

Phys 506 Lecture 3.

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In this lecture, we use the identities we just developed to determine the simple harmonic oscillator wave functions and other properties. The approach given here is a little different from what you will see in text books.

The SHO Hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2$$

Many text books postulate ladder operators as a "trick" solution, but IF we think of factorizing, like with polynomials, we would try

$$\frac{1}{\sqrt{2m}} (\hat{p} + im\omega\hat{x}) \frac{1}{\sqrt{2m}} (\hat{p} - im\omega\hat{x})$$

You might ask, why not factor as $\hat{A}\hat{A}^\dagger$. We will answer the ordering question later.

But, when we work out the product, because they are operators, we find

$$\begin{aligned} \hat{A}^\dagger \hat{A} &= \frac{1}{2m} (\hat{p}^2 - im\omega [\hat{p}, \hat{x}] + m^2 \omega^2 \hat{x}^2) \\ &= \hat{H} - \frac{1}{2} \hbar \omega \end{aligned}$$

so, we have

$$\hat{H} = \hat{A}^\dagger \hat{A} + \frac{1}{2} \hbar \omega$$

If we recall, for an eigenstate $|\psi\rangle$, $E = \langle \psi | \hat{H} | \psi \rangle$ with normalized $|\psi\rangle$, then we see for this case

$$E = \langle \psi | \hat{H} | \psi \rangle = \langle \psi | \hat{A}^\dagger \hat{A} | \psi \rangle + \frac{1}{2} \hbar \omega$$

$$\Rightarrow E \geq \frac{1}{2} \hbar \omega, \text{ since } \langle \psi | \hat{A}^\dagger \hat{A} | \psi \rangle = \| \hat{A} | \psi \rangle \|^2 \geq 0$$

If we can find a state with $\hat{A} | 0 \rangle = 0$, then this would be the ground state with $E_{gs} = \frac{1}{2} \hbar \omega$.

We assume such a state exists. (Later we see that it does)

We next work out the interesting relation (moving \hat{A}^\dagger through \hat{H})

$$\hat{H} \hat{A}^\dagger = (\hat{A}^\dagger \hat{A} + \frac{1}{2} \hbar \omega) \hat{A}^\dagger = \hat{A}^\dagger (\hat{A} \hat{A}^\dagger + \frac{1}{2} \hbar \omega)$$

$$\begin{aligned} \text{but } [\hat{A}, \hat{A}^\dagger] &= \frac{1}{2m} [\hat{p} - im\omega\hat{x}, \hat{p} + im\omega\hat{x}] \\ &= \frac{1}{2m} 2 im\omega [\hat{p}, \hat{x}] = \hbar \omega \end{aligned}$$

so, we have

$$\hat{H} \hat{A}^\dagger = \hat{A}^\dagger (\hat{H} + \hbar \omega)$$

We use this to find other eigenstates.

claim: $(\hat{A}^\dagger)^n | 0 \rangle$ is an eigenstate

Proof: $\hat{H} (\hat{A}^\dagger)^n | 0 \rangle = \hat{H} \hat{A}^\dagger (\hat{A}^\dagger)^{n-1} | 0 \rangle = \hat{A}^\dagger (\hat{H} + \hbar \omega) (\hat{A}^\dagger)^{n-1} | 0 \rangle$
repeat n-1 more times

$$= (\hat{A}^\dagger)^n (\hat{H} + n\hbar\omega_0) |0\rangle = (\hat{A}^\dagger)^n \left(\frac{1}{2}\hbar\omega_0 + n\hbar\omega_0\right) |0\rangle \quad (2)$$

$$= (n + \frac{1}{2})\hbar\omega_0 (\hat{A}^\dagger)^n |0\rangle = E_n (\hat{A}^\dagger)^n |0\rangle$$

