Quantum Harmonic Oscillator

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A harmonic oscillator can be imagined as a particle attached to the origin by a spring. If the particle is displaced a small amount, *x*, the restoring force varies proportional to distance, but in the opposing direction, $F = -kx$, where k is the spring stiffness (force per unit displacement). The associated potential energy is positive, because energy is stored in the spring which could do work. So $V = -\int F dx = \frac{k}{2}x^2$. The 1D Schrodinger equation is thus,

$$\hat{H}\psi = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{k}{2}x^2 \right]\psi = E\psi \tag{1}$$

There's a neat trick to solving this equation using ladder operators. These are defined as,

$$U_{\pm} = \frac{\hat{p}}{\sqrt{2m}} \pm i\sqrt{\frac{k}{2}} \cdot x \tag{2}$$

where $\hat{p} = -i\hbar\frac{\partial}{\partial x}$ and so $[x, \hat{p}] = i\hbar$. So we find,

$$\begin{aligned} U_+U_- &= \left(\frac{\hat{p}}{\sqrt{2m}} + i\sqrt{\frac{k}{2}} \cdot x \right)\left(\frac{\hat{p}}{\sqrt{2m}} - i\sqrt{\frac{k}{2}} \cdot x \right) = \frac{\hat{p}^2}{2m} + \frac{k}{2}x^2 + \frac{i}{2}\sqrt{\frac{k}{m}}(x\hat{p} - \hat{p}x) \\ &= \frac{\hat{p}^2}{2m} + \frac{k}{2}x^2 - \frac{\hbar}{2}\sqrt{\frac{k}{m}} = \hat{H} - \frac{\hbar\omega}{2} \end{aligned} \tag{3}$$

where we have defined $\omega = \sqrt{\frac{k}{m}}$. (Classically this would be the natural frequency of vibration of the mass on the end of the spring). In the same way we find,

$$U_-U_+ = \hat{H} + \frac{\hbar\omega}{2} \tag{4}$$

Taking the sum and difference of (3) and (4) gives,

$$\hat{H} = \frac{1}{2}(U_+U_- + U_-U_+) \tag{5}$$

$$[U_-, U_+] = \hbar\omega \tag{6}$$

From these we find,

$$\begin{aligned} [\hat{H}, U_+] &= \frac{1}{2}(U_+U_- + U_-U_+)U_+ - \frac{1}{2}U_+(U_+U_- + U_-U_+) = \frac{1}{2}(U_-U_+U_+ - U_+U_+U_-) \\ &= \frac{1}{2}([U_+U_- + \hbar\omega]U_+ - U_+[U_-U_+ - \hbar\omega]) = \hbar\omega U_+ \end{aligned} \tag{7}$$

We can now show using (7) that U_+ acts as a ladder operator, converting an energy eigenstate into another energy eigenstate of higher energy. So, assuming an energy eigenstate, $|\psi\rangle$, of energy *E*, so that $\hat{H}|\psi\rangle = E|\psi\rangle$, we get,

$$\hat{H}U_+|\psi\rangle = [U_+\hat{H} + \hbar\omega U_+]|\psi\rangle = [U_+E + \hbar\omega U_+]|\psi\rangle = [E + \hbar\omega]U_+|\psi\rangle \tag{8}$$

So that the state $U_+|\psi\rangle$ is also an energy eigenstate, with energy $(E+\hbar\omega)$. Repeating the process gives an infinite number of states with ever increasing energy,

$$U_+^n|\psi\rangle \text{ has energy } (E+n\hbar\omega) \tag{9}$$

In the same way we find that U_- is a downward-going ladder operator which reduces the energy by $\hbar\omega$, thus,

$$\hat{H}U_-|\psi\rangle = (E-\hbar\omega)|\psi\rangle \tag{10}$$

However, because the potential energy is positive, and because the kinetic energy must also be positive, it follows that there is a lowest energy state (because, at worst, it cannot be smaller than zero). Consequently, (10) cannot always be true. In the case that the state in (1) is chosen to be the ground state, $|\psi\rangle = |GS\rangle$, there is no lower energy state available. So the only possibility is that the action of U_- on the ground state is to give a zero result. Hence,

$$U_-|GS\rangle = 0 \tag{11}$$

But this means that $U_+U_-|GS\rangle = 0$, and using (3) this becomes,

$$\left(\hat{H} - \frac{\hbar\omega}{2}\right)|GS\rangle = \left(E_{GS} - \frac{\hbar\omega}{2}\right)|GS\rangle = 0 \tag{12}$$

