Simple Harmonic Oscillator

CLASSICAL

center of mass coordinates

\[ x_{cm} = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2} \]

location of cm.

\[ \mu = \frac{m_1 m_2}{m_1 + m_2} \]

reduced mass

\[ F = -k x \]

\[ x = [x_1(t) + x_2(t)] - [x_1 + x_2]_{equilibrium} \]

\( \leq \) for relative notions respect to one another
\[ F = \mu a = \mu \frac{d^2x}{dt^2} \]

\[ \kappa = \kappa_1 - \kappa_2 - l_0 \]

\[ x(t) = b_1 \cos \sqrt{\frac{k}{\mu}} t + b_2 \sin \sqrt{\frac{k}{\mu}} t \]

\[ x(0) = b_1 \cos \sqrt{\frac{k}{\mu}} \times 0 = b_1 = 0 \]

\[ v(0) = \left( \frac{dx(t)}{dt} \right)_{t=0} = b_2 \sqrt{\frac{k}{\mu}} \cos \sqrt{\frac{k}{\mu}} \times 0 = b_2 \sqrt{\frac{k}{\mu}} \]

\[ b_2 = \sqrt{\frac{\mu}{k}} v_0 \]

\[ x(t) = \sqrt{\frac{\mu}{k}} v_0 \sin \sqrt{\frac{k}{\mu}} t \]
Energy

\[ E_{\text{tot}} = E_{\text{pot}} + E_{\text{kin}} \]

\[ E_{\text{potential}} = \frac{1}{2} kx^2 \quad \text{and} \quad E_{\text{kinetic}} = \frac{1}{2} \mu v^2 \]

\[ \overline{E_{\text{pot}}} = \frac{1}{2} \overline{E_{\text{tot}}} \]

\[ \mathcal{V} \]

\[ \frac{1}{2} \mathcal{E}_{\text{tot}} \]

\[ \Rightarrow \text{Continuous Energy Spectrum} \]
Vibrational motion of a diatomic molecule

\[ F = -\frac{dV}{dx} = kx \]

\[ k = -\frac{d^2V}{dx^2} \]

\[ V(x) = \frac{1}{2} kx^2 \]

A good approximation

\[ \mu, x \rightarrow \text{like classical center of mass coord.} \]

\[ \hat{H}\psi_n(x) = E_n\psi_n(x) \]

\[ \frac{\hbar^2}{2\mu} \frac{d^2\psi_n(x)}{dx^2} + \frac{kx^2}{2} \psi_n(x) = E_n \psi_n(x) \]
Solutions:

\[ \psi_n(x) = A_n H_n(\alpha^{1/2} x)e^{-\alpha x^2/2}, \text{ for } n = 0, 1, 2, \ldots \]

\[ A_n = \frac{1}{\sqrt{2^n n!}} \left( \frac{\alpha}{\pi} \right)^{1/4} \]

\[ \int_{-\infty}^{\infty} \psi_n^*(x) \psi_n(x) \, dx = 1 \]

Hermite Polynomials

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

\[ \psi_1(x) = \left( \frac{4\alpha^3}{\pi} \right)^{1/4} x e^{-(1/2)\alpha x^2} \]

\[ \psi_2(x) = \left( \frac{\alpha}{4\pi} \right)^{1/4} (2\alpha x^2 - 1)e^{-(1/2)\alpha x^2} \]

\[ \psi_3(x) = \left( \frac{\alpha^3}{9\pi} \right)^{1/4} (2\alpha x^3 - 3x)e^{-(1/2)\alpha x^2} \]
\( \psi_0, \psi_2, \psi_4, \ldots \)

Even functions
\( \psi(x) = \psi(-x) \)

\( \psi_1, \psi_3, \psi_5, \ldots \)

Odd functions
\( \psi(x) = -\psi(-x) \)

\( f(-x) = -f(x) \)
\[ |\psi(x)|^2 = \psi^*(x)\psi(x) \]

**probability density**
Q: How about the eigenvalues?

$$E_n = \hbar \sqrt{\frac{k}{\mu} \left(n + \frac{1}{2}\right)} = h\nu \left(n + \frac{1}{2}\right) \text{ with } n = 0, 1, 2, 3, ...$$