So

$$E_n = (n + \frac{1}{2})\hbar\omega_0.$$

We also use this to normalize:

$$\begin{aligned} \langle 0 | (\hat{A})^n (\hat{A}^\dagger)^n |0\rangle &= \langle 0 | (\hat{A})^{n-1} \hat{A} \hat{A}^\dagger (\hat{A}^\dagger)^{n-1} |0\rangle \\ &= \langle 0 | (\hat{A})^{n-1} (\hat{H} + \frac{1}{2}\hbar\omega_0) (\hat{A}^\dagger)^{n-1} |0\rangle \\ &= \langle 0 | (\hat{A})^{n-1} (\hat{A}^\dagger)^{n-1} (\hat{H} + (n - \frac{1}{2})\hbar\omega_0) |0\rangle \\ &= n\hbar\omega_0 \langle 0 | (\hat{A})^{n-1} (\hat{A}^\dagger)^{n-1} |0\rangle \\ &\quad \text{repeat } n-1 \text{ more times} \\ &= n! (\hbar\omega_0)^n \langle 0 | 0 \rangle \end{aligned}$$

↑ assume normalized

So $|n\rangle = \frac{(\hat{A}^\dagger)^n}{\sqrt{n! (\hbar\omega_0)^n}} |0\rangle$ has $E_n = \hbar\omega_0 (n + \frac{1}{2})$

It is conventional to redefine

$$\hat{a}^\dagger = \frac{-i}{\sqrt{\hbar m \omega_0}} \hat{A}^\dagger \quad \hat{a} = \frac{i}{\sqrt{\hbar m \omega_0}} \hat{A}$$

$$\hat{a}^\dagger = \sqrt{\frac{m\omega_0}{2\hbar}} \left(\hat{x} - i \frac{1}{m\omega_0} \hat{p} \right) \quad \hat{a} = \sqrt{\frac{m\omega_0}{2\hbar}} \left(\hat{x} + i \frac{1}{m\omega_0} \hat{p} \right)$$

Then $[\hat{a}, \hat{a}^\dagger] = 1$, $\hat{H} = \hbar\omega_0 (\hat{a}^\dagger \hat{a} + \frac{1}{2})$, $\hat{a} |0\rangle = 0$, $|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}} |0\rangle$

↑ we removed an inconsequential phase of $(-i)^n$

Next up, we calculate the wave function.

Recall, the eigenstate of position satisfies

$$\hat{x} |x\rangle = x |x\rangle$$

claim:

$$|x\rangle = e^{-i \frac{x \hat{p}}{\hbar}} |x=0\rangle$$

↑ number operator

Proof:

$$\hat{x} |x\rangle = \hat{x} \left(e^{-i \frac{x \hat{p}}{\hbar}} |x=0\rangle \right)$$

↑ insert $e^{-i \frac{x \hat{p}}{\hbar}} e^{i \frac{x \hat{p}}{\hbar}} = 1$

$$\hat{x} |x\rangle = e^{-i \frac{x \hat{p}}{\hbar}} e^{i \frac{x \hat{p}}{\hbar}} \hat{x} e^{-i \frac{x \hat{p}}{\hbar}} |x=0\rangle$$

↑ Hadamard

$$= e^{-i \frac{x \hat{p}}{\hbar}} \left(\hat{x} + \frac{i x}{\hbar} [\hat{p}, \hat{x}] + \frac{1}{2} \left(\frac{i x}{\hbar}\right)^2 [\hat{p}, [\hat{p}, \hat{x}]] \dots \right) |x=0\rangle$$

$$= e^{-i \frac{x \hat{p}}{\hbar}} (\hat{x} + x) |x=0\rangle$$

But $\hat{x} |x=0\rangle = 0 |x=0\rangle = 0 \Rightarrow$

$$\hat{x} |x\rangle = x e^{-i \frac{x \hat{p}}{\hbar}} |x=0\rangle = x |x\rangle$$

so it is an eigenfunction!

$e^{-i \frac{x \hat{p}}{\hbar}}$ is called the translation operator.

Before we calculate the wave function, it is worthwhile to talk about what it really is. The wave function is constructed by the overlap of two eigenfunctions from non commuting operators. We should not think of this as a physical state the particle is in between measurements. It is instead a calculational tool used to determine the results of experiments. Often times conventional QM instruction overemphasizes the importance of the wave function in coordinate space. You should not. We can interpret the overlap in two ways. For example $\psi_n(x) = \langle x | n \rangle$ can be thought of as the probability amplitude to find a particle that has energy E_n to be found in the region near x (we assume the energies are non degenerate for simplicity here). It is similarly, the probability amplitude (technically the complex conjugate of the probability amplitude) to find a particle located near x to have energy E_n . It is important to note that

$$|\langle x | n \rangle|^2 = |\langle n | x \rangle|^2$$

so the probabilities of both statements are the same.

