(15) QHO, Part 2

1 Last Time

- Solved the Schrödinger Equation to find the Energy Eigenstates of the Quantum Harmonic Oscillator
- Discovered that $E_n = \hbar\omega(n + \frac{1}{2})$

2 This Time

- Raising and Lowering Operators the Quantum Harmonic Oscillator
- Commutation Relations of $\hat{a}^\dagger$ and $\hat{a}$

3 Raising and Lowering Operators

We ended last time with normalizable solutions to the Schrödinger equation with a quadratic potenial. So, to summarize, the energy eigenstates of the simple harmonic oscillator potential are

EES of SHO potential

$$\begin{aligned}
\phi_n(x) &= N_n\, H_n\left(x/\lambda\right) e^{-x^2/2\lambda^2} \\
\text{with} \quad & \lambda = \sqrt{\frac{\hbar}{m\omega}} \;\; \text{and} \;\; N_n = \frac{1}{\sqrt{2^n n!\, \lambda\sqrt{\pi}}} \\
\text{and} \quad & E_n = \hbar\omega(n + \tfrac{1}{2}) \\
\psi_n(x,t) &= \phi_n(x) e^{-i(n+\frac{1}{2})\omega t}
\end{aligned}$$

Note that the energies associated with these solutions, that is the energy eigenvalues required to make normalizable solutions, are evenly spaced by $\hbar\omega$ starting with the ground state at $\frac{1}{2}\hbar\omega$.

Today we will take a different approach to solving the Schrödinger equation with this potential. This approach is less direct, so you will have to bear with me for a while. We start by noting that the energy operator can be written as

Energy Operator for SHO

$$\begin{aligned}\hat{E} &= \frac{1}{2m}\hat{p}^2 + \frac{m\omega^2}{2}\,\hat{x}^2 \\ &= \hbar\omega\left[\left(\frac{\hat{p}}{p_0}\right)^2 + \left(\frac{\hat{x}}{x_0}\right)^2\right] \\ \text{with} \qquad & p_0^2 = 2m\hbar\omega, \;\; x_0^2 = \frac{2\hbar}{m\omega} = 2\lambda^2\end{aligned}$$

Much like last time, the first step is to make things dimensionless, though we have done it slightly differently this time.

If $\hat{p}$ and $\hat{x}$ were just numbers, we could use $a^2 + b^2 = (a+ib)(a-ib) = cc^*$ to simplify our lives, but here it doesn't quite work because $\hat{p}$ is an operator. Let's try anyway:

Operators with $\hat{p}$ and $\hat{x}$

$$\begin{aligned}\hat{a} &\equiv \frac{\hat{x}}{x_0} + i\frac{\hat{p}}{p_0} \\ \Rightarrow \hat{a}^\dagger &= \frac{\hat{x}}{x_0} - i\frac{\hat{p}}{p_0} \qquad \because \;\; \hat{x} = \hat{x}^\dagger, \;\; \hat{p} = \hat{p}^\dagger \\ \hat{a}^\dagger\hat{a} &= \left(\frac{\hat{x}}{x_0} - i\frac{\hat{p}}{p_0}\right)\left(\frac{\hat{x}}{x_0} + i\frac{\hat{p}}{p_0}\right) \\ &= \left(\frac{\hat{x}}{x_0}\right)^2 + \left(\frac{\hat{p}}{p_0}\right)^2 + i\frac{\hat{x}}{x_0}\frac{\hat{p}}{p_0} - i\frac{\hat{p}}{p_0}\frac{\hat{x}}{x_0} \\ &= \frac{\hat{E}}{\hbar\omega} + \frac{i}{2\hbar}\left[\hat{x},\hat{p}\right] \qquad \because \;\; x_0 p_0 = 2\hbar \\ &= \frac{\hat{E}}{\hbar\omega} - \frac{1}{2} \qquad \because \;\; [\hat{x},\hat{p}] = i\hbar \\ \Rightarrow \hat{E} &= \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\end{aligned}$$

So far I've only rewritten the energy operator, and yet we see that the form already resembles the answer we worked so hard for in the last lecture.

But what is this new operator $\hat{a}$?

Operator $\hat{a}$

$\hat{a} \neq \hat{a}^\dagger$ tell us that $\hat{a}$ is:

- Not Hermitian
- No constrained to have real eigenvalues
- Not associated with an Observable

Using our solution from last time, we can get a glimpse of what is to come.

