1 Harmonic Oscillator (HO)

The classical Hamiltonian for the HO is given by $H = \frac{p^2}{2m} + \frac{1}{2}kx^2$. The frequency ($\omega$) of the oscillation is independent of the amplitude. It is given by $\omega = \sqrt{k/m}$. Therefore the QMHamiltonian could be written as $H = \frac{P^2}{2m} + \frac{m\omega^2}{2}X^2$. From this equation, one can guess that there is a symmetry in position and momentum space solutions. The solution will not be easy in either momentum or position space; here we solve in position space.

We are looking for the bound state solutions which satisfy the Schrödinger equation $H\psi = E\psi$. All the eigenstates of the Hamiltonian must be bound states and all energies must be greater than zero. Again we will use the natural units, but what are the suitable natural units for this problem? The easiest parameter that can be used as a scale for this problem is the energy $E_0 = \hbar\omega$.

$$\frac{H}{\hbar\omega} = \frac{P^2}{2m\hbar\omega} + \frac{m\omega}{2\hbar}X^2$$

The second natural unit is $p_0 = \sqrt{mE_0} = \sqrt{m\hbar\omega}$. Finally, the proper scale for the position is $x_0 = \sqrt{\hbar/m\omega} = \hbar/p_0$. Using $\hat{P} = P/p_0$ and $\hat{X} = X/x_0$ as well as $\hat{H} = H/E_0$, $E/E_0 = \epsilon$ we have

$$\hat{H} = \frac{1}{2}\hat{P}^2 + \frac{1}{2}\hat{X}^2.$$

We note that in coordinate representation

$$\hat{X} = \hat{x} = x/x_0;\ \hat{P} = \frac{\hbar}{ip_0}\frac{\partial}{\partial x} = \frac{1}{i}\frac{\partial}{\partial \hat{x}}$$

Finally we write any eigenfunction of H as $\phi(x) = C\psi(\hat{x})$. The constant C is set by the requirement that both ϕ and ψ are normalized to one:

$$\int_{-\infty}^{\infty} |\psi(\hat{x})|^2 d\hat{x} = 1$$

and

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1 = x_0 C^2 \int_{-\infty}^{\infty} |\psi(\hat{x})|^2 d\hat{x}$$

from which we conclude

$$C = \sqrt{1/x_0} = \left(\frac{m\omega}{\hbar}\right)^{1/4}$$

Therefore, the eigenfunctions of the Hamiltonian fulfill

$$\epsilon\psi(\hat{x}) = -\frac{1}{2}\frac{\partial^2\psi(\hat{x})}{\partial\hat{x}^2} + \frac{1}{2}\hat{x}^2\psi(\hat{x})$$

First, we will find the solution for this PDE as $\hat{x} \to \infty$. Therefore, we can ignore the LHS.

$$\frac{\partial^2 \psi(\hat{x})}{\partial \hat{x}^2} = \hat{x}^2 \psi(\hat{x})$$

Let us try the following solution $y_\infty(\hat{x}) = e^{-\hat{x}^2/2}$

$$\frac{\partial \psi_\infty}{\partial \hat{x}} = -\hat{x} e^{-\hat{x}^2/2}$$

$$\frac{\partial^2 y_\infty}{\partial \hat{x}^2} = \hat{x}^2 e^{-\hat{x}^2/2} + e^{-\hat{x}^2/2}$$

The last term of the RHS can be ignored as $\hat{x} \to \infty$, and are we left with the Gaussian solution of unit σ. Therefore, the general solution $\psi(\hat{x})$ can be written as:

$$\psi(\hat{x}) = f(\hat{x}) \psi_\infty(\hat{x})$$

where $f(\hat{x})$ is a finite polynomial [1] which has the form $\sum_{k=0}^{n} c_k \hat{x}^k$

$$\psi(\hat{x}) = \sum_{k=0}^{n} c_k \hat{x}^k e^{-\hat{x}^2/2}$$

Substitute in the Schrödinger equation, one gets:

$\sum_{k=0}^{n} \epsilon c_k \hat{x}^k e^{-\hat{x}^2/2} = \frac{1}{2} \sum_{k=0}^{n} c_k \hat{x}^{k+2} e^{-\hat{x}^2/2} - \frac{1}{2} \frac{\partial^2 \psi(\hat{x})}{\partial \hat{x}^2}$ .....(I)

$$\frac{\partial^2 \psi(\hat{x})}{\partial \hat{x}^2} = \frac{\partial}{\partial \hat{x}} \sum_{k=0}^{n} c_k e^{-\hat{x}^2/2} (k \hat{x}^{k-1} - \hat{x}^{k+1})$$

$$\frac{\partial^2 \psi(\hat{x})}{\partial \hat{x}^2} = \sum_{k=0}^{n} c_k (k(k-1)\hat{x}^{k-2} - k\hat{x}^k - (k+1)\hat{x}^k + \hat{x}^{k+2}) e^{-\hat{x}^2/2}$$

