Quantum harmonic oscillator (in 1D)

A harmonic oscillator is a system with a quadratic potential:

$$V(x) = \frac{kx^2}{2}$$ (k is sometimes referred to as "spring" or "force" constant)

Such a simple potential has great importance in physics and quantum mechanics in particular. The reason for this is that this potential can serve as the first approximation (which suffices in many practical applications) to a more realistic interaction, provided that the amplitude of the motion is small enough.

Let us consider a particle trapped near the minimum of a smooth potential. A smooth potential can be approximated as a Taylor Series

$$V(x-x_0) = V(x_0) + V'(x_0)(x-x_0) + \frac{1}{2!}V''(x_0)(x-x_0)^2 + \ldots$$

The first term in this expansion is just a constant. It resuts in a trivial shift of the total energy. The second term, $V'(x_0)$, vanishes as we are at a point of minimum. This leaves only terms proportional to $(x-x_0)^2$, $(x_0-x_0)^3$, and so on. If $x-x_0$ is small then we can ignore the higher powers of $x-x_0$.

Now the point of the minimum, x_0, can be shifted with a simple transformation $x-x_0 \rightarrow x'$. Therefore we will assume for simplicity $x_0=0$.

Then $V(x) \approx \frac{V'(0)\,x^2}{2} = \frac{kx^2}{2} = \frac{m\omega^2x^2}{2}$ $\omega = \sqrt{\frac{k}{m}}$

The time idependent Schrödinger equation for 1D harmonic oscillator takes the form

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

It is convenient to introduce the natural scale for x in this problem. We set

$$\xi\equiv\alpha x=\sqrt{\frac{m\omega}{\hbar}}\,x$$ where $\frac{1}{\alpha}$ is the natural length scale

Let us also define new "energy" expressed in units of $\frac{1}{2}\hbar\omega$:

$$\epsilon=\frac{2E}{\hbar\omega}$$

The Schrödinger equation then reads

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

In order to simplify things a little we can make a substitution

$$\psi(\xi)=h(\xi)e^{-\frac{\xi^2}{2}}$$

This substitution is motivated by the fact that at large ξ the Schrödinger equation 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 a finite and integrable function at $\xi\to\infty$

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

$$\frac{d^2h(\xi)}{d\xi^2}-2\xi\frac{dh(\xi)}{d\xi}+(\epsilon-1)h=0 \qquad \leftarrow \text{the Hermite equation}$$

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

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

Its derivatives are:

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

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

Plugging these into the equation for $h(\xi)$ yields

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

Now, this relation must be true for any value of ξ. Therefore we must require that each coefficient before ξ^j vanish:

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

more specifically,

ξ^0: $2a_2 + (\epsilon - 1) a_0 = 0$

ξ^1: $2 \cdot 3 a_3 + (\epsilon - 1 - 2) a_1 = 0$

ξ^2: $3 \cdot 4 a_4 + (\epsilon - 1 - 4) a_2 = 0$

and so on

We can see that

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

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

As the potential is symmetric (even) in x, i.e. $V(-x) = V(x)$, the eigenstates must be either even or odd functions. Indeed, this can be proven as follows. Suppose $\psi(x)$ is a solution of the stationary SE with energy E:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x)$$

which we can also write as

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(-x)}{\partial x^2} + V(x)\psi(-x) = E\psi(-x) \qquad [\text{we used } V(-x) = V(x)]$$

So if $\psi(x)$ is a solution then $\psi(-x)$ is also a solution. The solution of the SE corresponding to a particular energy E is unique (see appendix) up to an arbitrary phase factor. This implies that

$$\psi(x) = C\psi(-x) \quad \text{where } C \text{ is a constant}$$

But

$$\psi(-x) = C\psi(x) = C \cdot C\psi(-x) \Rightarrow C^2 = 1 \Rightarrow C = \pm 1$$

Hence $\psi(x)$ must be either even or odd if $V(x) = V(-x)$

Let us now go back to our harmonic oscillator.
For even eigenstates $a_1 = 0$, $a_0 = 1$ (or any other nonzero value; since the wave function has to be normalized we do not need to worry about the actual value of a_0 now)

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 recall that $e^{\xi^2} = 1 + \xi^2 + \frac{\xi^4}{2!} + \frac{\xi^6}{3!} + \dots$

The coefficient of ξ^j in the expansion of e^{ξ^2} is

$$b_j = \frac{1}{\left(\frac{j}{2}\right)!} \quad \text{and} \quad \frac{b_{j+2}}{b_j} = \frac{\left(\frac{j}{2}\right)!}{\left(\frac{j}{2}+1\right)!} = \frac{1}{\frac{j}{2}+1} \rightarrow \frac{2}{j} \quad \text{when } j \to \infty$$

Therefore $h(\xi)$ goes as e^{ξ^2} if the power series is infinite. This is a disaster because then

$$\psi(\xi) = e^{-\frac{\xi^2}{2}} h(\xi) = e^{+\frac{\xi^2}{2}} \to \infty \quad \text{when } \xi \to \infty$$

For normalizable states this not really an option. Hence, the only way to keep the wave function normalizable is to require that the series is finite (e.g. $h(\xi)$ is a polynomial). The series will terminate if

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

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

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

These are the energy levels for a harmonic oscillator. Determining the corresponding wave functions is straightforward

For the allowed ϵ's 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 $h=1$ we take $a_0 = 0$ (symmetry consideration) and