Number Operator $\hat{N} = \hat{a}^\dagger \hat{a}$

$$\begin{aligned}
\hat{E}\phi_n(x) &= E\phi_n(x) = \hbar\omega\left(n + \frac{1}{2}\right)\phi_n(x) \\
\hat{E}\phi_n(x) &= \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\phi_n(x) \\
\Rightarrow \hat{a}^\dagger\hat{a}\phi_n(x) &= \hat{N}\phi_n(x) = n\phi_n(x)
\end{aligned}$$

So we expect that $\hat{N}$ applied to an energy eigenstate must give us the occupation number n of that state. We'll show how this comes about in a minute, but before we go on, note that last time we attributed the ground state energy to the uncertainty principle, but without real evidence. Here we see that it is a direct result of the failure of $\hat{x}$ and $\hat{p}$ to commute (which is also the source of the uncertainty principle), since this is what gave rise to the $\frac{1}{2}$ in our new equation for $\hat{E}$.

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4 Commutation Relations

I admit that it is not yet clear why $\hat{a}$ is of interest, but a little more math will get us there. In particular, the relationships of interest are the commutators involving $\hat{a}$.

Commutators of $\hat{a}$

$$\begin{aligned}
\left[\hat{a},\hat{a}^\dagger\right] &= \left[\frac{\hat{x}}{x_0}+i\frac{\hat{p}}{p_0},\frac{\hat{x}}{x_0}-i\frac{\hat{p}}{p_0}\right] \\
\text{use}\quad \left[\hat{A},\hat{B}+\hat{C}\right] &= \hat{A}(\hat{B}+\hat{C})-(\hat{B}+\hat{C})\hat{A} \\
&= \left[\hat{A},\hat{B}\right]+\left[\hat{A},\hat{C}\right] \\
\Rightarrow \left[\hat{a},\hat{a}^\dagger\right] &= \left[\frac{\hat{x}}{x_0},\frac{\hat{x}}{x_0}-i\frac{\hat{p}}{p_0}\right]+i\left[\frac{\hat{p}}{p_0},\frac{\hat{x}}{x_0}-i\frac{\hat{p}}{p_0}\right] \\
&= -\frac{i}{2\hbar}\left[\hat{x},\hat{p}\right]+\frac{i}{2\hbar}\left[\hat{p},\hat{x}\right] \\
&= 1 \quad \because \quad \left[\hat{x},\hat{p}\right]=i\hbar
\end{aligned}$$

With this in hand we are ready to find the commutator of $\hat{a}$ with $\hat{E}$.

Commutator with $\hat{E}$

$$\begin{aligned}
\left[\hat{E},\hat{a}\right] &= \hbar\omega\left[\hat{a}^\dagger\hat{a}+\frac{1}{2},\hat{a}\right] \\
&= \hbar\omega\left(\hat{a}^\dagger\hat{a}\hat{a}-\hat{a}\hat{a}^\dagger\hat{a}\right) \\
&= \hbar\omega\left[\hat{a}^\dagger,\hat{a}\right]\hat{a} \\
&= -\hbar\omega\ \hat{a} \\
&\ \text{similarly for}\quad \hat{a}^\dagger \\
\left[\hat{E},\hat{a}^\dagger\right] &= \hbar\omega\left[\hat{a}^\dagger\hat{a},\hat{a}^\dagger\right] \\
&= \hbar\omega\left(\hat{a}^\dagger\hat{a}\hat{a}^\dagger-\hat{a}^\dagger\hat{a}^\dagger\hat{a}\right) \\
&= \hbar\omega\ \hat{a}^\dagger\left[\hat{a},\hat{a}^\dagger\right] \\
&= \hbar\omega\ \hat{a}^\dagger
\end{aligned}$$

We have seen commutation relationships like this before. Recall the boost operator and its commutation with momentum.

Boost and Momentum

$$\begin{aligned}
\left[\hat{p}, \hat{B}_q\right] &= -i\hbar\left[\partial_x, e^{iqx}\right] \\
&= -i\hbar\left(\partial_x e^{iqx} - e^{iqx}\partial_x\right) \\
&= -i\hbar\left((\partial_x e^{iqx}) + e^{iqx}\partial_x - e^{iqx}\partial_x\right) \\
&= -i\hbar(iq)e^{iqx} = \hbar q\,\hat{B}_q
\end{aligned}$$

Which indicates that $\hat{a}$ must change the energy of a state by $-\hbar\omega$, and $\hat{a}^\dagger$ changes it by $\hbar\omega$, much like the boost operator changes the momentum by $\hbar q$.

