A. Quantum Mechanical Linear Harmonic Oscillator

- In an earlier lecture we covered the classical linear harmonic oscillator that has an energy

\[ E = \frac{p^2}{2m} + \frac{\kappa x^2}{2} \]  

(6.1)

where the frequency of the oscillator is defined by the equation \( \omega = 2\pi \nu = \frac{\sqrt{\kappa}}{\sqrt{m}} \).

- (6.1) has the form of an ellipse, with parametric equations

\[ x(t) = A \cos(\omega t) \text{ and } p(t) = -\omega m A \sin(\omega t), \]

where \( A \) is the amplitude of the oscillatory motion.

- The quantum mechanical oscillator has features very distinct from the classical oscillator. The quantum mechanical treatment of the linear harmonic oscillator (LHO) is one of the most important applications of quantum mechanics. The LHO is used as a simple approximation to molecular bond vibrations.

- The time-independent Schroedinger equation for the LHO is

\[ -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{\kappa x^2}{2}\psi = E\psi \]  

(6.2)

or

\[ \frac{d^2\psi}{dx^2} - \frac{m\kappa x^2}{\hbar^2}\psi = -\frac{2mE}{\hbar^2}\psi \]

- Equation (6.2) can be simplified even further by change of variable \( q = x\sqrt{\alpha} \) where \( \alpha = \frac{\omega m}{\hbar} \). Using these definitions Schroedinger’s equation may be rewritten as simply

\[ \frac{d^2\psi(q)}{dq^2} - q^2\psi(q) = -\epsilon\psi(q) \]  

(6.3)

where \( \epsilon = \frac{2E}{\hbar \nu} = \frac{2E}{\hbar \omega} \)

- Although there are no solid boundary conditions as there was with the particle in the box...the wave function is localized in the sense that it must approach zero as \( x \) increases toward infinity. This just means the probability of finding the particle must decrease as we move toward very large extensions.

- Equation (6.3) can be shown to be equivalent to a well-known differential equation called Hermite’s equation assuming \( \epsilon = \frac{2E}{\hbar \nu} = \frac{2E}{\hbar \omega} = 2n + 1 \) where \( n=0,1,2,3… \)
• This gives rise to the energy quantization equation: \( E_n = \hbar \omega (n + \frac{1}{2}) = \hbar \nu (n + \frac{1}{2}) \). Note this is shifted by \( \frac{1}{2} \hbar \nu \) from Planck’s energy. This is called the zero point energy \( \frac{1}{2} \hbar \nu \), the existence of which is required by the Heisenberg Uncertainty Principle.
• Note also \( \Delta E = E_{n+1} - E_n = \hbar \nu \) which means the energy levels are equally spaced for the LHO.
• The solution to Schrödinger’s equation for the LHO is \( \psi_n(q) = A_n e^{-q^2/2} H_n(q) \). \( A_n \) is a constant and \( H_n(q) \) is called a Hermite polynomial of the nth order.
  • The Hermite polynomials can be generated from the expression
    \[
    H_n(q) = (-1)^n e^{q^2} \frac{\partial^n}{\partial q^n} (e^{-q^2})
    \]
  • For example:
    \[
    H_0(q) = (-1)^0 e^{q^2} \frac{\partial^0}{\partial q^0} (e^{-q^2}) = e^{q^2} (e^{-q^2}) = 1
    \]
    \[
    H_1(q) = (-1)^1 e^{q^2} \frac{\partial^1}{\partial q^1} (e^{-q^2}) = -e^{q^2} (-2q)(e^{-q^2}) = 2q
    \]
    \[
    H_2(q) = (-1)^2 e^{q^2} \frac{\partial^2}{\partial q^2} (e^{-q^2}) = 4q^2 - 2
    \]
  • See text for Hermite polynomial illustrations.

B. Quantum Mechanical Oscillator: Probabilities
• As with the Particle-in-a-Box, the probability of finding a particle at \( q = x \alpha \) is
  \[
P_n(q) = |\psi_n(q)|^2.
  \]
  We require that \( \int_{-\infty}^{\infty} |\psi_n(q)|^2 dq = 1 \), and this requires that the arbitrary constant
  \[
  A_n = \left( \frac{1}{2^n n! \sqrt{\pi}} \right)^{1/2}
  \]
• The final form for the wave function is
  \[
  \psi_n(q) = \left( \frac{1}{2^n n! \sqrt{\pi}} \right)^{1/2} e^{-q^2/2} H_n(q)
  \]
  or in terms of \( x \).
  \[
  \psi_n(x) = \left( \frac{\sqrt{\alpha}}{2^n n! \sqrt{\pi}} \right)^{1/2} e^{-ax^2/2} H_n(x \sqrt{\alpha})
  \]
It is interesting to calculate probabilities $P_n(x)$ for finding a harmonically oscillating particle with energy $E_n$ at $x$. It is easiest to work with the coordinate $q$. For $n=0$ we have:

