Lecture 9:
The harmonic oscillator: Part 1

The potential for a one-dimensional harmonic oscillator is:

$$V(x) = \frac{1}{2}m\omega^2x^2, \tag{1}$$

with ω being the angular frequency of the oscillation. The time-independent Schrödinger equation thus reads:

$$\frac{\mathrm{d}^2}{\mathrm{d\,x}^2}\psi + \frac{2m}{\hbar^2}(E - \frac{1}{2}\omega^2x^2)\psi = 0. \tag{2}$$

By introducing the new dimensionless variable ξ:

$$\xi = \sqrt{\frac{m\omega}{\hbar}}x \quad\rightarrow\quad \frac{\mathrm{d}^2\psi}{\mathrm{d}\xi^2} + (\lambda - \xi^2)\psi = 0, \tag{3}$$

with $\lambda = 2E/(\hbar\omega) \geq 0$. To solve this equation, we first note that the asymptotic limit ($\xi \to \infty$) of the equation is:

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}\xi^2} \simeq \xi^2\psi, \tag{4}$$

with solution:

$$\psi \simeq g(\xi)e^{-\xi^2/2}, \tag{5}$$

being $g(\xi)$ a polynomial in ξ. The equation for $g(\xi)$ is then:

$$g(\xi)'' - 2\xi g(\xi)' + (\lambda - 1)g(\xi) = 0 \tag{6}$$

This differential equation is not trivially solvable. We will thus assume that the polynomial $g(\xi)$ is represented by the following series:

$$g(\xi) = \xi^s(a_0 + a_1\xi + a_2^2\xi^2 + ...) \text{ with } a_0 \neq 0; \; s \geq 0. \tag{7}$$

The substitution of Eq. 7 into Eq. 6 must give zero identically (i.e., regardless of the particular value of ξ). This is equivalent to say that all the coefficients of ξ^{s-2+n} $(n = 1, 2, ...)$ must be zero. We thus obtain the following set of conditions:

$$\begin{cases} s(s-1)a_0 = 0 \\ (s+1)sa_1 = 0 \\ (s+2)(s+1)a_2 - (2s+1-\lambda)a_0 = 0 \\ (s+3)(s+2)a_3 - (2s+3-\lambda)a_1 = 0 \\ .... \\ (s+\ell+2)(s+\ell+1)a_{\ell+2} - (2s+2\ell+1-\lambda)a_\ell = 0 \end{cases} \tag{8}$$

The first condition requires $s = 0$ or $s = 1$ (remember that $a_0 \neq 0$) whereas the second condition requires $a_1 = 0$ or/and $s = 0$ (remember that $s \geq 0$). The series then starts either with a constant factor ($a_0 \neq 0$ and $s = 0$) or with a term proportional to ξ ($s = 1$, $a_1 = 0$). In order to determine the polynomial $g(\xi)$, it is useful to remind that the wavefunction must be normalisable and we start by analysing the sub-series formed by the even terms $(a_0, a_2, a_4....)$. If this were an infinite series, the convergence of its sum will be determined by the factors with large ℓ. Using the recursive expression for a_ℓ (last equation in Eq. 8), it is easy to see that they will behave as:

$$\frac{a_{\ell+2}}{a_\ell} \to \frac{2}{\ell} \tag{9}$$

Without going into the details of the derivation, it is sufficient here to say that such a behaviour is respected by the series:

$$\sum_{n=1}^{\infty} \frac{1}{(n-1)!} \xi^{2n} \approx \xi^2 e^{\xi^2} \tag{10}$$

This behaviour is not acceptable, since it implies a divergent (i.e. not normalisable) wavefunction. The series must then have a finite number of terms and this is equivalent to say that the recursive condition expressed in the last equation of Eq. 8 must be zero for some even value of ℓ:

$$2s + 2\ell + 1 - \lambda = 0 \tag{11}$$

We now focus our attention on the other sub-series, the one with odd coefficients (ℓ is an odd number). If the condition in Eq. 11 is zero for some even value of ℓ it cannot be so for any odd value of ℓ. This implies that the sub-series with odd coefficients must be infinite. Again, it is sufficient for the sake of this derivation to say, without demonstration, that the asymptotic behaviour of this series is:

$$a_{2n+1} \simeq \frac{2^n}{(2n-1)!!} \quad \to \quad a_1\xi + a_3\xi^3 + a_5\xi^5 + ... \simeq \xi e^{\xi^2} \tag{12}$$

It is straightforward to note that this leads to an un-normalisable wave function [1]. The only possibility is to have $a_1 = 0$ that, recursively, implies that all the odd coefficients must be zero: $a_3 = a_5 = a_7 = ... = 0$. Summarising, the wavefunction is normalisable only if the condition in Eq. 11 is satisfied for $s = 0$ and $s = 1$. This is equivalent to imposing $\lambda = 2n + 1$ with $n = 0, 1, 2, ...$ Remembering the definition of λ ($\lambda = 2E/\hbar\omega$), the eigenvalues of energy for a harmonic oscillator are:

$$E_n = \hbar\omega(n + \frac{1}{2}) \quad \text{with} \quad n = 0, 1, 2, ... \tag{13}$$

We now recall that the associated wavefunction will be the product of a polynomial in ξ ($g(\xi)$), multiplied by $e^{-\xi^2/2}$. The equation for the polynomial $g(\xi)$ is:

$$g_n''(\xi) - 2\xi g_n'(\xi) + 2n\, g(\xi) = 0 \tag{14}$$

This equation is solved by a special class of polynomials called the *Hermite* polynomials $H_n(\xi)$. There are different ways to define these polynomials, and probably the most practical one is:

$$H_n(\xi) = (-)^n e^{\xi^2} \frac{\mathrm{d}^n}{\mathrm{d}\,\xi^n} e^{-\xi^2} \tag{15}$$

So the eigenfunctions and eigenvalues of the harmonic oscillator are:

$$\psi_n(\xi) = C_n H_n(\xi) e^{-\xi^2/2} \quad \text{with} \quad E_n = \hbar\omega(n + 1/2) \tag{16}$$

with C_n being the normalisation constant:

$$C_n = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \left(\frac{1}{2^n n!}\right)^{1/2} \tag{17}$$

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[1] Note: the semi-factorial !! requires to multiply every other element of a series. For instance: $8!! = 2 \times 4 \times 6 \times 8$.