We can show this explicitly as follows:

Action of $\hat{a}$

$$\begin{aligned}
\hat{E}\hat{a}\,\phi_n(x) &= (\hat{E}\hat{a} - \overbrace{\hat{a}\hat{E} + \hat{a}\hat{E}}^{=0})\phi_n(x) \\
&= \left(\left[\hat{E}, \hat{a}\right] + \hat{a}\hat{E}\right)\phi_n(x) \\
&= \left(-\hbar\omega\,\hat{a} + \hat{a}\hat{E}\right)\phi_n(x) \\
&= (E_n - \hbar\omega)\,\hat{a}\,\phi_n(x) \\
\hat{E}\;(\hat{a}\,\phi_n(x)) &= E_{n-1}\,(\hat{a}\,\phi_n(x))
\end{aligned}$$

*So the state $\hat{a}\,\phi_n(x)$ **must be** proportional to the state $\phi_{n-1}(x)$!*

Note that I say “proportional” because there is no guarantee that this new state is properly normalized, and we will see in a minute that it is not.

What about $\hat{a}^\dagger$? We can apply the same approach:

Action of $\hat{a}^\dagger$

$$
\begin{aligned}
\hat{E}\hat{a}^\dagger\,\phi_n(x) &= (\hat{E}\hat{a}^\dagger - \hat{a}^\dagger\hat{E} + \hat{a}^\dagger\hat{E})\phi_n(x) \\
&= \left(\left[\hat{E},\hat{a}^\dagger\right] + \hat{a}^\dagger\hat{E}\right)\phi_n(x) \\
&= \left(\hbar\omega\,\hat{a}^\dagger + \hat{a}^\dagger\hat{E}\right)\phi_n(x) \\
&= (E_n + \hbar\omega)\,\hat{a}^\dagger\,\phi_n(x) \\
\hat{E}\,\left(\hat{a}^\dagger\,\phi_n(x)\right) &= E_{n+1}\left(\hat{a}^\dagger\,\phi_n(x)\right)
\end{aligned}
$$

And we get a similar result, but in the other direction.

While $\hat{a}$ lowers the energy of a state by $\hbar\omega$, $\hat{a}^\dagger$ raises the energy of a state by the same amount. These operators are called "raising" and "lowering" operators.

Before going on, let's nail down the normalization factor so that I don't have to keep saying "proportional to". I'll leave the proof of the following to the reader.

Normalization

$$
\begin{aligned}
\hat{a}\,\phi_n(x) &= \sqrt{n}\,\phi_{n-1}(x) \\
\hat{a}^\dagger\,\phi_n(x) &= \sqrt{n+1}\,\phi_{n+1}(x) \\
\text{such that}\quad \hat{a}^\dagger\hat{a}\,\phi_n(x) &= \sqrt{n}\,\hat{a}^\dagger\,\phi_{n-1}(x) \\
&= \sqrt{n}\sqrt{(n-1)+1}\,\phi_n(x) \\
&= n\,\phi_n(x)
\end{aligned}
$$

With this last bit, we can write the explicit action of these operators on the energy eigenstates.

Climbing the Ladder

$$
\begin{aligned}
\hat{a}^{\dagger\,n}\phi_0(x) &= \sqrt{n!}\,\phi_n(x) \\
\hat{a}^n\phi_n(x) &= \sqrt{n!}\,\phi_0(x) \\
\hat{a}^{\dagger\,m}\hat{a}^n\phi_n(x) &= \sqrt{m!\,n!}\,\phi_m(x)
\end{aligned}
$$

The operators $\hat{a}$ and $\hat{a}^\dagger$, through repeated application, can be used to reach ***any energy eigenstate*** *from any other.*

Of course, you can do this without going all the way to the ground state, but the normalization factor is a little more complicated.

The implication of the existence of these "ladder operators" is that the energy eigenvalues are separated by $\hbar\omega$, which is the same thing we learned by solving the Schrödinger equation directly last time. While I made occasional reference to last lecture's derivation along the way, I didn't actually use it anywhere to obtain this result.

The commutation relation between $\hat{E}$ and $\hat{a}$ directly implies a ladder of evenly spaced energy eigenstates.

Recall that in the last lecture we ended up with a recursion relation for the coefficient in a polynomial, such that given the a_0 or a_1 and the energy all of the other a_n could be found recursively.

You may think of $\hat{a}^\dagger$ and $\hat{a}$ as a kind of recursion relation, expressed in terms of derivative operators, which relates each energy eigenfunction to the adjacent eigenfunctions.

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5 Finding the Ground State

So, we have shown that we have a ladder of states. We have not, however, shown that the ladder of states is fixed to any particular value, or that there is any reason why we can't use the lowering operator to step down into negative energies. To avoid negative energy states, which are unphysical, we require that $\hat{a}$ gives zero when applied to some state, which we will identify as the ground state.

