Physics 491: Quantum Mechanic I

Lecture 18: Simple Harmonic Oscillator Continued

In lecture 17 we used algebraic methods to solve the T.I.S.E. We found

$$\hat{H}|n\rangle = \underbrace{\hbar\omega(n+\tfrac{1}{2})}_{E_n}|n\rangle$$

where $n = 0, 1, 2, 3, \ldots$

with $\hat{a}|0\rangle = 0$ and $|n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^{+})^{n}|0\rangle$

so $\hat{a}|n\rangle = \sqrt{n}\,|n\rangle$ and $\hat{a}^{+}|n\rangle = \sqrt{n+1}\,|n+1\rangle$

What are the wave functions?

Recall: Wave function = position representation

$$u_n(x) = \langle x|n\rangle$$

Consider ground state $u_0(x) = \langle x|0\rangle$
Defined by $\langle x|\hat{a}|0\rangle = 0$

Now $\langle x|\hat{a}|0\rangle = \langle x|\hat{X} + i\hat{P}|0\rangle = \langle x|\frac{\hat{x}}{x_c} + i\frac{\hat{p}}{p_c}|0\rangle$

$$= \left(\frac{x}{x_c} + i\frac{\hbar}{ip_c}\frac{\partial}{\partial x}\right)u_0(x) = 0$$

$$\Rightarrow \quad \frac{d}{dx}u_0(x) = -\frac{2}{x_c^2}\,x\,u_0(x)$$

Ground state $\Rightarrow$ $$\boxed{u_0(x) = A_0 e^{-\frac{x^2}{x_c^2}} \quad : \text{Gaussian wave packet}}$$

Normalization $\int_{-\infty}^{\infty} dx\, |u_0(x)|^2 = 1$

$$|u_0(x)|^2 = |A_0|^2 e^{-\frac{2x^2}{x_c^2}}$$

Recall Gaussian $\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{x^2}{2\sigma^2}}$

$$\Rightarrow \quad \sigma^2 = \frac{x_c^2}{4} \qquad |A_0|^2 = \frac{1}{\sqrt{\pi x_c^2/2}}$$

$\Rightarrow$ Choosing A_0 real $\quad A_0 = \frac{1}{\pi^{1/4}} \left(\frac{m\omega}{\hbar}\right)^{1/4}$

<u>Excited states</u> $\quad u_n(x) = \langle x | n \rangle = \frac{1}{\sqrt{n!}} \langle x | (\hat{a}^\dagger)^n | 0 \rangle$

$$\Rightarrow u_n(x) = \frac{1}{\sqrt{n!}} \langle x | (\hat{X} - i\hat{P})^n | 0 \rangle$$

$$= \frac{1}{\sqrt{n!}} \left(\frac{x}{x_c} - i \frac{\hbar}{i p_c} \frac{\partial}{\partial x}\right)^n \langle x | 0 \rangle$$

$$\boxed{u_n(x) = \frac{1}{\sqrt{n!}} \left(\frac{x}{x_c} - \frac{x_c}{2} \frac{\partial}{\partial x}\right)^n u_0(x)}$$

$$\Rightarrow u_n(x) = \frac{A_0}{\sqrt{n!}}\left(\mathrm{X} - \frac{1}{2}\frac{\partial}{\partial \mathrm{X}}\right)^n e^{-\mathrm{X}^2}, \quad \mathrm{X} = \frac{x}{x_c}$$

$$u_1(x) = A_0\left(\mathrm{X} - \frac{1}{2}(-2\mathrm{X})\right) e^{-\mathrm{X}^2} = A_0(2\mathrm{X})e^{-\mathrm{X}^2}$$

$$u_2(x) = \frac{A_0}{\sqrt{2}}\left(\mathrm{X} - \frac{1}{2}\frac{\partial}{\partial \mathrm{X}}\right)\left(2\mathrm{X}e^{-\mathrm{X}^2}\right) = \frac{A_0}{\sqrt{2}}\left(4\mathrm{X}^2 - 1\right)e^{-\mathrm{X}^2}$$

etc.

