Harmonic Oscillator Energies and Wavefunctions via Raising and Lowering Operators

We can rearrange the Schrödinger equation for the HO into an interesting form ...

$$\frac{1}{2m}\left[\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2+(m\omega x)^2\right]\psi=\frac{1}{2m}\left[p^2+(m\omega x)^2\right]\psi=E\psi$$

with

$$H=\frac{1}{2m}\left[p^2+(m\omega x)^2\right]$$

which has the same form as

$$u^2+v^2=(iu+v)(-iu+v).$$

We now define two operators

$$\boxed{a_\pm\equiv\frac{1}{\sqrt{2\hbar m\omega}}(\mp ip+m\omega x)}$$

that operate on the test function f(x) to yield

$$(a_-a_+)f(x)=\left(\frac{1}{2\hbar m\omega}(ip+m\omega x)(-ip+m\omega x)\right)f(x)$$

$$=\frac{1}{2\hbar m\omega}\left[p^2+(m\omega x)^2-im\omega(xp-px)\right]f(x)$$

$$=\left\{\frac{1}{2\hbar m\omega}\left(p^2+(m\omega x)^2\right)-\frac{i}{2\hbar}[x,p]\right\}f(x)$$

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

Which leads to a new form of the Schrödinger equation in terms of a_+ and a_- …

$$\boxed{H\psi=\hbar\omega\left(a_-a_+-\frac{1}{2}\right)\psi}$$

If we reverse the order of the operators-- $a_-a_+\Rightarrow a_+a_-$ -- we obtain …

$$H\psi = \hbar\omega\left(a_+a_- + \frac{1}{2}\right)\psi$$

or

$$\hbar\omega\left(a_\pm a_\mp \pm \frac{1}{2}\right)\psi = E\psi$$

and the interesting relation

$$a_-a_+ - a_+a_- = \left[a_-a_+\right] = 1$$

A CLAIM: If ψ satisfies the Schrödinger equation with energy E, then $a_+\psi$ satisfies it with energy $(E+\hbar\omega)$!

$$H\left(a_+\psi\right) = \hbar\omega\left(a_+a_- + \frac{1}{2}\right)\left(a_+\psi\right) = \hbar\omega\left(a_+a_-a_+ + \frac{1}{2}a_+\right)\psi$$

$$= \hbar\omega a_+\left(a_-a_+ + \frac{1}{2}\right)\psi = a_+\left\{\hbar\omega\left(a_+a_- + 1 + \frac{1}{2}\right)\psi\right\} = a_+\left\{\hbar\omega\left(a_+a_- + \frac{1}{2}\right) + \hbar\omega\right\}\psi$$

$$= a_+\left(H + \hbar\omega\right)\psi = (E + \hbar\omega)\left(a_+\psi\right)$$

$$H\left(a_+\psi\right) = (E + \hbar\omega)\left(a_+\psi\right)$$

Likewise, $a_-\psi$ satisfies the Schrödinger equation with energy $(E-\hbar\omega)$ ...

$$H\left(a_-\psi\right) = \hbar\omega\left(a_-a_+ - \frac{1}{2}\right)\left(a_-\psi\right) = \hbar\omega\left(a_-a_+a_- - \frac{1}{2}a_-\right)\psi = a_-\hbar\omega\left(a_+a_- - \frac{1}{2}\right)\psi$$

$$= a_-\left\{\hbar\omega\left(a_-a_+ - 1 - \frac{1}{2}\right)\psi\right\} = a_-\left(H - \hbar\omega\right)\psi = a_-\left(E - \hbar\omega\right)\psi$$

$$H\left(a_-\psi\right) = \left(E - \hbar\omega\right)\left(a_-\psi\right)$$

So, these are operators connecting states and if we can find one state then we can use them to generate other wavefunctions and energies. In the parlance of the trade the $a_\pm$ are known as LADDER operators or

a_+ = RAISING and a_- = LOWERING operators.

