infty}^{\infty} \psi_0(x) \psi_1(x) \, dx \]

\[ <x>(t) \] oscillates at the vibrational frequency, like the classical H.O.!

Vibrational amplitude is \[ \int_{-\infty}^{\infty} \psi_0(x) \psi_1(x) \, dx \]

\[ \psi_0(x) = \left( \frac{\alpha}{\sqrt{\pi}} \right)^\frac{1}{2} e^{-\alpha x^2 / 2} \quad \psi_1(x) = \frac{1}{\sqrt{2}} \left( \frac{\alpha}{\sqrt{\pi}} \right)^\frac{1}{4} (2\alpha^{1/2} x) e^{-\alpha x^2 / 2} \]

\[ \Rightarrow x \psi_0(x) = \left( \frac{\alpha}{\sqrt{\pi}} \right)^\frac{1}{2} x e^{-\alpha x^2 / 2} = (2\alpha)^{-1/2} \psi_1(x) \]

\[ \therefore \int_{-\infty}^{\infty} \psi_0(x) \psi_1(x) \, dx = (2\alpha)^{-1/2} \int_{-\infty}^{\infty} \psi_0^2(x) \, dx = (2\alpha)^{-1/2} \langle x \rangle(t) = (2\alpha)^{-1/2} \cos(\omega_{vib} t) \]

Relations among Hermite polynomials

Recall H.O. wavefunctions

\[ \psi_n(x) = \frac{1}{(2^n n!)^{1/2}} \left( \frac{\alpha}{\sqrt{\pi}} \right)^\frac{1}{4} H_n(\alpha^{1/2} x) e^{-\alpha x^2 / 2} \quad n = 0, 1, 2, ... \]

Normalization \quad Gaussian \quad Hermite polynomial
\[ H_0(y) = 1 \quad \text{even (} n = 0 \text{)} \]
\[ H_1(y) = 2y \quad \text{odd (} n = 1 \text{)} \]
\[ H_2(y) = 4y^2 - 2 \quad \text{even (} n = 2 \text{)} \]
\[ H_3(y) = 8y^3 - 12y \quad \text{odd (} n = 3 \text{)} \]
\[ H_4(y) = 16y^4 - 48y^2 + 12 \quad \text{even (} n = 4 \text{)} \]
\[ \vdots \]

Generating formula for all the \( H_n \):
\[ H_n(y) = (-1)^n y^{n-1} e^{ny} \frac{d^n}{dy^n} e^{-y^2} \]

A useful derivative formula is:
\[ \frac{dH_n(y)}{dy} = (-1)^n 2y^n e^{ny} \frac{d^n}{dy^n} e^{-y^2} + (-1)^n y^{n-1} e^{ny} \frac{d^{n+1}}{dy^{n+1}} e^{-y^2} = 2yH_n(y) - H_{n+1}(y) \]

Another useful relation among the \( H_n \)'s is the recursion formula:
\[ H_{n+1}(y) - 2yH_n(y) + 2nH_{n-1}(y) = 0 \]

Substituting \( 2yH_n(y) = H_{n+1}(y) + 2nH_{n-1}(y) \) above gives
\[ \frac{dH_n(y)}{dy} = 2nH_{n-1}(y) \]

Use these relations to solve for momentum \( \langle p \rangle(t) \)
\[ \langle p \rangle(t) = \int_{-\infty}^{\infty} \Psi^*(x,t) \hat{p} \Psi(x,t) \, dx \]
\[ = \frac{1}{2} \left[ \int_{-\infty}^{\infty} \psi_0^*(x) e^{i\omega_0 t} + \psi_1^*(x) e^{i\omega_1 t} \right] \hat{p} \left[ \psi_0(x) e^{-i\omega_0 t} + \psi_1(x) e^{-i\omega_1 t} \right] \, dx \]
\[ = \frac{1}{2} \left[ \int_{-\infty}^{\infty} \psi_0^* \hat{p} \psi_0 \, dx + \int_{-\infty}^{\infty} \psi_1^* \hat{p} \psi_1 \, dx + \int_{-\infty}^{\infty} \psi_0^* \hat{p} \psi_0 e^{-i(\omega_1 - \omega_0)t} \, dx + \int_{-\infty}^{\infty} \psi_1^* \hat{p} \psi_1 e^{-i(\omega_0 - \omega_0)t} \, dx \right] \]
\[ \langle p \rangle_0 = 0 \quad \langle p \rangle_1 = 0 \]
\[
\frac{d}{dx} \psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/2} (-\alpha x) e^{-\alpha x^2/2} = - \left(\frac{\alpha}{2}\right)^{1/2} \psi_1(x)
\]