We see $u_n(x) = (\text{Polynomial of degree } n) * e^{-\mathrm{X}^2}$

Aside: Hermite polynomial: Special function

$$\mathcal{H}_n(\mathrm{X}) = e^{\mathrm{X}^2/2}\left(\mathrm{X} - \frac{\partial}{\partial \mathrm{X}}\right)^n e^{-\mathrm{X}^2}$$

Polynomial of degree n.

$$\Rightarrow \mathcal{H}_n(\sqrt{2}\,\mathrm{X}) = e^{\mathrm{X}^2}\left(\sqrt{2}\,\mathrm{X} - \frac{1}{\sqrt{2}}\frac{\partial}{\partial \mathrm{X}}\right)^n e^{-\mathrm{X}^2}$$

$$= (\sqrt{2})^n e^{\mathrm{X}^2}\left(\mathrm{X} - \frac{1}{2}\frac{\partial}{\partial x}\right) e^{-\mathrm{X}^2}$$

$$\Rightarrow \left(\mathrm{X} - \frac{1}{2}\frac{\partial}{\partial \mathrm{X}}\right)^n e^{-\mathrm{X}^2} = \frac{1}{\sqrt{2^n}}\mathcal{H}_n(\sqrt{2}\,\mathrm{X})$$

$$\Rightarrow \boxed{u_n(x) = A_n \mathcal{H}_n\left(\sqrt{2}\frac{x}{x_c}\right) e^{-(x/x_c)^2}}$$

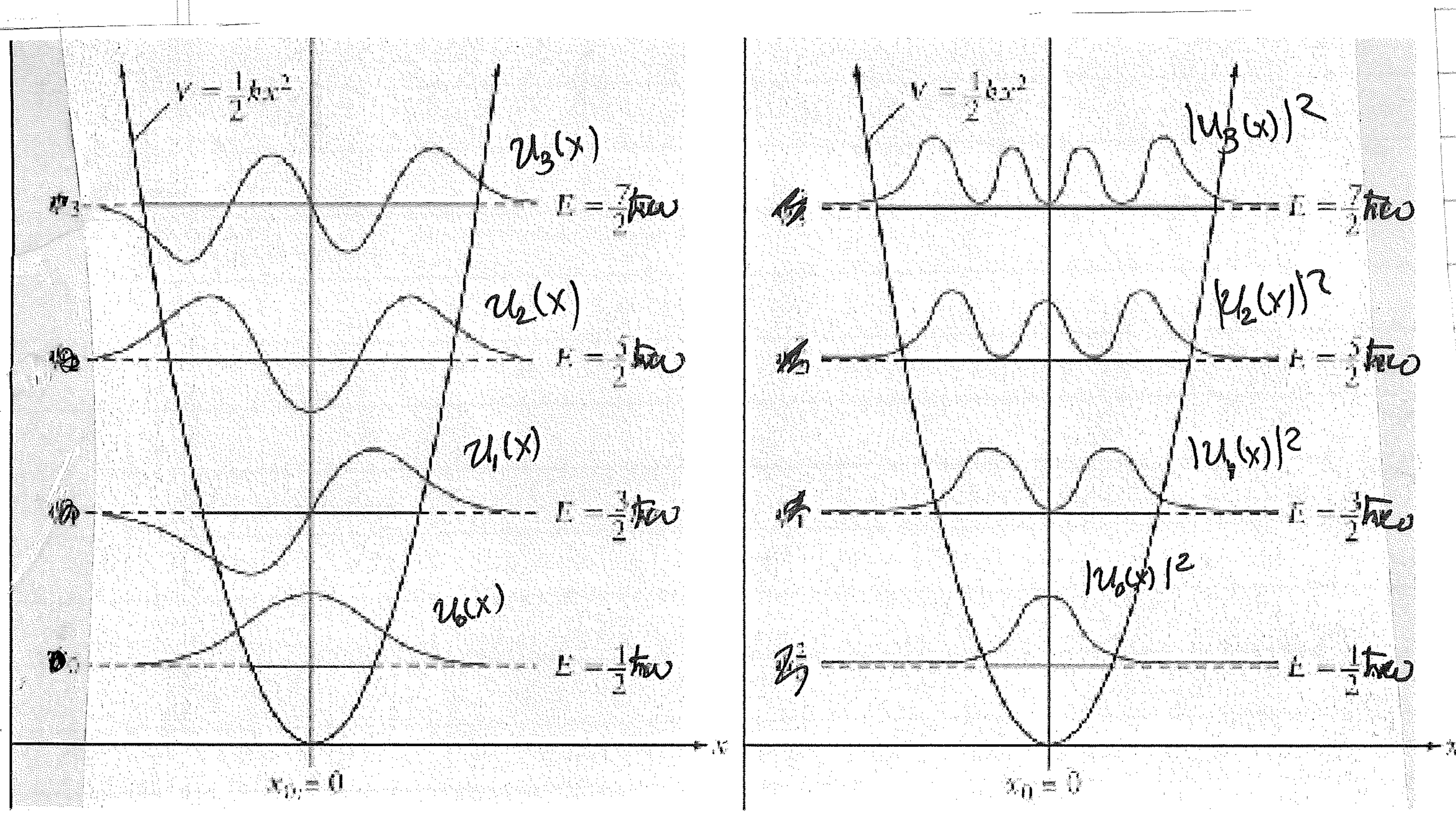
$\mathcal{H}_n$ = n^{th} order Hermite polynomial