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

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

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

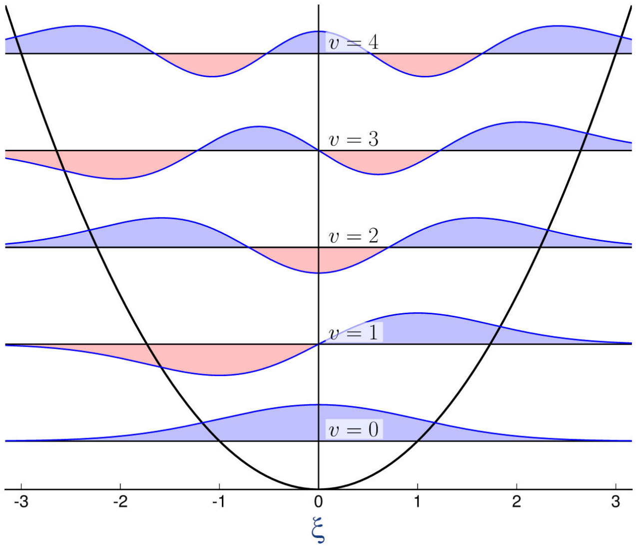
By continuing this way we can determine ψ_n for any n. In general,

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

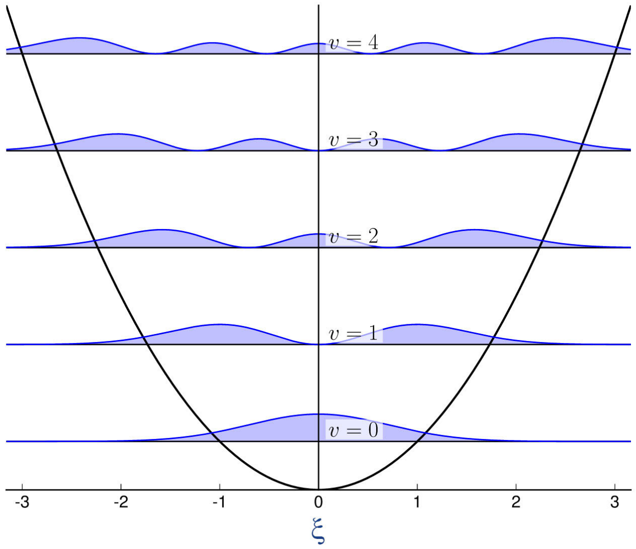
Polynomials $H_n(\xi)$ are called the Hermite polynomials. They can be generated using the Rodrigues formula:

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

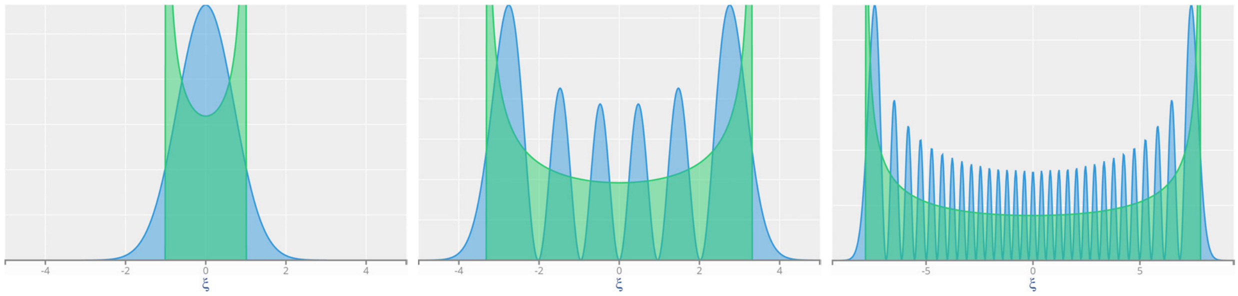
$H_0(\xi) = 1$ $\quad H_1(\xi) = 2\xi$ $\quad H_2(\xi) = e^{\xi^2} \frac{d^2}{d\xi^2} e^{-\xi^2} = -2 + 4\xi^2$



Harmonic oscillator wavefunctions, $\psi_n(\xi)$ for $n = 0, 1, 2, 3, 4$



Harmonic oscillator probability distributions, $|\psi_n(\xi)|^2$ for $n = 0, 1, 2, 3, 4$



Comparison of quantum (blue) and classical (green) probability distributions for $n = 0, 5, 30$

Appendix: non-degeneracy of bound state solutions in 1D

Suppose we have two bound state solutions, $\psi_1(x)$ and $\psi_2(x)$, to the Schrödinger equation in 1D that correspond to the same energy eigenvalue E. The Shrödinger equation for each reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx} + V(x)\psi_1 = E\psi_1$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx} + V(x)\psi_2 = E\psi_2$$

If we multiply the first equation by ψ_2 and subtract from it the second equation multiplied by ψ_1 we will get

$$\psi_2\frac{d^2\psi_1}{dx^2} - \psi_1\frac{d^2\psi_2}{dx^2} = 0$$

or

$$\frac{d}{dx}\left(\psi_2\frac{d\psi_1}{dx} - \psi_1\frac{d\psi_2}{dx}\right) = 0$$

which gives

$$\psi_2\frac{d\psi_1}{dx} - \psi_1\frac{d\psi_2}{dx} = \text{const}$$

The latter expression must hold for any value of argument x. At the same time we know that for bound states both the wave function and its derivative approaches zero when $x \to \pm\infty$. So const = 0. With that we can write that

$$\frac{1}{\psi_1}\frac{d\psi_1}{dx} = \frac{1}{\psi_2}\frac{d\psi_2}{dx}$$

This can only hold if $\psi_1 = C\psi_2$ (where C is a constant). Therefore, we can see that ψ_1 and ψ_2 must be the same up to a phase factor (the magnitude comes from the normalization of the wave function). This proves that there cannot be any degeneracy for bound state solutions of the Schrödinger equation in 1D