\[
\therefore \int_{-\infty}^{\infty} \psi_1^* \hat{\psi}_0 e^{i(\omega_1 - \omega_0) t} \, dx = i \hbar \left(\frac{\alpha}{2}\right)^{1/2} e^{i(\omega_1 - \omega_0) t} \int_{-\infty}^{\infty} \psi_1^* \psi_1 \, dx = i \hbar \left(\frac{\alpha}{2}\right)^{1/2} e^{i\omega_{1}\text{vib} t}
\]

To solve integral \( \int_{-\infty}^{\infty} \psi_0^* \hat{\psi}_1 e^{-i(\omega_1 - \omega_0) t} \, dx \) use relations among \( H_n \)'s

\[
\frac{d}{dx} \psi_1(x) = \frac{d}{dx} \left[ N_1 H_1(\alpha^{1/2} x) e^{-\alpha x^2/2} \right] = \alpha^{1/2} N_1 \frac{d}{dy} \left[ H_1(y) e^{-y^2/2} \right]
\]

with \( y \equiv \alpha^{1/2} x \quad dy = \alpha^{1/2} dx \quad dx = \alpha^{-1/2} dy \quad \frac{d}{dx} = \alpha^{1/2} \frac{d}{dy} \)

\[
\frac{d}{dy} H_1(y) = 2n H_0(y) = 2 H_0(y)
\]

\[
y H_1(y) = \frac{1}{2} \left[ 2n H_0(y) + H_2(y) \right] = H_0(y) + \frac{1}{2} H_2(y)
\]

\[
\frac{d}{dx} \psi_1(x) = \alpha^{1/2} N_1 \left[ H_0(y) e^{-y^2/2} - \frac{1}{2} H_2(y) e^{-y^2/2} \right] = \alpha^{1/2} N_1 \left[ \frac{1}{N_0} \psi_0(x) - \frac{1}{2 N_2} \psi_2(x) \right]
\]

\[
\int_{-\infty}^{\infty} \psi_0^* \hat{\psi}_1 e^{-i(\omega_1 - \omega_0) t} \, dx = e^{-i(\omega_1 - \omega_0) t} \left( -i \hbar \right) \alpha^{1/2} N_1 \int_{-\infty}^{\infty} \psi_0^* \psi_0 \, dx - \frac{1}{2 N_2} \int_{-\infty}^{\infty} \psi_0^* \psi_2 \, dx
\]

\[
= e^{-i(\omega_1 - \omega_0) t} \left( -i \hbar \right) \alpha^{1/2} N_1 \left[ \frac{1}{N_0} \int_{-\infty}^{\infty} \psi_0^* \psi_0 \, dx - \frac{1}{2 N_2} \int_{-\infty}^{\infty} \psi_0^* \psi_2 \, dx \right]
\]

\[
= e^{-i(\omega_1 - \omega_0) t} \left( -i \hbar \right) \frac{N_1}{N_0} = -i \hbar \left(\frac{\alpha}{2}\right)^{1/2} e^{-i\omega_{1}\text{vib} t}
\]

Finally
Average momentum also oscillates at the vibrational frequency.

\[
\langle p \rangle(t) = \frac{1}{2} \left[ i\hbar \left( \frac{\alpha}{2} \right)^{\frac{1}{2}} \left( e^{i\omega_{\text{vib}}t} - e^{-i\omega_{\text{vib}}t} \right) \right] = -\hbar \left( \frac{\alpha}{2} \right)^{\frac{1}{2}} \sin(\omega_{\text{vib}}t)
\]