$$A_n = \frac{1}{\left(\pi \frac{\hbar}{m\omega}\right)^{1/4}} \frac{1}{\sqrt{n!\,2^n}}$$

The Hermite Polynomial

- Eigenstate of Parity: $\mathcal{H}_n(-\mathbb{X}) = (-1)^n \mathcal{H}_n(\mathbb{X})$
- $\mathcal{H}_0(\mathbb{X}) = 1, \quad \mathcal{H}_1(\mathbb{X}) = 2\mathbb{X}, \quad \mathcal{H}_2(\mathbb{X}) = 4\mathbb{X}^2 - 2$
  etc.

Below is a plot of the energy eigenfunctions



Properties of the stationary states

- Mean position: $\boxed{\begin{array}{l}\langle \hat{x} \rangle_n = \langle n | \hat{x} | n \rangle = 0 \\ \text{(no off-diagonal elements)}\end{array}}$

Using wave functions:

$$\langle n | \hat{x} | n \rangle = \int_{-\infty}^{\infty} dx \; \underbrace{x}_{\text{odd}} \; \underbrace{|u_n(x)|^2}_{\text{even}} = 0$$

- Mean momentum: $\boxed{\begin{array}{l}\langle \hat{p}_n \rangle = \langle n | \hat{p} | n \rangle = 0 \\ \text{no off-diagonal elements}\end{array}}$

$$\langle n | \hat{p} | n \rangle = \int_{-\infty}^{\infty} dx \; u_n(x) \frac{\hbar}{-i} \frac{\partial}{\partial x} u_n(x)$$

This is pretty complicated to calculate. We could notice that

$u_n(x)$ has parity $(-1)^n$

and $\frac{du_n}{dx}(x)$ has parity $(-1)^{n+1}$

$\Rightarrow$ Overlap of even and odd $= 0$

Uncertainty: $\Delta x_n^2 = \langle \hat{x}^2 \rangle_n - \cancel{(\langle \hat{x} \rangle_n)^2} \to 0$

$$\Delta p_n^2 = \langle \hat{p}^2 \rangle_n - \cancel{(\langle \hat{p} \rangle_n)^2} \to 0$$

Ground state: $\langle \hat{x}^2 \rangle_0 = \langle 0| \left(\frac{x_c}{2} (\hat{a} + \hat{a}^\dagger) \right)^2 |0\rangle$

$$\Rightarrow \langle \hat{x}^2 \rangle_0 = \frac{x_c^2}{4} \langle 0| \left(\hat{a}^2 + \hat{a}^{\dagger 2} + \hat{a}^\dagger \hat{a} + \hat{a}\hat{a}^\dagger \right) |0\rangle$$

