Physics 492 – Quantum II

Lecture 7 – SHO Continued

In lecture 6 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 $\langle x|\hat{a}|0\rangle = \langle x|\hat{X} + i\hat{P}|0\rangle = \langle x|\frac{\hat{x}}{x_c} + i\frac{\hat{p}}{p_c}|0\rangle$

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

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

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

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 $\quad A_0 = \frac{1}{\pi^{1/4}} \sqrt{\frac{m\omega}{\hbar}}$

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

$$\Rightarrow u_n(x) = \frac{1}{\sqrt{n!}} \langle x | \left(\frac{\hat{X} - i\hat{P}}{\sqrt{2}} \right)^n | 0 \rangle$$

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

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

Hermite polynomials:

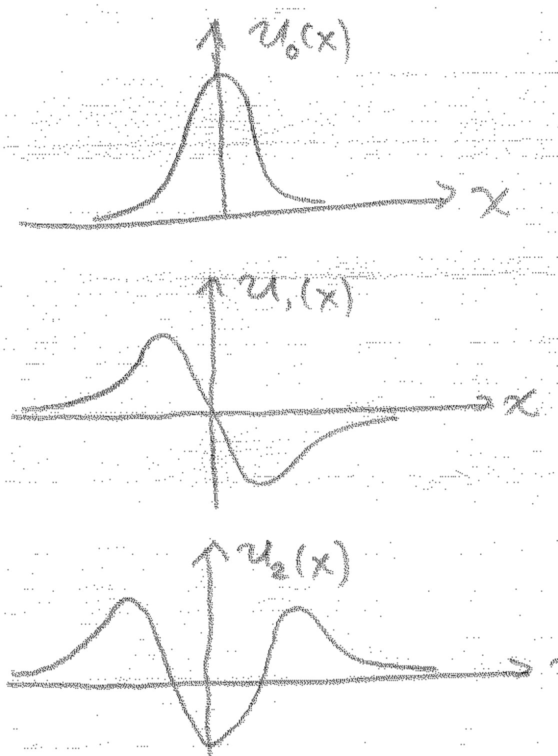
$$u_n(x) = \frac{A_0}{\sqrt{n!}} \left(\frac{x}{x_c} - \frac{x_c}{2} \frac{\partial}{\partial x} \right)^n e^{-x^2/x_c^2}$$

$$\boxed{\begin{aligned} u_n(x) &= A_n \, \mathcal{H}_n\!\left(\frac{\sqrt{2}\,x}{x_c}\right) e^{-x^2/x_c^2} \\ \mathcal{H}_n(y) &= n^{th} \text{ order Hermite polynomial,} \\ A_n &= \frac{1}{\pi^{1/4}} \frac{1}{\sqrt{2^n n!}} \sqrt{\frac{m\omega}{\hbar}} \end{aligned}}$$

$$\mathcal{H}_0(y) = 1, \quad \mathcal{H}_1(y) = 2y, \quad \mathcal{H}_2(y) = 4y^2 - 2$$

Parity $\mathcal{H}_n(-y) = (-1)^n \mathcal{H}_n(y)$

Sketch of stationary states



Matrix representations

Let us write the matrix representations of our observables in the Fock basis $\{|n\rangle\}$

Energy: $\langle n' | \hat{H} | n \rangle = (n + \frac{1}{2}) \hbar\omega \, \delta_{n'n}$ (diagonal)

$$\hat{H} \doteq \begin{bmatrix} \frac{\hbar\omega}{2} & & & \\ & \frac{3\hbar\omega}{2} & & 0 \\ & 0 & \frac{5\hbar\omega}{2} & \\ & & & \ddots \end{bmatrix}$$

Creation / Annihilation

$$\langle n' | \hat{a} | n \rangle = \sqrt{n} \, \langle n' | n-1 \rangle = \sqrt{n} \, \delta_{n', n-1}$$

or

$$= \sqrt{n'+1} \, \langle n'+1 | n \rangle = \sqrt{n'+1} \, \delta_{n'+1, n}$$

$$\hat{a} \doteq \begin{array}{cc} \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & \\ 0 & 0 & \sqrt{3} & 0 & \\ \vdots & \vdots & \vdots & \vdots & \end{bmatrix} & \begin{array}{c} |0\rangle \\ |1\rangle \\ |2\rangle \\ |3\rangle \\ \vdots \end{array} \end{array}$$

$$\hat{a}^\dagger = \langle n' | \hat{a}^\dagger | n \rangle = \sqrt{n+1} \, \langle n' | n+1 \rangle$$

$$= \sqrt{n+1} \, \delta_{n', n+1}$$

$$
\hat{a}^{\dagger} \doteq
\begin{array}{c c}
\begin{array}{cccccc} \langle 0| & \langle 1| & \langle 2| & \langle 3| & & \end{array} & \\
\begin{bmatrix}
0 & \sqrt{1} & 0 & 0 & \cdots \\
0 & 0 & \sqrt{2} & 0 & \cdots \\
0 & 0 & 0 & \sqrt{3} & \cdots \\
0 & 0 & 0 & 0 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \ddots
\end{bmatrix}
&
\begin{array}{c} |0\rangle \\ |1\rangle \\ |2\rangle \\ |3\rangle \\ \end{array}
\end{array}
$$

$$
\text{Position:} \quad \hat{x} = x_c \left(\frac{\hat{a} + \hat{a}^{\dagger}}{2} \right)
$$

$$
\Rightarrow \quad \hat{x} = \sqrt{\frac{\hbar}{2m\omega}}
\begin{bmatrix}
0 & 1 & 0 & 0 & \cdots \\
1 & 0 & \sqrt{2} & 0 & \cdots \\
0 & \sqrt{2} & 0 & \sqrt{3} & \cdots \\
0 & 0 & \sqrt{3} & 0 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \ddots
\end{bmatrix}
$$

$$
\text{Momentum:} \quad \hat{p} = P_c \left(\frac{\hat{a} - \hat{a}^{\dagger}}{2i} \right)
$$

$$
\Rightarrow \quad \hat{p} = -i \sqrt{\frac{m\omega\hbar}{2}}
\begin{bmatrix}
0 & -\sqrt{1} & 0 & 0 & \cdots \\
\sqrt{1} & 0 & -\sqrt{2} & 0 & \cdots \\
0 & \sqrt{2} & 0 & -\sqrt{3} & \cdots \\
0 & 0 & \sqrt{3} & 0 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \ddots
\end{bmatrix}
$$

