A. Quantum Mechanical Linear Harmonic Oscillator

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

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

(5.1)

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

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

\[ x(t) = A \cos(\omega t) \] 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 Schrödinger equation for the LHO is

\[ -\frac{\hbar^2}{8m\pi^2} \frac{\partial^2 \psi(x)}{\partial x^2} + \frac{\kappa x^2}{2} \psi(x) = E \psi(x) \]

or

\[ -\frac{\hbar^2}{8m\pi^2} \frac{\partial^2 \psi(x)}{\partial x^2} + \frac{m\omega^2 x^2}{2} \psi(x) = E \psi(x) \]

- Schrödinger’s equation may be rewritten as simply

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

where \( \alpha = \frac{2\pi \nu m}{\hbar}, q = x\sqrt{\alpha}, \) and \( \epsilon = \frac{4\pi E}{\omega \hbar} \).

- 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.

- 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:

\[ H_0(q) = (-1)^0 e^{q^2} \frac{\partial^0}{\partial q^0} (e^{-q^2}) = e^{q^2} (e^{-q^2}) = 1 \]
• \( H_1(q) = (-1)^1 e^{\frac{q^2}{2}} \frac{\partial}{\partial q} \left( e^{-q^2} \right) = -e^{\frac{q^2}{2}} (-2q)(e^{-q^2}) = 2q \)

• \( H_2(q) = (-1)^2 e^{\frac{q^2}{2}} \frac{\partial^2}{\partial q^2} \left( e^{-q^2} \right) = 4q^2 - 2 \)

• The energy has the form \( \varepsilon = \frac{4\pi E}{\omega h} = 2n + 1 \Rightarrow E_n = h \nu (n + \frac{1}{2}), n = 0, 1, 2, 3, \ldots \) Note this is shifted by \( \hbar \nu /2 \) from Planck’s energy. This is called the zero point energy, the existence of which is required by the Heisenberg Uncertainty Principle.

End of Lecture 20

B. Quantum Mechanical Oscillator: Probabilities

• As with the Particle-in-a-Box, the probability of finding a particle at \( q = x\sqrt{\alpha} \) 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

\[
A_n = \left( \frac{1}{2^n n! \sqrt{\pi}} \right)^{1/2} \tag{5.2}
\]

• The final form for the wave function is

\[
\psi_n(q) = \left( \frac{1}{2^n n! \sqrt{\pi}} \right)^{1/2} e^{-\frac{q^2}{2}} H_n(q) \tag{5.3}
\]

or in terms of \( x \)... \( \psi_n(x) = \left( \frac{\sqrt{\alpha}}{2^n n! \sqrt{\pi}} \right)^{1/2} e^{-\frac{\alpha x^2}{2}} H_n\left( x\sqrt{\alpha} \right) \)

• 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:

![Graph of P(q) for n=0,1,2](image_url)
\[ \psi_0(q) = \left( \frac{1}{\sqrt{\pi}} \right)^{1/2} e^{-q^2/2} \]  

(5.4)

and so

\[ \psi_0(q) = A_0 \left( \frac{1}{\sqrt{\pi}} \right)^{1/2} e^{-q^2/2} \Rightarrow P_0(q) = |\psi_0(q)|^2 \propto \frac{1}{\sqrt{\pi}} e^{-q^2} \]

\[ \psi_1(q) = A_1 \left( \frac{2}{\sqrt{\pi}} \right)^{1/2} q e^{-q^2/2} \Rightarrow P_1(q) = |\psi_1(q)|^2 \propto \frac{2q^2}{\sqrt{\pi}} e^{-q^2} \]

\[ \psi_2(q) = A_2 \left( \frac{1}{2\sqrt{\pi}} \right)^{1/2} (2q^2 - 1) e^{-q^2/2} \Rightarrow P_2(q) = |\psi_2(q)|^2 \propto \frac{(2q^2 - 1)^2}{2\sqrt{\pi}} e^{-q^2} \]

\[ \psi_3(q) = A_3 \left( \frac{1}{3\sqrt{\pi}} \right)^{1/2} (2q^3 - 3q) e^{-q^2/2} \Rightarrow P_3(q) = |\psi_3(q)|^2 \propto \frac{(2q^3 - 3q)^2}{3\sqrt{\pi}} e^{-q^2} \]

(5.5)

- The classical amplitude is obtained by

\[ E_n = \hbar v (n + \frac{1}{2}) = \frac{\kappa A_n^2}{2} \Rightarrow A_n = \pm \sqrt{\frac{2n + 1}{\alpha}} \]

(5.6)

- \( A_0 = \pm \sqrt{\frac{1}{\alpha}} \), \( A_1 = \pm \sqrt{\frac{3}{\alpha}} \), \( A_2 = \pm \sqrt{\frac{5}{\alpha}} \), Note the wave functions can extend beyond the classical limits for the motion…

C. Expectation Values

- The expectation value of a dynamical variable \( O \) can be calculated for a quantum system using expression

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

- \( \psi^*(x) \) 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

\[ f^* f = |f|^2 = |a|^2 + |b|^2 \]

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 \( \langle p^2_x \rangle \) for a linear harmonic oscillator in the nth energy level.

\[ \langle x^2 \rangle = \frac{\langle q^2 \rangle}{\alpha} = \frac{1}{\alpha} \int_{-\infty}^{\infty} \psi_0(q) q^2 \psi_0(q) dq = \frac{1}{\alpha} \int_{-\infty}^{\infty} q^2 \left( \frac{1}{\sqrt{\pi}} \right) e^{-q^2} dq = \frac{2}{\alpha \sqrt{\pi}} \int_0^{\infty} q^2 e^{-q^2} = \frac{1}{2\alpha} \]

(5.7)

In general
\[
\langle x^2 \rangle = \frac{\langle q^2 \rangle}{\alpha} = \frac{1}{\alpha} \int_{-\infty}^{\infty} \psi_n(q)^2 \psi_n(q) dq = \frac{1}{\alpha} (n + \frac{1}{2}) \tag{5.8}
\]

\[
\langle p_x^2 \rangle = \alpha \left( \frac{h}{2\pi} \right)^2 (n + \frac{1}{2}) \tag{5.9}
\]