Aside $\hat{a}|0\rangle = 0$ and $\langle 0| \hat{a}^\dagger = 0$

$$\Rightarrow \langle 0| \hat{a}^2 |0\rangle = 0 \qquad \langle 0| \hat{a}^\dagger \hat{a} |0\rangle = 0$$
$$\langle 0| \hat{a}^{\dagger 2} |0\rangle = 0$$

$$\langle 0| \hat{a}\hat{a}^\dagger |0\rangle = \langle 0| (\hat{a}^\dagger \hat{a} + 1) |0\rangle = 1$$

$$\Rightarrow \langle \hat{x}^2 \rangle_0 = \frac{x_c^2}{4} = \frac{\hbar}{2m\omega}$$

$$\Rightarrow \boxed{\text{Uncertainty } \Delta X_0 = \sqrt{\frac{\hbar}{2m\omega}}}$$

Similarly $\langle \hat{p}^2 \rangle_0 = \langle 0| \left(\frac{p_c}{2i} (\hat{a} - \hat{a}^\dagger) \right)^2 |0\rangle$

$$\Rightarrow \langle \hat{p}^2 \rangle_0 = \frac{p_c^2}{4} \langle 0| -\hat{a}^2 - \hat{a}^{\dagger 2} + \hat{a}^\dagger \hat{a} - \hat{a}\hat{a}^\dagger |0\rangle$$

$$\Rightarrow \langle \hat{p}^2 \rangle_0 = \frac{p_c^2}{4} = \frac{m\omega\hbar}{2}$$

$\Rightarrow$ Uncertain in momentum in the ground-state $\boxed{\Delta p_0 = \sqrt{\frac{m\omega\hbar}{2}}}$

Uncertain product in ground state

$$\boxed{\Delta x_0 \, \Delta p_0 = \frac{\hbar}{2}}$$

Gaussian minimum uncertainty product

In excited states, we can show

$$\boxed{\begin{aligned} \Delta x_n &= \sqrt{(n+\tfrac{1}{2})\frac{\hbar}{m\omega}} \\ \Delta p_n &= \sqrt{(n+\tfrac{1}{2})\, m\omega\hbar} \end{aligned}}$$

Time Dependence:

If $|\psi(0)\rangle = |n\rangle$, $|\psi(t)\rangle = e^{-iE_n t/\hbar}|n\rangle$

$$\Rightarrow \quad |\psi(t)\rangle = \underbrace{e^{-i\omega t/2}}_{\text{same phase for all states}} \; e^{-in\omega t}|n\rangle$$

Stationary state

Given $|\psi(0)\rangle = |n\rangle \Rightarrow \langle \hat{x}(t)\rangle_n = \langle \psi(t)|\hat{x}|\psi(t)\rangle$

$$\Rightarrow \langle \hat{x}(t)\rangle_n = \langle n| e^{+iE_n t/\hbar} \, \hat{x} \, e^{+iE_n t/\hbar}|n\rangle$$

Stationary states [illegible]

"Correspondence Principle"

Though the stationary states do not exhibit the oscillator behavior of the expected values of x and p familiar in the classical SHO, there are aspects of the classical solution buried in the energy eigenfunctions as $n \to \infty$. This is known as Bohr's correspondence principle.

Loosely, for "large quantum numbers", the solutions "look" classical.

