Solution of Schrödinger's equation for SHO

The classical 1-dim simple harmonic oscillator (SHO) of mass m and spring constant k is described by *Hooke's law* and the equation of motion is,

$$F = -kx = m\frac{d^2x}{dt^2} \quad\Rightarrow\quad x = A\,e^{ikx} + B\,e^{-ikx}. \tag{1}$$

The potential energy of such a SHO is,

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

where ω is the angular frequency of the oscillator, $\omega = \sqrt{k/m}$. The quantum problem is to solve the Schrödinger equation for the potential (2). The time-independent Schrödinger equation for SHO is,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\,\psi. \tag{3}$$

Generally there are two entirely different ways to solve this problem. The first is the canonical approach involving solving differential equations as is exclusively done before. The second one is the novel technique called *factorization method*.

One thing to note in brute force solving of the differential equation (3) is apparent absent of boundary (and hence boundary condition(s)). Because of x^2 in the potential, the equation has singular points at $\pm\infty$ and therefore the boundary condition is equivalent to having well-behaved wave function. In order to solve this differential equation, we need to get its form right, *i.e.* equivalent to some standard form, at least to attempt series solution. To do that let,

$$\xi = \alpha x \quad\rightarrow\quad \frac{d}{dx} = \alpha\frac{d}{d\xi} \quad\text{and}\quad \frac{d^2}{dx^2} = \alpha^2\frac{d^2}{d\xi^2}.$$

The Schrödinger equation (3) becomes,

$$\frac{d^2\psi(\xi)}{d\xi^2} + \frac{2mE}{\hbar^2\alpha^2}\,\psi(\xi) - \frac{m^2\omega^2}{\hbar^2\alpha^4}\,\xi^2\,\psi(\xi) = 0.$$

The SHO Schrödinger equation can be written in terms of dimensionless varible by making the coefficient of ξ^2 unity and introducing a dimensionless number ϵ,

$$\frac{m^2\omega^2}{\hbar^2\alpha^4} = 1 \quad\Rightarrow\quad \alpha^2 = \frac{m\omega}{\hbar} \quad\text{therefore,}\quad \xi = \sqrt{\frac{m\omega}{\hbar}}\,x, \tag{4}$$

$$\epsilon = \frac{2mE}{\hbar^2\alpha^2} = \frac{2E}{\hbar\omega} \tag{5}$$

Hence, the equation (3) in terms of dimensionless variable becomes,

$$\frac{d^2\psi}{d\xi^2} + (\epsilon - \xi^2)\,\psi = 0. \tag{6}$$

At very large ξ, hence at large x, the $\xi^2 \gg \epsilon$ and the asymptotic form of the solution is,

$$\frac{d^2\psi}{d\xi^2} \approx \xi^2\,\psi \quad \Rightarrow \quad \psi(\xi) \sim \xi^n\, e^{-\xi^2/2}, \tag{7}$$

where ξ^n is the polynomial part of the solution. This suggest the general solution to be

$$\psi(\xi) = u(\xi)\, e^{-\xi^2/2}. \tag{8}$$

Substituting the general solution (8) in (6), the Schrödinger equation for SHO becomes,

$$\begin{aligned} \frac{d\psi}{d\xi} &= \left(\frac{du}{d\xi} - \xi\, u\right) e^{-\xi^2/2}, \\ \text{and} \quad \frac{d^2\psi}{d\xi^2} &= \left(\frac{d^2u}{d\xi^2} - 2\xi\,\frac{du}{d\xi} + (\xi^2-1)u\right) e^{-\xi^2/2}, \\ \Rightarrow \quad \frac{d^2u}{d\xi^2} - 2\xi\,\frac{du}{d\xi} &+ (\epsilon-1)u = 0. \end{aligned} \tag{9}$$

This form of Schrödinger equation (9) is rather similar to the differential equation

$$\frac{d^2H}{d\xi^2} - 2\xi\,\frac{dH}{d\xi} + 2n\,H = 0, \tag{10}$$

whose solution H is known to be *Hermite polynomials* if n is an integer. But whether $\epsilon - 1 = 2n$ is an integer, is the question we want to address. For this, power series solution in ξ, known as *Frobenius method*, is sought (assuming Frobenius method is applicable in the present problem),

$$u(\xi) = \xi^s \sum_{r=0}^{\infty} a_r\,\xi^r, \quad a_0 \neq 0. \tag{11}$$

Putting the power series solution (11) into Schrödinger equation (9), we find

$$\sum_r \left[(r+s)(r+s-1)\,a_r\,\xi^{r+s-2} - \{2(r+s)-(\epsilon-1)\}\,a_r\,\xi^{r+s}\right] = 0. \tag{12}$$

Since the above is valid for all ξ, coefficients of each power of ξ can be equated to zero (uniqueness of power series expansions). Thus for $r = 0$ and $r = 1$ we get two *indicial equations*,

$$\left.\begin{aligned} s(s-1)a_0 &= 0 \\ s(s+1)a_1 &= 0 \end{aligned}\right\} \quad a_0 \neq 0 \quad \Rightarrow \quad s = 0 \text{ or } 1. \tag{13}$$