Properties of the stationary states

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

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: $\boxed{\langle \hat{p}_n \rangle = \langle n | \hat{p} | n \rangle = 0 \quad \text{no off-diagonal elements}}$

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

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

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

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

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

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

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

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

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

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

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

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

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

$$= \langle \hat{x}(0)\rangle_n = 0 \qquad \underline{\text{Stationary}}$$

Similarly, $\langle \hat{p}(t)\rangle_n = 0$ for all times

$\Rightarrow$ Stationary states "don't move"

In order to have dynamics we must have a <u>superposition</u> of energy eigenstates

Example: Let $|\psi(0)\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{2}|1\rangle + \frac{i}{2}|2\rangle$

$$\langle\psi(0)|\psi(0)\rangle = \left|\frac{1}{\sqrt{2}}\right|^2 + \left|\frac{1}{2}\right|^2 + \left|\frac{i}{2}\right|^2 = \frac{1}{2} + \frac{1}{4} + \frac{1}{4} = 1 \checkmark$$

What is $\langle \hat{x}\rangle_{t=0}$?

$$\langle \hat{x}\rangle_{t=0} = \langle\psi(0)|\,\hat{x}\,|\psi(0)\rangle$$

Use matrix representation in energy basis.
Restrict to subspace spanned by $\{|0\rangle, |1\rangle, |2\rangle\}$

$$\hat{x} \doteq \sqrt{\frac{\hbar}{2m\omega}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{bmatrix}$$

$$|\psi(0)\rangle \doteq \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{2} \\ \frac{i}{2} \end{bmatrix} = \frac{1}{2}\begin{bmatrix} \sqrt{2} \\ 1 \\ i \end{bmatrix}$$

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

$$x \to x + dx \, ?$$

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

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

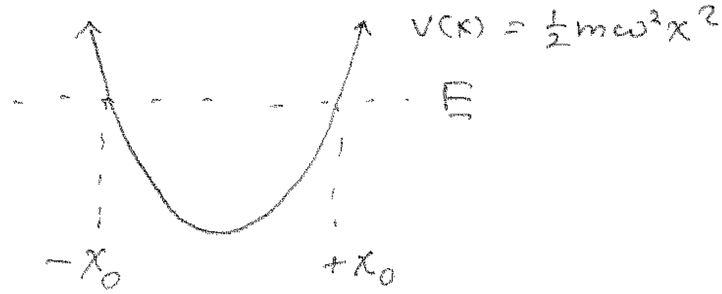
T ← period of oscillator

$\Rightarrow$ Classical probability density

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

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

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

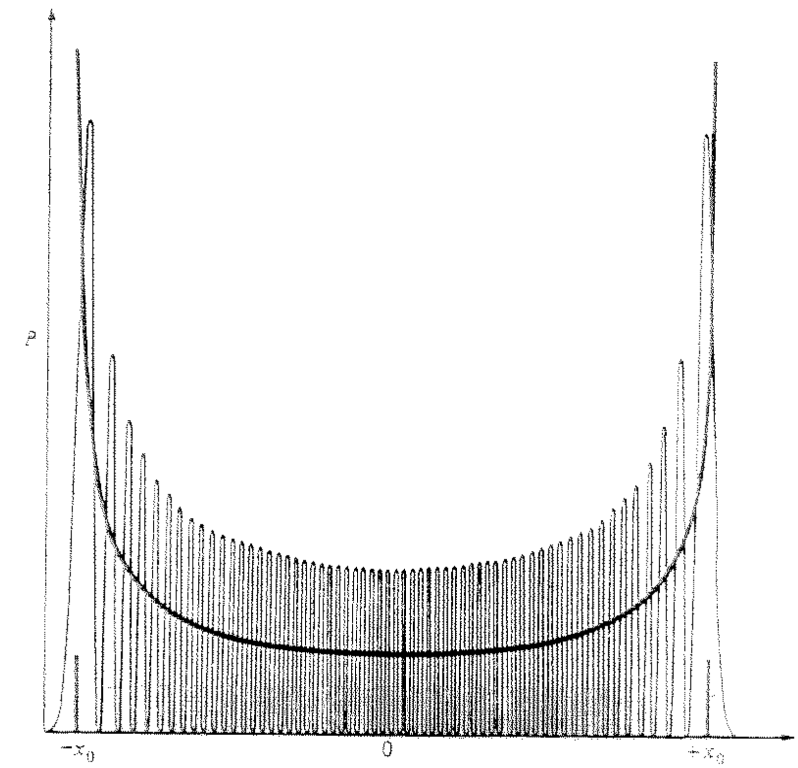


At these turning points $V(x_0) = E \Rightarrow E = \frac{1}{2}m\omega^2 x^2$

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

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

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

$$\Psi(x) \approx \frac{C}{\sqrt{v_{class}(x)}} e^{\frac{i}{\hbar}\int_0^x dx' \, p_{class}(x)} \quad : \text{ WKB approximation}$$