# Harmonic Oscillator

In classical physics we have Hooke's law $F = -kx = m\frac{d^2x}{dt^2}$ which is solved with $x(t) = A\sin(\omega t) + B\cos(\omega t)$ where $\omega = \sqrt{\frac{k}{m}}$

In the case of a harmonic oscillator, we consider a particle in a potential $V(x) = \frac{1}{2}kx^2$.

$$V(x) = \frac{1}{2}kx^2 \Rightarrow V(x) = \frac{1}{2}m\omega^2x^2 \quad \text{by subbing in } \omega = \sqrt{\tfrac{k}{m}}$$

If we substitute this into the TISE: $-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = E\psi$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi$$

$$\Rightarrow \frac{1}{2m}\left[-\hbar^2\frac{\partial^2\psi}{\partial x^2} + (m\omega x)^2\psi\right] = E\psi$$

$$\Rightarrow \frac{1}{2m}\left[\left(-i\hbar\frac{\partial}{\partial x}\right)^2\psi + (m\omega x)^2\psi\right] = E\psi$$

$$\Rightarrow \frac{1}{2m}\left(\hat{p}^2 + (m\omega x)^2\right)\psi = E\psi$$

There is no obvious way to solve this so we will have to struggle through some algebra:

Let's define 2 new operators:

$$\boxed{\hat{a}_\pm = \frac{1}{\sqrt{2\hbar m\omega}}\left(\mp i\hat{p} + m\omega\hat{x}\right)}$$

These two new operators are linear combinations of $\hat{p}$ and $\hat{x}$.

Let's play around a little bit to learn some of the properties of $\hat{a}_\pm$:

$$\hat{a}_-\hat{a}_+ = \frac{1}{2\hbar m\omega}(i\hat{p} + m\omega\hat{x})(-i\hat{p} + m\omega\hat{x})$$

$$= \frac{1}{2\hbar m\omega}\left(\hat{p}^2 + (m\omega\hat{x})^2 + im\omega\hat{p}\hat{x} - im\omega\hat{x}\hat{p}\right)$$

$$= \frac{1}{2\hbar m\omega}\left(\hat{p}^2 + (m\omega\hat{x})^2 - im\omega\underbrace{(\hat{x}\hat{p} - \hat{p}\hat{x})}\right)$$

This is called the commutator of $\hat{x}$ and $\hat{p}$ and is denoted $[\hat{x}, \hat{p}]$

$$= \frac{1}{2\hbar m\omega}\left(\hat{p}^2 + (m\omega\hat{x})^2 - im\omega[\hat{x}, \hat{p}]\right) \quad (*)$$

But what exactly is this commutator?

we can find out what the "value" of a commutator of two operators is if we apply the commutator to a dummy function $f(x)$:

$$[\hat{x},\hat{p}]f(x) = (\hat{x}\hat{p} - \hat{p}\hat{x})f$$

$$= \hat{x}\hat{p}f - \hat{p}\hat{x}f \qquad \text{now apply operators } \hat{x} = x \quad \hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

$$= x\frac{\hbar}{i}f'(x) - \frac{\hbar}{i}\frac{\partial}{\partial x}\left(xf(x)\right)$$

$$= x\frac{\hbar}{i}f'(x) - \frac{\hbar}{i}f(x) - \frac{\hbar}{i}xf'(x) \qquad \text{by using product rule}$$

$$= -\frac{\hbar}{i}f(x) = i\hbar f(x)$$

so if $[\hat{x},\hat{p}]f = i\hbar f$, then $[\hat{x},\hat{p}] = i\hbar$ — we call this the canonical commutation relation.

Subbing this back into (*)

$$\hat{a}_-\hat{a}_+ = \frac{1}{2\hbar m\omega}\left(\hat{p}^2 + (m\omega\hat{x})^2 - im\omega \cdot i\hbar\right)$$

$$= \frac{1}{2\hbar m\omega}\left(\hat{p}^2 + (m\omega\hat{x})^2 + m\omega\hbar\right)$$

$$= \frac{1}{\hbar\omega}\left(\frac{\hat{p}^2}{2m} + \frac{m\omega\hat{x}^2}{2}\right) + \frac{1}{2}$$

$$= \frac{1}{\hbar\omega}\left(\frac{\hat{p}^2}{2m} + V(x)\right) + \frac{1}{2}$$

$$\therefore \boxed{\hat{a}_-\hat{a}_+ = \frac{1}{\hbar\omega}\hat{H} + \frac{1}{2}} \quad \text{or} \quad \boxed{\hat{H} = \hbar\omega\left(\hat{a}_-\hat{a}_+ - \frac{1}{2}\right)}$$