Finding the Ground State

$$\begin{aligned}
\hat{a}\phi_0(x) &= 0 \\
\Rightarrow \left(\frac{\hat{x}}{x_0} + i\frac{\hat{p}}{p_0}\right)\phi_0(x) &= 0 \\
\Rightarrow \left(\frac{x}{x_0} + \frac{\hbar}{p_0}\partial_x\right)\phi_0(x) &= 0 \ \because\ \hat{p} = -i\hbar\partial_x \\
\Rightarrow \partial_x\phi_0(x) &= -\frac{p_0}{\hbar x_0}x\phi_0(x) \\
\Rightarrow \partial_x\phi_0(x) &= -\frac{2}{x_0^2}x\phi_0(x) \\
&\quad \because \quad x_0 p_0 = 2\hbar
\end{aligned}$$

We have our first differential equation of the day, and the ground state must solve it. Let's we try our favorite wavefunction, the Gaussian.

Finding the Ground State, continued

$$\begin{aligned}
\text{try} \quad \phi_0(x) &= N_0 e^{-x^2/x_0^2} \\
\Rightarrow \partial_x N_0 e^{-x^2/x_0^2} &= -N_0\frac{2x}{x_0^2}e^{-x^2/x_0^2}
\end{aligned}$$

So, in agreement with the more direct approach, the ground state is a Gaussian.

Lastly, we use this to tie our ladder to a particular energy scale.

Ground State Energy

$$\begin{aligned}
\hat{E}\phi_0(x) &= \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\phi_0(x) \\
&= \hbar\omega\left(0 + \frac{1}{2}\phi_0(x)\right) \\
&= \frac{1}{2}\hbar\omega\ \phi_0(x) \\
\Rightarrow E_0 &= \frac{1}{2}\hbar\omega
\end{aligned}$$

And that wraps it up. We have the ground state and its energy. From there we can find any state by applying the raising operator n times, and we know the energy of the new state will be $\hbar\omega(n + \frac{1}{2})$.

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6 Example: First Excited State

If all of that seems a bit too abstract, you might try to use the raising operator to find the first excited state. It should agree with the direct derivation from last lecture.

Finding the First Excited State

$$\begin{aligned}
\hat{a}^\dagger \phi_0(x) &= \left(\frac{\hat{x}}{x_0} - i\frac{\hat{p}}{p_0}\right)\phi_0(x) \\
&= \left(\frac{x}{x_0} - \frac{\hbar}{p_0}\partial_x\right)\phi_0(x) \\
&= \left(\frac{x}{x_0} + \frac{\hbar}{p_0}\frac{2x}{x_0^2}\right) N_0 e^{-x^2/x_0^2} \\
\Rightarrow \phi_1(x) &= N_0 \frac{2x}{x_0} e^{-x^2/x_0^2} \quad \because \quad x_0 p_0 = 2\hbar \\
&= \sqrt{2} N_1 \frac{2x}{\sqrt{2}\lambda} e^{-x^2/2\lambda^2} \\
& \quad \because \quad x_0 = \sqrt{2}\lambda, \quad N_0 = \sqrt{2} N_1 \\
&= N_1 H_1(x/\lambda) e^{-x^2/2\lambda^2} \quad \because \quad H_1(u) = 2u
\end{aligned}$$

Which is what we started the day with.

And we can lower this state to return to the ground state.

Returning to the Ground State

$$
\begin{aligned}
\hat{a}\phi_1(x) &= N_0 \left(\frac{x}{x_0} + \frac{\hbar}{p_0}\partial_x \right) \frac{2x}{x_0} e^{-x^2/x_0^2} \\
&= N_0 \left[\frac{x}{x_0}\frac{2x}{x_0} + \frac{\hbar}{p_0}\left(\frac{2}{x_0} - \frac{2x}{x_0}\frac{2x}{x_0^2} \right) \right] e^{-x^2/x_0^2} \\
&= N_0 \left[\frac{2x^2}{x_0^2} + \frac{x_0}{2}\left(\frac{2}{x_0} - \frac{4x^2}{x_0^3} \right) \right] e^{-x^2/x_0^2} \\
&= N_0\, e^{-x^2/x_0^2} = \phi_0(x)
\end{aligned}
$$

From all of this you probably get the impression that while we have a way to find all of the eigenstates from the ground state, the work is not really as "done" as it was with the direct approach. Despite this fact, the operator method gave us the energy eigenvalues without having to do the work of finding the actual wavefunctions!

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7 Brief Discussion of Potentials

I have been talking a lot about various potentials. How are these related to real life? What are some physical examples?

Piece of metal or wire (step or well).

Mass on spring, or any other linear restoring force (QHO).

Crystal lattice (delta wells).

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8 Next Time

- The Schrödinger Equation in the real word of 3D