So the ground state energy must be,

$$E_{GS} = \frac{\hbar\omega}{2} \tag{13}$$

This is the infamous "zero point energy" of the harmonic oscillator. It equals half a quantum of energy, where the quantum of energy, $\hbar\omega$, is the spacing between energy levels. The absolute energy levels now follow from (9) by substituting in the ground state energy for *E*,

$$E_n = \left(\frac{1}{2} + n\right)\hbar\omega \tag{14}$$

Having found the energy levels, what is the explicit form of the wavefunctions as functions of *x*? The ground state wavefunction can be found by substituting (2) into (11), which becomes,

$$\left[\frac{\hat{p}}{\sqrt{2m}} - i\sqrt{\frac{k}{2}}\cdot x\right]\psi_{GS} = 0 \tag{15}$$

Re-arranging gives, $$\frac{\partial\psi_{GS}}{\partial x} = -\frac{\sqrt{mk}}{\hbar}x\psi_{GS} = -\frac{m\omega}{\hbar}x\psi_{GS} \tag{16}$$

Integrating: $$\int\frac{d\psi_{GS}}{\psi_{GS}} = \log\psi_{GS} = -\frac{m\omega}{\hbar}\int x dx = -\frac{m\omega}{\hbar}\cdot\frac{x^2}{2} \tag{17}$$

Hence, $$\psi_{GS} = A\exp\left\{-\frac{m\omega}{2\hbar}x^2\right\} \tag{18}$$

The constant is found by requiring normalisation, $\int_{-\infty}^{+\infty} |\psi|^2 \, dx = 1$. Using the standard integral,

$$\int_{-\infty}^{+\infty} \exp\left\{-\alpha x^2\right\} \cdot dx = \sqrt{\frac{\pi}{\alpha}} \tag{19}$$

this gives the normalised ground state wavefunction,

$$\psi_{GS} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left\{-\frac{m\omega}{2\hbar} x^2\right\} \tag{20}$$

Explicit expressions for the wavefunctions of higher energy are then found using (2) in (9), which gives us,

$$\psi_n = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \left(-\frac{\hbar}{\sqrt{2m}} \frac{\partial}{\partial x} + \sqrt{\frac{k}{2}} \cdot x\right)^n \exp\left\{-\frac{m\omega}{2\hbar} x^2\right\} \tag{21}$$

The general form of these solutions is a polynomial times the exponential factor. The polynomials are called Hermite polynomials. The ground state has $n = 0$.

Harmonic Oscillator in 3D

The solution for the 3D harmonic oscillator is obtained with no further effort. This is because the 3D Hamiltonian can simply be written as the sum of three 1D Hamiltonians,

$$\begin{aligned} \hat{H} &= -\frac{\hbar^2}{2m}\nabla^2 + \frac{k}{2}r^2 = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{k}{2}x^2\right) + \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{k}{2}y^2\right) + \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + \frac{k}{2}z^2\right) \\ &= \hat{H}_x + \hat{H}_y + \hat{H}_z \end{aligned} \tag{22}$$

So the solution is just a product of 1D wavefunctions, $\psi(\bar{r}) = \psi_x(x)\psi_y(y)\psi_z(z)$. This follows because,

$$\hat{H}\psi = \left(\hat{H}_x + \hat{H}_y + \hat{H}_z\right)\psi_x(x)\psi_y(y)\psi_z(z) = \left(E_x + E_y + E_z\right)\psi_x(x)\psi_y(y)\psi_z(z) \tag{23}$$

This also shows that the energy levels of the 3D oscillator are just the sum of three 1D energy levels. The 3D ground state must therefore have zero point energy $\frac{3}{2}\hbar\omega$, i.e., an amount $\hbar\omega/2$ for each coordinate direction. The general 3D state is given in terms of three quantum numbers, n, m, q, each of which takes the possible values 0, 1, 2, 3…, so that the energy level is,

$$E_{nmq} = \left(n + m + q + \frac{3}{2}\right)\hbar\omega \tag{24}$$

The corresponding wavefunction is given by $\psi(\bar{r}) = \psi_x(x)\psi_y(y)\psi_z(z)$ where each of the three terms is given by (21), i.e.,

$$\psi_{nmq}(\bar{r}) = \psi_n(x)\psi_m(y)\psi_q(z) \tag{25}$$

So, once again, just like a particle in a 3D box or an atom, in the 3D harmonic oscillator there are three quantum numbers that define the state and energy level.