Alternatively, if we had started with $\hat{a}_+\hat{a}_-$

$$\boxed{\hat{a}_+\hat{a}_- = \frac{1}{\hbar\omega}\hat{H} - \frac{1}{2}} \quad \text{or} \quad \boxed{\hat{H} = \hbar\omega\left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right)}$$

if we subtract the $\hat{a}_+\hat{a}_-$ from $\hat{a}_-\hat{a}_+$ we find

$$\hat{a}_-\hat{a}_+ - \hat{a}_+\hat{a}_- = 1 \qquad \therefore \qquad [\hat{a}_-,\hat{a}_+] = 1$$

We can therefore write the TISE ($\hat{H}\psi = E\psi$) as:

$$\underline{\underline{\hbar\omega\left(\hat{a}_-\hat{a}_+ - \tfrac{1}{2}\right)\psi = E\psi}} \quad \text{or} \quad \underline{\underline{\hbar\omega\left(\hat{a}_+\hat{a}_- + \tfrac{1}{2}\right)\psi = E\psi}}$$

So why is this great? Well now we have the tools to calculate all solutions of the harmonic oscillator completely algebraically. Let's see how:

From the TISE $\hat{H}\psi = E\psi$, let's see what happens if the $\psi$ is acted on by $\hat{a}_+$:

$$\begin{aligned}
\hat{H}(\hat{a}_+\psi) &= \hbar\omega\left(\hat{a}_+\hat{a}_- + \tfrac{1}{2}\right)(\hat{a}_+\psi) \\
&= \hbar\omega\left(\hat{a}_+\hat{a}_-\hat{a}_+ + \tfrac{1}{2}\hat{a}_+\right)\psi \\
&= \hbar\omega\,\hat{a}_+\left(\hat{a}_-\hat{a}_+ + \tfrac{1}{2}\right)\psi
\end{aligned}$$

since $\hat{a}_-\hat{a}_+ - \hat{a}_+\hat{a}_- = 1$
$\hat{a}_-\hat{a}_+ = 1 + \hat{a}_+\hat{a}_-$

$$\begin{aligned}
&= \hbar\omega\,\hat{a}_+\left(\hat{a}_+\hat{a}_- + 1 + \tfrac{1}{2}\right)\psi \\
&= \hat{a}_+\left[\hbar\omega\left(\hat{a}_+\hat{a}_- + \tfrac{1}{2}\right) + \hbar\omega\right]\psi \\
&= \hat{a}_+(\hat{H} + \hbar\omega)\psi = \hat{a}_+(E + \hbar\omega)\psi
\end{aligned}$$

$\therefore\ \hat{H}(\hat{a}_+\psi) = (E + \hbar\omega)(\hat{a}_+\psi)$ This is in the form of the TISE so this tells us that $\hat{a}_+\psi$ also corresponds to a solution of the TISE but this time with an energy $E + \hbar\omega$.

Doing the same for $\hat{a}_-$:

$$\begin{aligned}
\hat{H}(\hat{a}_-\psi) &= \hbar\omega\left(\hat{a}_-\hat{a}_+ - \tfrac{1}{2}\right)(\hat{a}_-\psi) \\
&= \hbar\omega\,\hat{a}_-\left(\hat{a}_+\hat{a}_- - \tfrac{1}{2}\right)\psi
\end{aligned}$$

but since $\hat{a}_+\hat{a}_- - \hat{a}_-\hat{a}_+ = -1$
$\hat{a}_+\hat{a}_- = \hat{a}_-\hat{a}_+ - 1$

$$\begin{aligned}
&= \hbar\omega\,\hat{a}_-\left(\hat{a}_-\hat{a}_+ - \tfrac{1}{2} - 1\right)\psi \\
&= \hat{a}_-\left[\hbar\omega\left(\hat{a}_-\hat{a}_+ - \tfrac{1}{2}\right) - \hbar\omega\right]\psi \\
&= \hat{a}_-(\hat{H} - \hbar\omega)\psi = \hat{a}_-(E - \hbar\omega)\psi
\end{aligned}$$

$\therefore\ \hat{H}(\hat{a}_-\psi) = (E - \hbar\omega)(\hat{a}_-\psi)$ so this gives a solution of the TISE with an energy of $E - \hbar\omega$.

So if we had 1 solution of the TISE, we could generate all the rest using $\hat{a}_+$ and $\hat{a}_-$

The operator $a_+$ and $a_-$ are thus called ladder operators since they provide solutions to the TISE that have corresponding energies either raised or lowered by $\hbar\omega$.

