1D Harmonic Oscillator

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

Here $\frac{m\omega^2}{2} = \frac{k}{2}$ $\quad \omega = \sqrt{\frac{k}{m}}$ is the angular frequency of the oscillator

It is useful to introduce the natural scale in this problem: $\xi \equiv \alpha x = \sqrt{\frac{m\omega}{\hbar}}\, x$ $\quad \frac{1}{\alpha}$ is the natural length scale

Let us also define ~~a~~ new "energy" expressed in units of $\frac{1}{2}\hbar\omega$: $\quad \mathcal{E} = \frac{2E}{\hbar\omega}$

The SE then reads

$$-\frac{d^2\psi}{d\xi^2} + \xi^2\psi = \mathcal{E}\psi \qquad \text{or} \qquad \frac{d^2\psi}{dx^2} = (\xi^2 - \mathcal{E})\psi$$

To simplify things we can write ψ as a product $\psi(\xi) = h(\xi)e^{-\frac{\xi^2}{2}}$ [there is no approximation here!]

This is because at large ξ the SE above becomes $\psi'' = \xi^2\psi$ and the solution of that is $\psi \approx Ae^{-\frac{\xi^2}{2}} + Be^{\frac{\xi^2}{2}}$. $B = 0$ since we require finite and square integrable function at $\xi \to \infty$

After the substitution $\psi = he^{-\frac{\xi^2}{2}}$ we obtain:

$$\frac{d^2h(\xi)}{d\xi^2} - 2\xi\frac{dh(\xi)}{d\xi} + (\mathcal{E}-1)h = 0$$

This is the Hermite equation

The solutions to Hermite's equation can be obtained with different techniques. The one we will employ is called the power series method. In this method we represent $h(\xi)$ as a power series:

$$h(\xi) = a_0 + a_1\xi + a_2\xi^2 + \dots = \sum_{j=0}^{\infty} a_j \xi^j$$

The derivatives are:

$$h'(\xi) = a_1 + 2a_2\xi + 3a_3\xi^2 + \dots = \sum_{j=0}^{\infty} j a_j \xi^{j-1}$$

$$h''(\xi) = 2a_2 + 6a_3\xi + 12a_4\xi + \dots \sum_{j=0}^{\infty} (j+1)(j+2)\, a_{j+2}\, \xi^j$$

Plugging those into the original equation for h yields:

$$\sum_{j=0}^{\infty} \left[(j+1)(j+2)a_{j+2} - 2ja_j + (\epsilon-1)a_j\right]\xi^j = 0$$

Since this must be true for any ξ value we must require that each coefficient in front of ξ^j vanish:

$$(j+1)(j+2)a_{j+2} - 2ja_j + (\epsilon-1)a_j = 0$$

e.g.

$$2a_2 + (\epsilon-1)a_0 = 0 \quad (1)$$

$$2\cdot 3a_3 + (\epsilon-1-2)a_1 = 0 \quad (2)$$

$$3\cdot 4a_4 + (\epsilon-1-4)a_2 = 0 \quad (3)$$

$\vdots$

We can see that

$$a_{j+2} = \frac{(2j+1-\epsilon)}{(j+1)(j+2)}a_j \quad \leftarrow \text{recursion relation}$$

The recursion relation relates all even coefficients to a_0 and all odd coefficienst to a_1. The even and odd coefficients are independent of each other.

As the potential is symmetric in x : $V(x) = V(-x)$ the eigenstates must be either even or odd functions. (in QM language that sounds as "the eigenstates of parity)

For even eigenstates $a_1 = 0$, $a_0 = 1$ (or any other nonzero value; since the wave function has to be normalized we need not worry about the actual value of a_0)

For odd eigenstates we choose $a_0 = 0$, $a_1 = 1$

If j is large we have

$$\frac{a_{j+2}}{a_j} = \frac{2}{j}$$

Now notice that $e^{\xi^2} = 1 + \xi^2 + \frac{\xi^4}{2!} + \frac{\xi^6}{3!} + \ldots$

The coefficient of ξ^j in the expansion of e^{ξ^2} is $b_j = \frac{1}{(\frac{j}{2})!}$ and $\frac{b_{j+2}}{b_j} = \frac{(\frac{j}{2})!}{(\frac{j}{2}+1)!} = \frac{1}{\frac{j}{2}+1} \to$

$\to \frac{2}{j}$ when $j \to \infty$

Therefore $h(\xi) \sim e^{\xi^2}$ if the power series is infinite. But then $\psi(\xi) = e^{-\frac{\xi^2}{2}} h(\xi) = e^{+\frac{\xi^2}{2}} \underset{\xi \to \infty}{\to} \infty$

For normalizable states this is not an option. Hence, the only way to keep the wave function normalizable is to require that the series is finite (i.e. polynom)

The series will terminate if

$$\epsilon - 1 - 2n = 0$$

This gives us the quantization of the energy. Only those values are allowed, which satisfy the condition

$$E = \frac{\hbar\omega}{2}\epsilon = \hbar\omega\left(n + \frac{1}{2}\right) \quad \text{where} \quad n = 0, 1, 2 \ldots \infty$$

Now let us turn to the wave function.

For allowed ϵ the recursion formula is

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

When $n = 0$ there is only one term:

$$h(\xi) = a_0 \Rightarrow \psi_0(\xi) = a_0 e^{-\frac{\xi^2}{2}}$$

When $n = 1$ we take $a_0 = 0$ (symmetry) and

$$h_1(\xi) = a_1\xi \Rightarrow \psi_1(\xi) = a_1\xi e^{-\frac{\xi^2}{2}}$$

When $n = 2$ at $j = 0$ we get $a_2 = -2a_0$, so

$$h_2(\xi) = a_0(1 - 2\xi^2) \Rightarrow \psi_2(\xi) = a_0(1 - 2\xi^2) e^{-\frac{\xi^2}{2}}$$

For an arbitrary n

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\frac{\xi^2}{2}}$$

Polynomials $H_n(\xi)$ are called Hermite polynomials

They can be obtained using the Rodrigues formula:

$$H_n(\xi) = (-1)^n e^{\xi^2} \left(\frac{d}{d\xi}\right)^n e^{-\xi^2}$$

$$H_0(\xi) = 1 \qquad H_1(\xi) = 2\xi$$

$$H_2(\xi) = e^{\xi^2} \frac{d^2}{d\xi^2} e^{-\xi^2} = -2 + 4\xi^2$$