$$P_n(q) = |\psi_n(q)|^2 = A_n^2 H_n^2(q) e^{-q^2}$$  \hspace{1cm} (6.7)$$

and so

$$\psi_0(q) = \left( \frac{1}{2^00!\sqrt{\pi}} \right)^{1/2} e^{-q^2/2} \Rightarrow P_0(q) = |\psi_0(q)|^2 = \frac{1}{\sqrt{\pi}} e^{-q^2}$$

$$\psi_1(q) = \left( \frac{1}{2^11!\sqrt{\pi}} \right)^{1/2} 2qe^{-q^2/2} \Rightarrow P_1(q) = |\psi_1(q)|^2 \propto \frac{2q^2}{\sqrt{\pi}} e^{-q^2}$$

$$\psi_2(q) = \left( \frac{1}{2^22!\sqrt{\pi}} \right)^{1/2} 2(2q^2-1)e^{-q^2/2} \Rightarrow P_2(q) = |\psi_2(q)|^2 \propto \frac{(2q^2-1)^2}{2\sqrt{\pi}} e^{-q^2}$$

$$\psi_3(q) = \left( \frac{1}{2^33!\sqrt{\pi}} \right)^{1/2} 4(2q^3-3q)e^{-q^2/2} \Rightarrow P_3(q) = |\psi_3(q)|^2 \propto \frac{(2q^3-3q)^2}{3\sqrt{\pi}} e^{-q^2}$$  \hspace{1cm} (6.8)$$

In classical mechanics $E = \frac{\kappa a^2}{2}$, where $a$ is the maximum extension of the LHO and $x = \pm a$ are the classical turning points…i.e. where the mass stops and turns around. In quantum mechanics the classical turning point $a$ is a function of $n$ and is obtained from

$$E_n = \hbar \nu \left(n + \frac{1}{2}\right) = \frac{\kappa a_n^2}{2} \Rightarrow a_n = \pm \sqrt[2n+1]{\frac{2n+1}{\alpha}}$$  \hspace{1cm} (6.9)$$
• Note the wave functions given in (6.7) can extend beyond the classical turning points for all \( n \). The wave functions however do approach zero as \( x \) (or \( q \)) approaches infinity.
• Also, for the classical LHO, the probability of locating the mass \( m \) is maximum at the turning points where the mass is stationary, and minimum at \( x=0 \) where the mass moves at maximum velocity. For \( n=0 \) quantum behavior reverses this trend, i.e. the probability is maximum at \( x=0 \) and decreases toward zero as \( x \) increases.
• Quantum behavior approaches classical behavior as \( n \) and the energy become large. See text figures 14.23 and 14.24. This is an example of the Correspondence Principle.

C. Expectation Values
• The expectation value of a dynamical variable \( O \) can be calculated for a quantum system using expression

\[
\langle O \rangle = \int \psi^*(x)O\psi(x)\,dx
\]

where \( \psi^*(x) \) is called the complex conjugate of the wave function. Given a function of a complex variable \( f = a + ib \), the complex conjugate \( f^* = a - ib \). Note \( f^* = f \), which is a real number. For the harmonic oscillator however, the wave functions \( \psi_n(x) \) are real.

• Calculations
  • Note as in the classical oscillator \( \langle x \rangle = \langle p_x \rangle = 0 \) (why?)
  • We can calculate the mean-square position \( \langle x^2 \rangle \) and the mean-square momentum \( \langle p_{x}^2 \rangle \) for a linear harmonic oscillator in the \( n \)th energy level.

\[
\langle x^2 \rangle = \frac{\langle q^2 \rangle}{\alpha} = \frac{1}{\alpha} \int_{-\infty}^{\infty} \psi_0(q)q^2\psi_0(q)\,dq = \frac{1}{\alpha} \int_{0}^{\infty} q^2 \left( \frac{1}{\sqrt{\pi}} \right) e^{-q^2} \,dq = \frac{2}{\alpha \sqrt{\pi}} \int_{0}^{\infty} q^2 e^{-q^2} = \frac{1}{2\alpha}
\]

In general

\[
\langle x^2 \rangle = \frac{\langle q^2 \rangle}{\alpha} = \frac{1}{\alpha} \int_{-\infty}^{\infty} \psi_n(q)q^2\psi_n(q)\,dq = \frac{1}{\alpha}(n + \frac{1}{2})
\]

\[
\langle p_{x}^2 \rangle = \alpha \left( \frac{\hbar}{2\pi} \right)^2 (n + \frac{1}{2})
\]

In calculating averages like \( \langle x^2 \rangle = \frac{\langle q^2 \rangle}{\alpha} = \frac{1}{\alpha} \int_{-\infty}^{\infty} q^2 \left( \frac{1}{\sqrt{\pi}} \right) e^{-q^2} \,dq \) the standard integral form

\[
\int_{0}^{\infty} x^n e^{-ax^2} \,dx = \frac{1 \times 3 \times 5 \cdots (2n-1)}{2^{n+1} a^n} \sqrt{\frac{\pi}{a}}
\]

is useful…