

Harmonic Oscillator

Classical HO

Particle mass m ; restoring force constant K ; equation

$$m \frac{d^2 x}{dt^2} = -Kx \quad (1)$$

or

$$m \frac{d^2 x}{dt^2} + \omega^2 x = 0; \quad \omega = \left(\frac{K}{m}\right)^{\frac{1}{2}} \quad (2)$$

Solution to this which has $x = 0$ at $t = 0$ is

$$x = A \sin \omega T \quad (3)$$

with frequency of oscillation $\nu = \frac{\omega}{2\pi}$; ω is called the angular frequency.

Quantum HO

Potential corresponding to force $-Kx$ is

$$V(x) = \frac{1}{2}Kx^2 \quad (4)$$

Schrödinger equation:

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + \frac{1}{2}Kx^2 \psi(x) = E\psi(x) \quad (5)$$

Change to dimensionless variables

$$y = \left(\frac{mK}{\hbar^2}\right)^{\frac{1}{4}} x = \alpha x; \quad \epsilon = \frac{2E}{\hbar} \left(\frac{m}{K}\right)^{\frac{1}{2}} = \frac{2E}{\hbar\omega} = \frac{2E}{h\nu} \quad (6)$$

giving

$$\frac{d^2 \psi}{dy^2} - y^2 \psi(y) = -\epsilon \psi(y) \quad (7)$$

Complimentary solution

First solve simpler equation

$$\frac{d^2 \psi}{dy^2} - y^2 \psi(y) = 0 \quad (8)$$

(can think of this as equation as $|y| \rightarrow \infty$). Gives

$$\psi(y) = A \exp\left(-\frac{1}{2}y^2\right) + B \exp\left(\frac{1}{2}y^2\right) \quad (9)$$

Boundary conditions for a localised problem give $B = 0$ so that $\psi \rightarrow 0$ as $|y| \rightarrow \infty$. Assume full solution of form

$$\psi(y) = H(y) \exp\left(-\frac{1}{2}y^2\right)$$

$$\begin{aligned}\frac{d\psi}{dy} &= \frac{dH}{dy} \exp\left(-\frac{1}{2}y^2\right) - y\psi \\ \frac{d^2\psi}{dy^2} &= \frac{d^2H}{dy^2} \exp\left(-\frac{1}{2}y^2\right) - y\frac{dH}{dy} \exp\left(-\frac{1}{2}y^2\right) - \psi - y\frac{dH}{dy} \exp\left(-\frac{1}{2}y^2\right) + y^2\psi\end{aligned}\quad (10)$$

which gives

$$\frac{d^2\psi}{dy^2} - y^2\psi(y) = -\epsilon\psi(y) = \exp\left(-\frac{1}{2}y^2\right) \left[\frac{d^2H}{dy^2} - 2y\frac{dH}{dy} - H \right] \quad (11)$$

so the equation to solve is

$$\frac{d^2H}{dy^2} - 2y\frac{dH}{dy} + (\epsilon - 1)H = 0 \quad (12)$$

This equation has $p(y) = -2y$ and $q(y) = -(\epsilon - 1)$, so there are no singular points. So can obtain two simple series solution about $y = 0$, these will have radius of convegence, $\rho = \infty$. Also note that the equation is **even** so expect separate even and odd solutions

$$\begin{aligned}H(y) &= \sum_{n=0}^{\infty} a_n y^n; \\ \frac{dH}{dy} &= \sum_{n=0}^{\infty} n a_n y^{n-1}; \\ \frac{d^2H}{dy^2} &= \sum_{n=0}^{\infty} n(n-1) a_n y^{n-2}\end{aligned}\quad (13)$$

so

$$\sum_{n=0}^{\infty} n(n-1) a_n y^{n-2} - 2 \sum_{n=0}^{\infty} n a_n y^{n-1} - (\epsilon - 1) \sum_{n=0}^{\infty} a_n y^n = 0 \quad (14)$$

tidying this up and changing the dummy variable on the first sum by $n \rightarrow n + 2$ gives

$$\sum_{n=-2}^{\infty} (n+1)(n+2) a_n y^n + \sum_{n=0}^{\infty} (\epsilon - 1 - 2n) a_n y^n = 0 \quad (15)$$

For this equation to be true for **all** values of y , the coefficient of each power of y must be **separately** equated to zero. This gives

$$\begin{aligned}2a_2 + (\epsilon - 1)a_0 &= 0 \quad \text{coef. of } y^0; \\ a_{j+2}(j+2)(j+1) - [\epsilon - 1 - 2j]a_j &= 0 \quad \text{coef. of } y^j.\end{aligned}\quad (16)$$

giving a recurrence relation

$$a_{j+2} = \frac{2j - \epsilon + 1}{(j+1)(j+2)} a_j \quad j = 0, 1, 2, \dots \quad (17)$$

The series must **terminate** otherwise $H(y)$ and hence $\psi(x)$ go as $\exp(y^2)$, ie as the solution already rejected. If highest power of y in a solution is y^n , then a_{n+1} and a_{n+2} **must be zero**. This means

$$a_{n+2} = 0 = \frac{2n - \epsilon + 1}{(n+1)(n+2)} a_n \quad (18)$$

which gives

$$2n - \epsilon + 1 = 0 \quad (19)$$

or $\epsilon = 2n + 1$ as the physically allowed levels of the HO, which are

$$E = \left(n + \frac{1}{2}\right)h\nu = \left(n + \frac{1}{2}\right)\hbar\omega \quad n = 0, 1, 2, \dots \quad (20)$$

The polynomials $H(y)$ are called **Hermite Polynomials**, generally written $H_n(y)$. By convention they are written so that $a_n = 2^n$. They have recurrence relation

$$a_{j+2} = \frac{2(j-n)}{(j+1)(j+2)}a_j. \quad (21)$$

First few Hermite polynomials

$$\begin{aligned} H_0(y) &= 1, \\ H_1(y) &= 2y, \\ H_2(y) &= 4y^2 - 2, \end{aligned} \quad (22)$$

Normalisation constant:

$$N_n = \left(\frac{\alpha}{\pi^{\frac{1}{2}}2^n n!}\right)^{\frac{1}{2}} \quad (23)$$