It is easy to overemphasize the importance of $\psi(x)$. But we can also find $\psi(p)$ and other wave functions. When we look at this from an operator perspective, we will see that we can employ translation to relate the amplitude at the origin to the amplitude anywhere else. Amazingly, the results come entirely from operator algebra and the fact that $[\hat{x}, \hat{p}] = i\hbar$. In particular, we do not need the Schrodinger equation or any other differential equation to tell us how to determine the wave function. It follows from the properties of the ground state and the ladder operators. This holds not just for the simple harmonic oscillator, but we will see it holds for all solvable problems later in the course!

Now we calculate the wave function in coordinate space

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$$\Psi_n(x) = \langle x | n \rangle = \langle x=0 | e^{i x \hat{p}} \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}} | 0 \rangle$$

But $\hat{p} = \frac{(\hat{a} - \hat{a}^\dagger) m \omega_0}{2i} \sqrt{\frac{2\hbar}{m \omega_0}} = -i \sqrt{\frac{\hbar m \omega_0}{2}} (\hat{a} - \hat{a}^\dagger)$

The operator $e^{i x \hat{p}} = e^{x \sqrt{\frac{m \omega_0}{2\hbar}} (\hat{a} - \hat{a}^\dagger)}$

So, the question is how do we use these operators to get the wave function. We only know two things about the states

$$\hat{a} | 0 \rangle = 0 \quad \text{and} \quad \hat{x} | x=0 \rangle = 0$$

This means

$$e^{\alpha \hat{a}} | 0 \rangle = | 0 \rangle \quad \text{for any } \alpha$$

and

$$e^{\beta \hat{x}} | x=0 \rangle = | x=0 \rangle \quad \text{for any } \beta$$

These relations are very important always look for such annihilation relations!

This then leads to a potential strategy to simplify this matrix element. We need to convert $e^{\alpha \hat{p}}$ into some kind of $e^{\alpha' \hat{x}}$

Recalling that $\hat{p} \propto \hat{a} - \hat{a}^\dagger$ and $\hat{x} \propto \hat{a} + \hat{a}^\dagger$ tells us we should

- 1.) split up $e^{\alpha \hat{p}} = e^{-\alpha \hat{a}^\dagger} e^{\alpha \hat{a}}$ * correction terms
- 2.) move $e^{\alpha \hat{a}}$ to the right until it disappears when it hits $| 0 \rangle$
- 3.) replace it by $e^{-\alpha \hat{a}^\dagger} | 0 \rangle = | 0 \rangle$
- 4.) move to the left until next to $e^{-\alpha \hat{a}^\dagger}$
- 5.) bring into the same exponent $e^{-c(\hat{a} + \hat{a}^\dagger)}$ * correction terms
- 6.) operate onto $\langle x=0 |$ where $\langle x=0 | e^{-c(\hat{a} + \hat{a}^\dagger)} = \langle x=0 |$

This will get rid of the exponential term. Then we need to determine how to deal with the rest of the expression. To do that we work again with the same two facts $\hat{a} | 0 \rangle = 0$ $\langle x=0 | \hat{x} = 0$ and use them to simplify until we get the final wave function.

Now, we go through the technical details carefully.

$$\text{Recall } e^{i \frac{x \hat{B}}{\hbar}} = \exp \left[x \sqrt{\frac{m\omega_0}{2\hbar}} (\hat{a} - \hat{a}^\dagger) \right]$$

$$= \exp \left[x \sqrt{\frac{m\omega_0}{2\hbar}} \left(\underset{\uparrow}{\hat{A}} - \underset{\uparrow}{\hat{B}} \right) \right]$$