Since there are infinite stationary state solutions, we could apply $\hat{a}_+$ infinite times. But what about $\hat{a}_-$?

If we let $\psi_0$ be the stationary state solution with the smallest energy larger than 0, then:

$$\hat{a}_- \psi_0 = 0 \rightarrow \frac{1}{\sqrt{2\hbar m\omega}}\left(i\hat{p} + m\omega\hat{x}\right)\psi_0 = 0$$

$$\frac{1}{\sqrt{2\hbar m\omega}}\left(\hbar\frac{\partial}{\partial x} + m\omega x\right)\psi_0 = 0$$

This is a differential equation which we can transform into:

$$\hbar\frac{\partial}{\partial x}\psi = -m\omega x\psi_0 \Rightarrow \frac{d\psi_0}{dx} = \frac{-m\omega}{\hbar}x\psi_0$$

$$\int\frac{d\psi_0}{\psi_0} = \frac{-m\omega}{\hbar}\int x\,dx \Rightarrow \ln\psi_0 = -\frac{m\omega}{2\hbar}x^2 + C$$

$$\therefore \psi_0 = Ae^{-\frac{m\omega}{2\hbar}x^2}$$ we find $A$ through normalisation:

$$\int|\psi_0|^2dx = 1 = |A|^2\int_{-\infty}^{\infty}e^{-\frac{m\omega}{\hbar}x^2}dx$$

This is a standard integral with result $\sqrt{\frac{\pi}{a}}$ where $a = \frac{m\omega}{\hbar}$

$$= |A|^2\sqrt{\frac{\pi\hbar}{m\omega}}$$

$$\Rightarrow A = \pm\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$$ we pick positive for convenience

So the ground state wave function of the harmonic oscillator is:

$$\underline{\underline{\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}e^{-\frac{m\omega}{2\hbar}x^2}}}$$

We can compute the corresponding energy of this ground state using the hamilton operator

$$\hat{H}\psi_0 = \hbar\omega(\hat{a}_+\hat{a}_- + \tfrac{1}{2})\psi_0 = E_0\psi_0$$

$$E_0\psi_0 = \hbar\omega\,\hat{a}_+\hat{a}_-\psi_0 + \hbar\omega\tfrac{1}{2}\psi_0 \qquad \text{but } \hat{a}_-\psi_0 = 0$$

$$= \hbar\omega\,\hat{a}_+(0) + \tfrac{1}{2}\hbar\omega\psi_0$$

$$E_0\psi_0 = \tfrac{1}{2}\hbar\omega\psi_0 \quad \Rightarrow \quad \underline{\underline{E_0 = \tfrac{1}{2}\hbar\omega}}$$

We can now construct the whole ladder of solutions by repeatedly applying the $\hat{a}_+$ operator:

$$\underline{\underline{\psi_n(x) = A_n(\hat{a}_+)^n\psi_0(x)}} \quad \text{with} \quad \underline{\underline{E_n = (n+\tfrac{1}{2})\hbar\omega}}$$

So what is a general expression for $A_n$ at any $\psi_n$?

Let's use the ladder operators to find an expression for this normalisation constant:

let $\hat{a}_+\psi_n = c_{n+1}\psi_{n+1}$ $\quad \hat{a}_-\psi_n = d_{n-1}\psi_{n-1}$ $\quad$ where $c_{n+1}$ and $d_{n-1}$ are normalisation constants to be determined.

Before we continue, let's make some observations about $\hat{a}_+$ and $\hat{a}_-$

a) if $f$ and $g$ are square integrable functions:

$$\int_{-\infty}^{\infty} f^*\hat{a}_\pm g\,dx = \frac{1}{\sqrt{2m\hbar\omega}}\int_{-\infty}^{\infty} f^*\left(\mp\hbar\frac{d}{dx} + m\omega x\right)g\,dx$$

$$= \frac{1}{\sqrt{2m\hbar\omega}}\left\{\left[\mp\hbar f^*g\right]_{-\infty}^{\infty} + \int_{-\infty}^{\infty}\pm\hbar\frac{d}{dx}f^*g\,dx + \int_{-\infty}^{\infty}m\omega x f^*g\,dx\right\}$$

$$= \frac{1}{\sqrt{2m\hbar\omega}}\int_{-\infty}^{\infty}\left(\pm\hbar\frac{d}{dx} + m\omega x\right)f^*g\,dx = \int_{-\infty}^{\infty}(\hat{a}_\mp f)^*g$$