We know there is a bottom rung on the ladder ψ_0 so that

$$a_-\psi_0 = 0$$

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

Integrating this equation yields

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

$$\int\frac{d\psi_0}{\psi_0}=-\frac{m\omega}{\hbar}\int xdx \qquad \Rightarrow \qquad \ln\psi_0=-\frac{m\omega}{2h}x^2+A_0$$

$$\boxed{\psi_0(x)=A_0e^{-\frac{m\omega}{2\hbar}x^2}} \text{ and } \boxed{E_0=\frac{1}{2}\hbar\omega}$$

E_0 comes from plugging ψ_0 into $H\psi=E\psi$. We will perform the normalization below.

Now that we are firmly planted on the bottom rung of the ladder, we can utilize a_+ repeatedly to obtain other wavefunctions, ψ_n, and energies, E_n. That is,

$$\boxed{\psi_n(x)=A_n(a_+)^n e^{-\frac{m\omega}{2\hbar}x^2},} \qquad \text{with } \boxed{E_n=\left(n+\frac{1}{2}\right)\hbar\omega}$$

Thus, for ψ_1 we obtain

$$\psi_1(x)=A_1\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\left(\frac{2m\omega}{\hbar}\right)^{\frac{1}{2}}xe^{-\frac{m\omega}{2\hbar}x^2}$$

where you still have to determine the normalization constant A_1.

Algebraic Normalization of the Wavefunctions: We can perform the normalization algebraically. We know that

$$a_+\psi_n = c_n\psi_{n+1} \qquad\qquad a_-\psi_n = d_n\psi_{n-1}$$

What are the proportionality factors c_n and d_n? For any functions $f(x)$ and $g(x)$

$$\int_{-\infty}^{\infty} f^*(a_\pm)g dx = \int_{-\infty}^{\infty}(a_\mp f)^* g\ dx$$

here $a_\mp$ is the **Hermitian conjugate** of $a_\pm$

Proof:

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

recall that

$$a_\pm = \frac{1}{(2\hbar m\omega)^{1/2}}\left[\mp ip+mwx\right] = \frac{1}{(2\hbar m\omega)^{1/2}}\left[\mp i\left(\frac{\hbar}{i}\frac{d}{dx}\right)+mwx\right] = \frac{1}{(2\hbar m\omega)^{1/2}}\left[\mp\hbar\frac{d}{dx}+mwx\right]$$

Integrate by parts

$$\int f^*(a_\pm g)\ dx = \frac{1}{(2\hbar mw)}\ dx = \int_{-\infty}^{\infty}\left[\left(\pm\hbar\frac{d}{dx}+mwx\right)f\right]^* gdx = \int_{-\infty}^{\infty}(a_\mp f)^* g\ dx$$

So we can write

$$\int_{-\infty}^{\infty}(a_\pm\psi_n)^*(a_\pm\psi_n)dx = \int_{-\infty}^{\infty}(a_\mp a_\pm\psi_n)^*\psi_n dx$$

We now use

$$\hbar\omega\left(a_\pm a_\mp \pm\frac{1}{2}\right)\psi_n = E_n\psi_n \quad \text{and} \quad E_n = \left(n+\frac{1}{2}\right)\hbar w$$

$$\left(a_+a_- \pm\frac{1}{2}\right)\psi_n = \left(n+\frac{1}{2}\right)\psi_n$$

and therefore

$$\boxed{a_+a_-\psi_n = n\psi_n}$$

And

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

$$\boxed{a_- a_+ \psi_n = (n+1)\psi_n}$$

We can now calculate c_n:

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

$$\boxed{c_n = \sqrt{n+1}}$$

The calculation for d_n proceeds in a similar manner :

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

$$\boxed{d_n = \sqrt{n}}$$

Thus we obtain the two normalization constants for the $a_\pm$

$$a_+\psi_n = (n+1)^{1/2}\,\psi_{n+1} \qquad\qquad a_-\psi_n = n^{1/2}\,\psi_{n-1}$$

<u>HO Wavefunctions:</u> Rearranging the equations to a slightly more useful form yields

$$\psi_{n+1} = \frac{1}{(n+1)^{1/2}} a_+\psi_n \qquad\qquad \psi_{n-1} = \frac{1}{n^{1/2}} a_-\psi_n$$