Recall as well $[\hat{a}, \hat{a}^\dagger] = 1$, so use BCH

$$e^{\hat{A}} e^{\hat{B}} = e^{\hat{A} + \hat{B} + \frac{1}{2}[\hat{A}, \hat{B}]} \text{ or } e^{\hat{A}} e^{\hat{B}} e^{-\frac{1}{2}[\hat{A}, \hat{B}]} = e^{\hat{A} + \hat{B}}$$

$$\text{here } \hat{A} = -x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}^\dagger \quad \hat{B} = x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a} \quad [\hat{A}, \hat{B}] = + \frac{m\omega_0}{2\hbar} x^2$$

$$\text{so } \psi_n(x) = \langle x=0 | \frac{e^{-\frac{m\omega_0 x^2}{4\hbar}}}{\sqrt{n!}} e^{-x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}^\dagger} e^{x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}} (\hat{a}^\dagger)^n |0\rangle$$

$$= \frac{e^{-\frac{m\omega_0 x^2}{4\hbar}}}{\sqrt{n!}} \langle x=0 | e^{-x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}^\dagger} \underbrace{\left(e^{x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}} \hat{a}^\dagger e^{-x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}} \right)^n}_{\text{Hadamard}} e^{x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}} |0\rangle$$

"multiply by 1" \leftarrow $e^{-x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}^\dagger} e^{x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}}$

$$= \frac{e^{-\frac{m\omega_0 x^2}{4\hbar}}}{\sqrt{n!}} \langle x=0 | e^{-x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}^\dagger} \left(\hat{a}^\dagger + x \sqrt{\frac{m\omega_0}{2\hbar}} \right)^n |0\rangle$$

"multiply by 1" \leftarrow $e^{-x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}^\dagger} e^{x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}}$ replace $\left(e^{-x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}^\dagger} \hat{a} e^{x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}^\dagger} \right)$ since $\hat{a}|0\rangle = 0 \Rightarrow \hat{a}^\dagger|0\rangle = |1\rangle$

$$= \frac{e^{-\frac{m\omega_0 x^2}{4\hbar}}}{\sqrt{n!}} \langle x=0 | e^{-x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}^\dagger} e^{-x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}} \left(e^{x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}} \hat{a}^\dagger e^{-x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}} + x \sqrt{\frac{m\omega_0}{2\hbar}} \right)^n |0\rangle$$

Hadamard \leftarrow \uparrow twice as much

$$= \frac{e^{-\frac{m\omega_0 x^2}{4\hbar}}}{\sqrt{n!}} \langle x=0 | e^{-x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}^\dagger} e^{-x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}} \left(\hat{a}^\dagger + x \sqrt{\frac{2m\omega_0}{\hbar}} \right)^n |0\rangle$$

BCH $\hat{A} = -x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}^\dagger \quad \hat{B} = -x \sqrt{\frac{m\omega_0}{2\hbar}} \hat{a}$

$$= \frac{e^{-\frac{m\omega_0 x^2}{4\hbar}}}{\sqrt{n!}} \langle x=0 | e^{-x \sqrt{\frac{m\omega_0}{2\hbar}} (\hat{a}^\dagger + \hat{a}) - \frac{1}{2} \frac{m\omega_0}{2\hbar} x^2} \left(\hat{a}^\dagger + x \sqrt{\frac{2m\omega_0}{\hbar}} \right)^n |0\rangle$$

$$\text{Recall: } \hat{a}^\dagger + \hat{a} = \sqrt{\frac{2m\omega_0}{\hbar}} \hat{x}$$

$$= \frac{e^{-\frac{m\omega_0 x^2}{2\hbar}}}{\sqrt{n!}} \langle x=0 | e^{-x \frac{m\omega_0}{\hbar} \hat{x}} \left(\hat{a}^\dagger + x \sqrt{\frac{2m\omega_0}{\hbar}} \right)^n |0\rangle$$

\leftarrow twice as large an exponent.

$$\text{but } \hat{x}|x=0\rangle = 0 \Rightarrow \langle x=0 | e^{-x \frac{m\omega_0}{\hbar} \hat{x}} = \langle x=0 |$$

$$\text{So } \psi_n(x) = \frac{e^{-\frac{m\omega_0 x^2}{2\hbar}}}{\sqrt{n!}} \langle x=0 | \left(\hat{a}^\dagger + x \sqrt{\frac{2m\omega_0}{\hbar}} \right)^n |0\rangle$$