substitute in equation I,putting every term with power k at the LHS,

$$\sum_{k=0}^{n} c_k \hat{x}^k (2\epsilon - 2k - 1) = -\sum_{k=2}^{n} c_k k(k-1) \hat{x}^{k-2}$$

re-lable the RHS, $k - 2 = k'$

$$RHS = -\sum_{k'=0}^{n-2} c_{k'+2} (k'+2)(k'+1) \hat{x}^{k'}$$

$$RHS = -\sum_{k=0}^{n-2} c_{k+2} (k+2)(k+1) \hat{x}^{k}$$

[1] It must be finite or the full wave function wouldn't go to zero at ∞ as it must to be normalizable.

$$\sum_{k=0}^{n} c_k \hat{x}^k (2\epsilon - 2k - 1) = -\sum_{k=0}^{n-2} c_{k+2}(k+2)(k+1)\hat{x}^k$$

Compare coefficient by coefficient, we get:

$$c_{k+2} = -c_k \frac{2\epsilon - (2k+1)}{(k+1)(k+2)} .....II$$

$$\psi(\hat{x}) = \sum_{k=0}^{n} c_k \hat{x}^k e^{-\hat{x}^2/2} = H_n(\hat{x}) e^{-\hat{x}^2/2}$$

H_n are called Hermite polynomials. We have to determine c_0 and c_1 and then any other constant can be calculated from the recursion relation. This recursion relation leads to an infinite set of c's. However, to retain the correct asymptotic behavior, we need to ascertain that there is a maximum power $\hat{x}^n$ for the Hermite polynomials. Therefore, the RHS in equation (II) must goes to zero for some value of k. So,

$$2\epsilon - (2k+1) = 0$$

$$\exists k : 2\epsilon = (2k+1)$$

$$\epsilon = k + \frac{1}{2} .....III$$

Therefore, we have conditions on our energy. Not every eigenvalue is possible for the energy.Only the values satisfy equation (III) are allowed.Write the energy in terms of the dimensional quantity, one gets;

$$E_n = (n + \frac{1}{2})\hbar\omega$$

We require $c_0 = 0$ if n is odd and $c_1 = 0$ if n is even; as well as (by convention) $c_n = 2^n$. The simple-most Hermite polynomial is $H_0(\hat{x})$, $c_0 = 2^0 = 1$.The ground state wave function is $< x|E_0 >= NCe^{-\hat{x}^2/2}$ with $N = \pi^{-1/4}$. It is the same as the asymptotic solution, a Gaussian. The eigenvalue of energy is $^1/_2\hbar\omega$ in this case. In contrast to the "Gaussian wave packet" discussed earlier, this eigenstate has a constant expectation value for position of $< x >= 0$ and a constant width in x-space. In momentum space the solution is also Gaussian and we have:

$$< p|E_0 >= NCe^{-(p/p_0)^2/2}$$

$\Delta\hat{x} = \sqrt{1/2}$, $\Delta x = \sqrt{1/2}\sqrt{\frac{\hbar}{m\omega}}$, $\Delta p = \sqrt{1/2}\sqrt{\hbar m\omega}$

$$\Delta p \Delta x = \frac{\hbar}{2}$$

So $E_0 = \frac{\hbar\omega}{2}$, the ground state has positive binding energy. The momentum square is not zero, while $< p >= 0$.

Further solutions exist for each n:
$H_1(\hat{x}) = 2\hat{x}$, $E_1 = \frac{3\hbar\omega}{2}$
$H_2(\hat{x}) = 4\hat{x}^2 - 2$, $E_2 = \frac{5\hbar\omega}{2}$
$H_3(\hat{x}) = 8\hat{x}^3 - 12\hat{x}$, $E_3 = \frac{7\hbar\omega}{2}$
...

In the QM Oscillator, nothing is going back and forth as for the classical oscillator because we have $< x >= 0$, and $< p >= 0$. The higher the energy of the system, the larger the width of the states becomes. This is expected because for a classical oscillator the energy is directly proportional to the amplitude. Classically, it is also more likely to find the oscillator close to one of its end points (lower kinetic energy and therefore lower velocity) than in the middle (higher kinetic energy). This turns out to be true only for the higher excited states for the quantum oscillator.

To normalize $\psi(\hat{x})$ we have

$$\int_{-\infty}^{\infty} |\psi(\hat{x})|^2 d\hat{x} = 1$$

$$\psi_n(\hat{x}) = \sqrt{\frac{1}{\sqrt{\pi}2^n n!}} H_n(\hat{x}) e^{-\hat{x}^2/2}$$

$$\phi_n(x) = (\frac{m\omega}{\hbar})^{\frac{1}{4}} \sqrt{\frac{1}{\sqrt{\pi}2^n n!}} H_n(x/x_0) e^{-(x/x_0)^2/2}$$