More precisely, if a bound particle is moving on a classical trajectory, we can ask the question, what is the probability of finding the particle in the interval

$$x \to x + dx \text{ ?}$$

Classically, we would say that the probability of finding a particle in a certain interval is equal to the fraction of time spent in that interval

$$P_{class}(x)\,dx = \frac{dt(x)}{\frac{T}{2}} = \frac{dx}{\left(\frac{dx}{dt}\right)}\,\frac{2}{T}$$

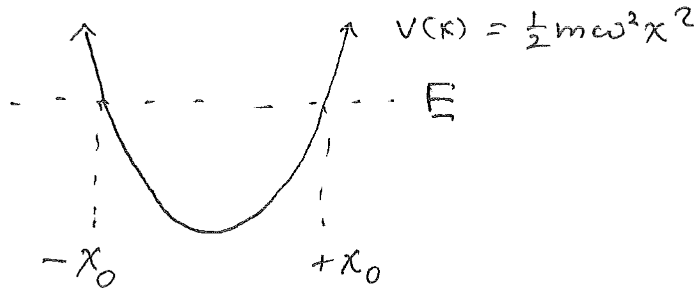
$T \leftarrow$ period of oscillator

$\Rightarrow$ Classical probability density

$$P_{class}(x) = \frac{2}{v_{class}(x)\,T}$$

where $v_{class}(x) = \dfrac{p_{class}(x)}{m} = \dfrac{\sqrt{2m(E - V(x))}}{m}$

Suppose the SHO has turning points at $\pm x_0$

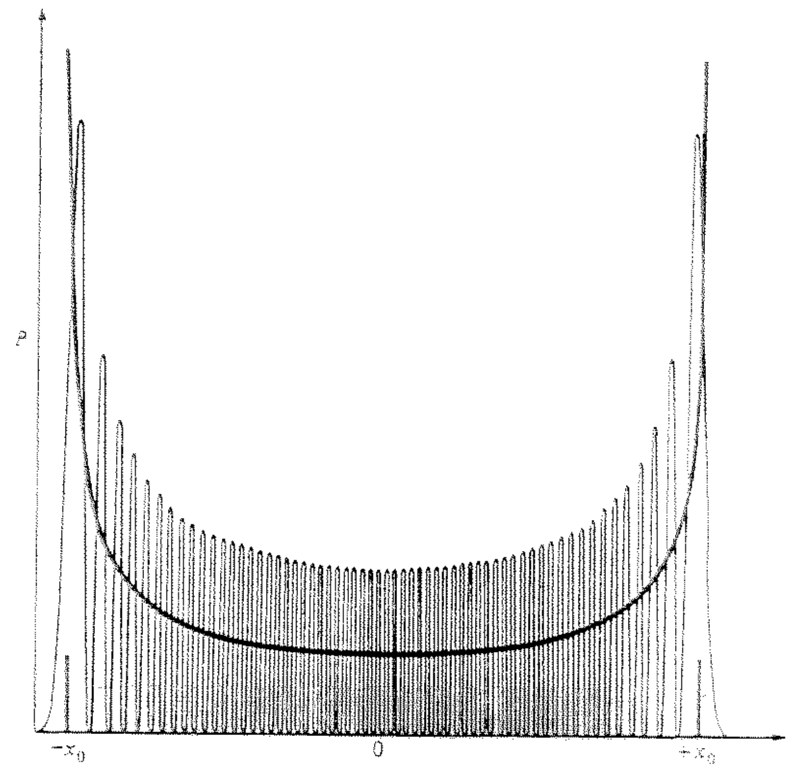


At these turning points $V(x_0) = E \Rightarrow E = \frac{1}{2}m\omega^2 x^2$

$$\Rightarrow v_{class}(x) = \omega\sqrt{x_0^2 - x^2}$$

and the oscillator period $T = \dfrac{2\pi}{\omega}$

Thus $P_{class}(x) = \frac{1}{\pi\sqrt{x_0^2-x^2}}$



Shown above is a plot of $P_{class}(x)$ sumperimposed on the square of the stationary state wave function for $n = 34$. Note the for this large quantum number the wavefunction is much larger near the turning points, as expected classically.

This is a universal feature of stationary states for large quantum numbers – the classical trajectories are reflected in some way in the nature of the wave function

Formally one can show that for large n

$$\psi(x) \approx \frac{c}{\sqrt{v_{class}(x)}} e^{\frac{i}{\hbar}\int_0^x dx' P_{class}(x)} \quad : \text{WKB approximation}$$