We can now use these equations to generate other wavefunctions. Thus, if we start with ψ_0 we obtain:

$$n=0 \qquad \psi_1 = \frac{1}{(0+1)^{1/2}} a_+\psi_0 = a_+\psi_0$$

$$n=1 \qquad \psi_2 = \frac{1}{\sqrt{2}} a_+\psi_1 = \frac{1}{\sqrt{2}} (a_+)^2 \psi_0$$

$$n=2 \qquad \psi_3 = \frac{1}{\sqrt{2+1}} a_+\psi_2 = \frac{1}{\sqrt{3\cdot 2}} a_+^3\psi_0$$

$$n=3 \qquad \psi_4 = \frac{1}{\sqrt{3+1}} a_+\psi_3 = \frac{1}{\sqrt{4\cdot 3\cdot 2}} a_+^4\psi_0$$

So that ψ_n is

$$\boxed{\psi_n = \frac{1}{\sqrt{n!}} (a_+)^n \psi_0}$$

Orthogonality of the HO Wavefunctions: Recall the orthogonality condition for two wave functions is

$$\boxed{\int_{-\infty}^{\infty} \psi_n^* \psi_m dx = \delta_{nm}}$$

Using the $a_\pm$ operators we can show this condition also holds for the HO wavefunctions. The proof is as follows.

$$\int \psi_m^* (a_+ a_-) \psi_n \, dx = n \int \psi_m^* \psi_n \, dx$$

$$\int (a_- \psi_m)^* (a_- \psi_m) dx = \int (a_+ a_- \psi_m)^* \psi_n \, dx = m \int \psi_m^* \psi_n \, dx$$

$$(n-m) \int \psi_m^* \psi_n \, dx = 0$$

The trivial case occurs when $n = m$; but when $n \neq m$ then

$$\int \psi_m^* \psi_n \, dx = 0$$

Potential Energy of the Harmonic Oscillator: We can now use the $a_\pm$ operators to perform some illustrative calculations. Consider the potential energy associated with the HO.

$$V = \frac{1}{2} k x^2 = \frac{1}{2} m\omega^2 x^2$$

and therefore

$$\langle V \rangle = \left\langle \frac{1}{2} m\omega^2 x^2 \right\rangle = \frac{1}{2} m\omega^2 \int \psi_n^* \hat{x}^2 \psi_n dx$$

First, we express $\hat{x}$ and $\hat{p}$ in terms of $a_\pm$ operators …

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

and

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

Dirac Notation: Before we evaluate this expression let's introduce some new notation that will make life simpler for us on future occasions. Instead of writing the integral between $\pm\infty$ we use brackets $\langle\ |\ \rangle$ to denote this integral. The first half is called a "bra" and the second a "ket". That is, "bra"-c-"ket" notation is

bra = $\langle\ |$ and ket = $|\ \rangle$

and for the probability density we would have an expression such as

$$\int_{-\infty}^{\infty} \psi_m^* \psi_n dx = \langle m|n\rangle$$

where the present of ψ_m^* is understood. Using this notation, integrals for $\langle x\rangle, \langle p\rangle, and \langle x^2\rangle$ assume the form

$$\int_{-\infty}^{\infty} \psi_m^* \hat{x} \psi_n dx = \langle m|\hat{x}|n\rangle \qquad \text{and} \qquad \int_{-\infty}^{\infty} \psi_m^* \hat{p} \psi_n dx = \langle m|\hat{p}|n\rangle$$

$$\langle V\rangle = \left\langle \frac{1}{2} m\omega^2 x^2 \right\rangle = \frac{1}{2} m\omega^2 \int \psi_n^* \hat{x}^2 \psi_n dx = \frac{1}{2} m\omega^2 \langle n|\hat{x}^2|n\rangle$$

$$\langle V\rangle = \left(\frac{\hbar}{2m\omega}\right)\frac{1}{2} m\omega^2 \left[\langle n|a_+a_+|n\rangle + \langle n|a_+a_-|n\rangle + \langle n|a_-a_+|n\rangle + \langle n|a_-a_-|n\rangle\right]$$

yielding

$$\boxed{\langle V\rangle = \frac{h\omega}{4}\left[n+n+1\right] = \frac{\hbar\omega}{2}\left(n+\frac{1}{2}\right)}$$

It is important to not get totally embroiled in the equations and neglect the chemistry and physics. Accordingly, we should ask the question as to the physical significance of this formula ?