Summarising: We see it is possible to "move" around the ladder operators:

$$\int_{-\infty}^{\infty} f^*(\hat{a}_\pm g)\,dx = \int_{-\infty}^{\infty}(\hat{a}_\mp f)^*g\,dx$$

We say that $\hat{a}_\pm$ is the hermitian conjugate of $\hat{a}_\mp$

More on what that means later in the course!

b) from $\hbar\omega(\hat{a}_\pm \hat{a}_\mp \pm \frac{1}{2})\psi_n = E_n\psi_n$, we can make the substitution $E_n = (n+\frac{1}{2})\hbar\omega$ that we showed earlier:

$$\hbar\omega(\hat{a}_\pm \hat{a}_\mp \pm \tfrac{1}{2})\psi_n = (n+\tfrac{1}{2})\hbar\omega\,\psi_n$$

$$\hat{a}_\pm \hat{a}_\mp \psi_n \pm \tfrac{1}{2}\psi_n = (n+\tfrac{1}{2})\psi_n$$

$$\Rightarrow \hat{a}_\pm \hat{a}_\mp \psi_n = (n + \tfrac{1}{2} \mp \tfrac{1}{2})\psi_n$$

we can now combine a) and b) together:

a) $\int_{-\infty}^{\infty} f^* \hat{a}_\pm g\, dx = \int_{-\infty}^{\infty} (\hat{a}_\mp f)^* g\, dx$

b) $\hat{a}_\pm \hat{a}_\mp \psi_n = (n + \frac{1}{2} \mp \frac{1}{2})\psi_n$

we can compute the normalisation of $\hat{a}_+\psi_n$:

$$\int_{-\infty}^{\infty} (\hat{a}_+\psi_n)^* (\hat{a}_+\psi_n)\, dx = \int_{-\infty}^{\infty} (\hat{a}_-\hat{a}_+\psi_n)^* \psi_n\, dx$$ we used a) for this

$$\int_{-\infty}^{\infty} (\hat{a}_-\hat{a}_+\psi_n)^* \psi_n\, dx = \int_{-\infty}^{\infty} ((n+\tfrac{1}{2}+\tfrac{1}{2})\psi_n)^* \psi_n\, dx$$

$$= (n+1)\int_{-\infty}^{\infty} |\psi_n|^2\, dx$$

$$(n+1) = |c_{n+1}|^2 \int_{-\infty}^{\infty} |\psi_{n+1}|^2\, dx$$ since the wave functions are normalised (don't really get this step, just go with it!)

we have thus showed that:

$$\hat{a}_+\psi_n = \sqrt{n+1}\,\psi_{n+1}$$ This is an important result.

so assuming we know the functional form of $\psi_n$, we can get a properly normalised $\psi_{n+1}$ by applying $\hat{a}_+$ once.

we can similarly show:

$$\int_{-\infty}^{\infty} (\hat{a}_-\psi_n)^* (\hat{a}_-\psi_n)\, dx = \int_{-\infty}^{\infty} (\hat{a}_+\hat{a}_-\psi_n)^* \psi_n\, dx = \int_{-\infty}^{\infty} ((n+\tfrac{1}{2}-\tfrac{1}{2})\psi_n)^* \psi_n\, dx$$

$$= n\int_{-\infty}^{\infty} |\psi_n|^2\, dx \qquad \therefore \quad n = |d_{n-1}|^2 \int_{-\infty}^{\infty} |\psi_{n-1}|^2\, dx$$

We have thus showed that:

$$\underline{\underline{\hat{a}_- \psi_n = \sqrt{n}\, \psi_{n-1}}}$$

We can then combine these to give us a general expression for normalised harmonic oscillator states:

$$\boxed{\psi_n = \frac{1}{\sqrt{n!}} (\hat{a}_+)^n \psi_0} \quad \text{where} \quad \underline{\underline{\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}}}$$

Just like for the infinite square well, the stationary states for the harmonic oscillator are orthogonal. We can show this by:

$$\int_{-\infty}^{\infty} \psi_m^* (\hat{a}_+\hat{a}_- \psi_n)\, dx = \int_{-\infty}^{\infty} (\hat{a}_- \psi_m)^* (\hat{a}_- \psi_n)\, dx = \int_{-\infty}^{\infty} (\hat{a}_+\hat{a}_- \psi_m)^* \psi_n \, dx$$

$$\rightarrow n \int_{-\infty}^{\infty} \psi_m^* \psi_n \, dx = \underline{\underline{n \delta_{mn}}} = \underline{\underline{m \delta_{mn}}}$$

So there is only a solution if $m = n$. So they are orthogonal.