$s = -1$ is not an acceptable condition since it introduces new singularity at $\xi = 0$. In general, for ξ^{r+s},

$$(r+s+2)(r+s+1)\,a_{r+2} = [2(r+s)-(\epsilon-1)]\,a_r \tag{14}$$

$$\frac{a_{r+2}}{a_r} = \frac{2r+2s+1-\epsilon}{(r+s+2)(r+s+1)}. \tag{15}$$

From the recursion relation (15) it follows that for $s = 0$ starting with a_0 (a_1) generates all the even (odd) numbered coefficients that go with the even (odd) powers of ξ,

$$
\begin{aligned}
a_2 &= \frac{1-\epsilon}{2}\,a_0, \quad a_4 = \frac{5-\epsilon}{12}\,a_2 = \frac{(5-\epsilon)(1-\epsilon)}{24}\,a_0, \quad \ldots \\
a_3 &= \frac{3-\epsilon}{6}\,a_1, \quad a_5 = \frac{7-\epsilon}{20}\,a_3 = \frac{(7-\epsilon)(3-\epsilon)}{120}\,a_1, \quad \ldots
\end{aligned}
$$

Actually without requiring $a_1 \neq 0$, we can generate the whole of the odd coefficients and hence odd powers of ξ from a_0 for $s = 1$ solution of the indicial equations (13). Obvious as it is, we have both even and odd solutions for (9) built on a_0 and a_1 for $s = 0$ or on a_0 for $s = 0$ and $s = 1$,

$$
\begin{aligned}
u(\xi)_{\text{even}} &= a_0 + a_2\,\xi^2 + a_4\,\xi^4 + \ldots && (16)\\
u(\xi)_{\text{odd}} &= a_1\,\xi + a_3\,\xi^3 + a_5\,\xi^5 + \ldots && (17)\\
&\text{or} \quad a_0\,\xi + a_3\,\xi^3 + a_5\,\xi^5 + \ldots && (18)\\
u(\xi) &= \xi^s\,\left[(a_0 + a_2\,\xi^2 + a_4\,\xi^4 + \ldots) + (a_1\,\xi + a_3\,\xi^3 + a_5\,\xi^5 + \ldots)\right]. && (19)
\end{aligned}
$$

Therefore, the full solution $u(\xi)$ can be determined from two constants a_0 and a_1 which is expected for a secon-order differential equation. However, not all the solutions so obtained are normailizable! For at very large r, the recursion formula (15) behaves as,

$$
\frac{a_{r+2}}{a_r} = \frac{2 + \frac{2s}{r} + \frac{1-\epsilon}{r}}{r\left(1+\frac{s+2}{r}\right)\left(1+\frac{s+1}{r}\right)} \stackrel{r\to\infty}{\longrightarrow} \frac{2}{r}. \qquad (20)
$$

Now if we look for a series,

$$
e^{\xi^2} = 1 + \xi^2 + \frac{\xi^4}{2!} + \ldots \equiv \sum_{r=0,2,4,\ldots} b_r\xi^r, \quad \text{where} \quad b_r = 1/(r/2)!
$$

Therefore the ratio of two adjacent coefficients is,

$$
\frac{b_{r+2}}{b_r} = \frac{(r/2)!}{[(r+2)/2]!} = \frac{1}{r/2+1} \stackrel{r\to\infty}{\longrightarrow} \frac{2}{r} \qquad (21)
$$

Hence asymptotically, $u(\xi)$ is behaving like $\exp(\xi^2)$ and, in turn, $\psi(\xi)$ in (8) goes like $\exp(\xi^2/2)$ something that we do not want as solution. Our requirement of normalizable solution can be met if the series is made to *terminate*. The series must end at some highest r, say $r = n'$ beyond which all other coefficients $a_{n'+2}$ are zero. This will truncate either the series $u(\xi)_{\text{even}}$ or the $u(\xi)_{\text{odd}}$ and the other one must be zero from the start. Because $s = 0$ and 1 give both even and odd solutions, we choose

$$
a_1 = 0 \quad \Rightarrow \quad a_3 = a_5 == a_7 = \cdots = 0.
$$

For acceptable, normalizable solutions, equation (15) requires,

$$
2r + 2s + 1 - \epsilon = 0 \quad \rightarrow \quad 2(n' + s) + 1 = \epsilon.
$$

Since $s = 0$ or 1 we can write $n' + s = n$ where n is any integer,

$$\epsilon \;=\; 2n + 1 \;=\; \frac{2E}{\hbar\omega} \quad \Rightarrow \quad E_n \;=\; \left(n + \frac{1}{2}\right)\hbar\omega, \quad n \;=\; 0,\, 1,\, 2,\, 3,\, \ldots \tag{22}$$

So the bottomline is, the energy eigenvalues of SHO are quantized and for $n = 0$ we have $E_0 = \hbar\omega/2$ as *zero-point energy*. The wave functions are,

$$\psi(\xi) \;=\; u(\xi)\, e^{-\xi^2/2} \;=\; e^{-\xi^2/2} \sum_r a_r\, \xi^{r+s} \quad \text{with} \quad \frac{a_{r+2}}{a_r} \;=\; \frac{2r + 2s - 2n}{(r+s+1)(r+s+2)}. \tag{23}$$

For the two solutions of the indicial equation (13), the wave functions are

$$\mathbf{s = 0}: \quad \psi(\xi)_{\text{even}} \;=\; \left(a_0 + a_2\xi^2 + a_4\xi^4 + \ldots + a_n\xi^n\right)\, e^{-\xi^2/2}, \quad n = 0, 2, 4, \ldots \tag{24}$$

$$\mathbf{s = 1}: \quad \psi(\xi)_{\text{odd}} \;=\; \left(a_0\xi + a_2\xi^3 + a_4\xi^5 + \ldots + a_{n-1}\xi^n\right)\, e^{-\xi^2/2}, \quad n = 1, 3, 5, \ldots \tag{25}$$

The coefficients a_0, a_2, a_4, ... in (24) are very different from those a_0, a_2, a_4, ... in (25).