Let's look at $n=0$ and $n=1$

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$$n=0 \quad \psi_0(x) = e^{-\frac{1}{2} \frac{m\omega_0}{\hbar} x^2} \quad \langle x=0 | 0 \rangle$$

number (norm const)

$$n=1 \quad \psi_1(x) = e^{-\frac{1}{2} \frac{m\omega_0}{\hbar} x^2} \quad \langle x=0 | (\hat{a}^\dagger + x \sqrt{\frac{2m\omega_0}{\hbar}}) | 0 \rangle$$

"add zero"

but $\hat{a}^\dagger = \hat{a}^\dagger + \hat{a} - \hat{a} = \sqrt{\frac{2m\omega_0}{\hbar}} \hat{x} - \hat{a}$

$$\psi_1(x) = e^{-\frac{1}{2} \frac{m\omega_0}{\hbar} x^2} \langle x=0 | \left(\sqrt{\frac{2m\omega_0}{\hbar}} \hat{x} - \hat{a} + x \sqrt{\frac{2m\omega_0}{\hbar}} \right) | 0 \rangle$$

← gives 0
← gives 0

$$\psi_1(x) = e^{-\frac{1}{2} \frac{m\omega_0}{\hbar} x^2} x \sqrt{\frac{2m\omega_0}{\hbar}} \langle x=0 | 0 \rangle$$

Define $H_n(\sqrt{\frac{m\omega_0}{\hbar}} x) = \frac{\sqrt{2^n}}{\langle x=0 | 0 \rangle} \langle x=0 | (\hat{a}^\dagger + x \sqrt{\frac{2m\omega_0}{\hbar}})^n | 0 \rangle$

← factors needed to relate to Hermite's work

we just showed that $H_0 = 1$

$$H_1 = 2 \sqrt{\frac{m\omega_0}{\hbar}} x$$

We find a recurrence relation for general n

$$\begin{aligned} H_n(\sqrt{\frac{m\omega_0}{\hbar}} x) &= \frac{\sqrt{2^n}}{\langle x=0 | 0 \rangle} \langle x=0 | (\hat{a}^\dagger + x \sqrt{\frac{2m\omega_0}{\hbar}}) (\hat{a}^\dagger + x \sqrt{\frac{2m\omega_0}{\hbar}})^{n-1} | 0 \rangle \\ &= \frac{\sqrt{2^n}}{\langle x=0 | 0 \rangle} \langle x=0 | \hat{a}^\dagger (\hat{a}^\dagger + x \sqrt{\frac{2m\omega_0}{\hbar}})^{n-1} | 0 \rangle \\ &\quad + 2x \sqrt{\frac{m\omega_0}{\hbar}} H_{n-1}(\sqrt{\frac{m\omega_0}{\hbar}} x) \end{aligned}$$

but $\langle x=0 | \hat{a}^\dagger = \langle x=0 | (-\hat{a})$ since $\langle x=0 | (\hat{a}^\dagger + \hat{a}) = 0$
↑ prop to \hat{x}

$$\begin{aligned} \text{and } \hat{a} (\hat{a}^\dagger + x \sqrt{\frac{2m\omega_0}{\hbar}})^{n-1} | 0 \rangle &= [\hat{a}, (\hat{a}^\dagger + x \sqrt{\frac{2m\omega_0}{\hbar}})^{n-1}] | 0 \rangle \quad \text{since } \hat{a} | 0 \rangle = 0 \\ &= (n-1) (\hat{a}^\dagger + x \sqrt{\frac{2m\omega_0}{\hbar}})^{n-2} | 0 \rangle \end{aligned}$$

$$\text{so } H_n(\sqrt{\frac{m\omega_0}{\hbar}} x) = 2 \sqrt{\frac{m\omega_0}{\hbar}} x H_{n-1}(\sqrt{\frac{m\omega_0}{\hbar}} x) - 2(n-1) H_{n-2}(\sqrt{\frac{m\omega_0}{\hbar}} x)$$

This, combined with the H_0 and H_1 values already found are the recurrence relations for the Hermite polynomials

n	$H_n(y)$
0	1
1	2y
2	4y ² - 2
3	8y ³ - 12y
4	16y ⁴ - 48y ² + 12
5	32y ⁵ - 160y ³ + 120y

Note, this is the physicist's convention. Mathematicians use a different one.