## Calculating Potential Energy

We can use ladder operators to compute the potential energy in the $n^{th}$ state. Without ladder operators we would try:

$$\langle V \rangle = \langle \tfrac{1}{2} m\omega^2 x^2 \rangle = \tfrac{1}{2} m\omega^2 \int_{-\infty}^{\infty} \psi_n^* x^2 \psi_n \, dx$$ and we would evaluate this by brute force.

We can instead do this more elegantly with ladder operators.

We know $\hat{a}_\pm = \frac{1}{\sqrt{2\hbar m\omega}} (\mp i\hat{p} + m\omega x)$

$$\hat{a}_+ + \hat{a}_- = \frac{1}{\sqrt{2\hbar m\omega}} (-i\hat{p} + i\hat{p} + 2m\omega x) = \frac{1}{\sqrt{2\hbar m\omega}} (2m\omega x)$$

$$\therefore \hat{a}_+ + \hat{a}_- = \sqrt{\frac{4m^2\omega^2}{2\hbar m\omega}}\, x = \sqrt{\frac{2m\omega}{\hbar}}\, x$$

$$\underline{\underline{\therefore x = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a}_+ + \hat{a}_-)}}$$

Similarly:

$$a_+ - a_- = \frac{1}{\sqrt{2\hbar m\omega}}\left(-i\hat{p} - i\hat{p}\right) = \frac{1}{\sqrt{2\hbar m\omega}}\left(-2i\hat{p}\right)$$

$$= -\sqrt{\frac{2}{\hbar m\omega}}\, i\hat{p} \qquad \therefore\ \hat{p} = -\sqrt{\frac{\hbar m\omega}{2}} \cdot \frac{1}{i} \cdot (a_+ - a_-)$$

$$\therefore\ \underline{\hat{p} = \sqrt{\frac{\hbar m\omega}{2}}\, i\,(a_+ - a_-)}$$

We don't actually need this, just demonstrating it's possible.

$$x^2 = \frac{\hbar}{2m\omega}\left(\hat{a}_+\hat{a}_+ + \hat{a}_+\hat{a}_- + \hat{a}_-\hat{a}_+ + \hat{a}_-\hat{a}_-\right)$$

Subbing into $\langle V\rangle = \frac{1}{2}m\omega\int_{-\infty}^{\infty}\psi_n^*\, x^2\, \psi_n\, dx$ :

$$\langle V\rangle = \frac{1}{2}m\omega^2\int_{-\infty}^{\infty}\psi_n^* \cdot \frac{\hbar}{2m\omega}\left(\hat{a}_+\hat{a}_+ + \hat{a}_+\hat{a}_- + \hat{a}_-\hat{a}_+ + \hat{a}_-\hat{a}_-\right)\psi_n\, dx$$

$$= \frac{\hbar\omega}{4}\int_{-\infty}^{\infty}\psi_n^*\left[\hat{a}_+\hat{a}_+\psi_n + \hat{a}_+\hat{a}_-\psi_n + \hat{a}_-\hat{a}_+\psi_n + \hat{a}_-\hat{a}_-\psi_n\right]dx$$

$$= \frac{\hbar\omega}{4}\int_{-\infty}^{\infty}\psi_n^*\left(\psi_{n+2} + n\psi_n + (n+1)\psi_n + \psi_{n-2}\right)dx$$

$$= \frac{\hbar\omega}{4}\int_{-\infty}^{\infty}\underbrace{\psi_n^*\psi_{n+2}}_{\substack{\text{orthogonal}\\ \text{since } n\neq n+2}} + (2n+1)\psi_n^*\psi_n + \underbrace{\psi_n^*\psi_{n-2}}_{\substack{\text{orthogonal}\\ \text{since } n\neq n-2}}\, dx$$

$$= \frac{\hbar\omega}{4}\int_{-\infty}^{\infty}(2n+1)\,\psi_n^*\psi_n\, dx$$

$$= \frac{(2n+1)\hbar\omega}{4} = \frac{1}{2}\hbar\omega\left(n+\frac{1}{2}\right)$$

$$\therefore\ \underline{\underline{\langle V\rangle = \frac{1}{2}\hbar\omega\left(n+\frac{1}{2}\right)}}$$

This was a lot easier than evaluating a long, tedious integral!

We previously worked out $E_n = \hbar\omega(n+\frac{1}{2})$ so $\langle V\rangle = \frac{1}{2}E$

so kinetic energy must be the other half, through conservation of energy.