Frequency of oscillation

Zero point energy?

$$E_0 = \frac{1}{2} h\nu$$

$$\Delta E = h\omega = h\nu$$
Exercise

Example Problem 2.2

(a) Is \( \Psi_1(x) = \left( \frac{4x^3}{\pi c} \right)^{1/4} x e^{-(x/2)^2} \) an eigenfunction of kinetic energy operator or potential energy operator?

\[ \hat{T} + \hat{V}(x) \]

\[ \{x, p\} \neq 0 \]

\[ \left[ \hat{H}, \hat{\hat{T}} \right] \neq 0 \]

\[ \left[ \hat{\hat{H}}, \hat{\hat{T}} \right] \neq 0 \]

\[ \left[ \hat{\hat{T}}, \hat{\hat{V}} \right] \]

\[ \Rightarrow \text{no! It is not an eigenfunction of these operators} \]
(b) What are the average values of the kinetic and potential energies for a quantum mechanical oscillator?

\[ \langle \Phi \rangle = \int \psi^* \psi \, dx \]

**Solution**

\[ \hat{E}_{\text{potential}} = \hat{V}(x), \quad \hat{E}_{\text{kinetic}} = -\frac{t_1^2 d^2}{2 m d x^2} \]

\[ \langle E_{pot} \rangle = \int \psi_1^* (x) V(x) \psi_1 (x) \, dx \]

\[
\begin{align*}
\int_\infty^{-\infty} \left( \frac{4 a^3}{l c} \right)^{1/4} e^{-\frac{1}{2} k x^2} \left( \frac{4 a^3}{l c} \right)^{1/4} e^{-(1/2) a x^2} \, dx \\
= \frac{1}{2} k \left( \frac{4 a^3}{l c} \right)^{1/2} \int_\infty^{-\infty} x^4 e^{-a x^2} \, dx \\
= k \left( \frac{4 a^3}{l c} \right)^{1/2} \int_0^\infty x^4 e^{-x^2} \, dx
\end{align*}
\]
Using \[ \int_0^\infty x^{2n-1} e^{-ax^2} \, dx = \frac{1 \times 3 \times 5 \times \ldots (2n-1)}{2^n \cdot a^n} \sqrt{\frac{\pi}{a}} \]

\[ \int_0^\infty x^3 e^{-ax^2} \, dx = 0 \]

\[ \Rightarrow \langle E_{\text{pot}} \rangle = \frac{1}{2} k \left( \frac{4\pi^3}{\sqrt{\alpha}} \right)^{1/2} \sqrt{\frac{\pi}{a}} \cdot \frac{3}{4\pi^2} \]

\[ \Rightarrow \langle E_{\text{pot}} \rangle = \frac{3 k}{4\pi} = \frac{3}{4} t \sqrt{\frac{k}{\mu}} \]

\[ \langle E_{\text{kin}} \rangle = \int \hat{r}^2 \langle x \rangle \left( -\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} \right) \hat{r} \langle x \rangle \, dx \]

Similar way \[ \frac{1}{2} E_1 \]

\[ \Rightarrow \langle E_{\text{kin}} \rangle = \frac{3}{4} t \sqrt{\frac{k}{\mu}} \]

in general \[ \langle E_{k,n} \rangle = \langle E_{\text{pot}} \rangle = \frac{t \sqrt{k}}{2 \mu} (n+1) \]

for \( n \)th state
Let \( \omega = \sqrt{\frac{k^2}{\mu}} \)

\[ \Rightarrow \quad \varepsilon_n = n \omega \left( n + \frac{1}{2} \right) \]

\[ \downarrow \quad e^{-i (\varepsilon / \hbar) t} \]

\[ \overrightarrow{\Psi}_n(x,t) = \Psi_n(x) e^{-i \omega t} \]

\[ \Delta \varepsilon = \hbar \omega \]

\[ \Rightarrow n \rightarrow \varepsilon_0 = \frac{1}{2} \hbar \omega \] spaced

energies equally