

# Lecture Notes in Quantum Mechanics

## Chapter-III : Linear Harmonic Oscillator

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## Chapter 3

# Linear Harmonic Oscillator

### 3.1 Introduction

The wave mechanical theory of the harmonic oscillator provides the basis for understanding a wide variety of physical systems like vibration of diatomic and polyatomic molecules, specific heat capacities of solids, electromagnetic field etc... Let us consider a free particle executing linear harmonic oscillations along the x-axis. The Hamiltonian for a this particle is given as

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2, \quad (3.1)$$

where

$$\begin{aligned} p &= -i\hbar \frac{d}{dx} \\ k &= m\omega^2. \end{aligned} \quad (3.2)$$

Here  $m$  is the mass and  $p$  is the momentum of the particle and  $k$  is the force per unit displacement and  $\omega$  is the critical angular frequency of oscillations. We know the time independent Schroedinger equation for the oscillator can be written as

$$Hu(x) = Eu(x). \quad (3.3)$$

Substituting Eqs. (3.1) & (3.2) in the above equation gives

$$\left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 \right) u(x) = Eu(x) \quad (3.4)$$

### 3.2 Dimensionless Form: Conversion to Hermite Differential Equation

Let us change the independent variable in Eq. (3.4) from  $x$  to  $\rho$  such that

$$\rho = \alpha x \quad (3.5)$$

$$\alpha = \sqrt{\frac{m\omega}{\hbar}} \quad (3.6)$$

$$\alpha^2 = \frac{m\omega}{\hbar}. \quad (3.7)$$

Then  $\frac{d}{dx} = \left(\frac{d\rho}{dx}\right) \frac{d}{d\rho}$ , hence  $\frac{d}{dx} = \alpha \frac{d}{d\rho}$  and  $\frac{d^2}{dx^2} = \alpha^2 \frac{d^2}{d\rho^2}$ .

Using these the Schroedinger equation, (3.4) can be converted into a dimensionless form as

$$\frac{d^2 u(\rho)}{d\rho^2} + (\lambda - \rho^2)u(\rho) = 0, \quad (3.8)$$

where

$$\lambda = \left(\frac{2E}{\hbar\omega}\right) \quad (3.9)$$

and

$$u(\rho) \simeq u(\alpha x). \quad (3.10)$$

Proof:

Replacing the independent variable  $x$  to  $\rho$ , in Eq. (3.4), gives

$$\left(-\frac{\hbar^2}{2m}\right) \frac{\alpha^2 d^2}{d\rho^2} u(\alpha x) + \frac{1}{2} m\omega^2 x^2 u(\alpha x) = Eu(\alpha x)$$

$$\left(-\frac{\hbar^2 \alpha^2}{2m}\right) \frac{d^2 u(\rho)}{d\rho^2} + \frac{1}{2} m\omega^2 x^2 u(\rho) = Eu(\rho)$$

Multiplying the above equation by  $\left(-\frac{2m}{\hbar^2 \alpha^2}\right)$  and rearranging it gives

$$\left(-\frac{2m}{\hbar^2 \alpha^2}\right) \times \left\{ \left(-\frac{\hbar^2 \alpha^2}{2m}\right) \frac{d^2 u(\rho)}{d\rho^2} + \frac{1}{2} m\omega^2 x^2 u(\rho) \right\} = \left(-\frac{2m}{\hbar^2 \alpha^2}\right) \times Eu(\rho)$$

But

$$\left(-\frac{2m}{\hbar^2\alpha^2}\right) \times \left(-\frac{\hbar^2\alpha^2}{2m}\right) = 1,$$

Further

$$\begin{aligned} \left(-\frac{2m}{\hbar^2\alpha^2}\right) \frac{1}{2}m\omega^2x^2 &= \left(\frac{m^2\omega^2}{\hbar^2}\right) \frac{x^2}{\alpha^2} \\ &= \frac{\alpha^4x^2}{\alpha^2} \\ &= \alpha^2x^2 \\ &= \rho^2 \end{aligned}$$

and

$$\begin{aligned} E \left(-\frac{2m}{\hbar^2\alpha^2}\right) &= E \left(-\frac{2m}{\hbar^2}\right) \frac{1}{\alpha^2} \\ &= E \left(-\frac{2m}{\hbar^2}\right) \left(\frac{\hbar}{m\omega}\right) \\ &= \left(\frac{2E}{\hbar\omega}\right). \end{aligned}$$

As  $E$ ,  $\hbar$  and  $\omega$  are constants, we can define the RHS as a new constant  $\lambda$  such that

$$\lambda = \left(\frac{2E}{\hbar\omega}\right).$$

Let the wavefunction  $u(\rho)$  be expressed in terms of a new function  $\nu(\rho)$ , such that

$$u(\rho) = e^{-\rho^2/2}\nu(\rho) \quad (3.11)$$

Finding the first order and second order derivatives of  $u(\rho)$  with respect to  $\rho$  gives

$$\dot{u}(\rho) = e^{-\rho^2/2} [\dot{\nu}(\rho) - \rho\nu(\rho)] \quad (3.12)$$

$$\ddot{u}(\rho) = e^{-\rho^2/2} [\ddot{\nu}(\rho) - 2\rho\dot{\nu}(\rho) + (\rho^2 - 1)\nu(\rho)]. \quad (3.13)$$

Substituting  $u(\rho)$  and its derivatives in Eq. (3.8) gives

$$e^{-\rho^2/2} [\ddot{\nu}(\rho) - 2\rho\dot{\nu}(\rho) + (\rho^2 - 1)\nu(\rho)] + (\lambda - \rho^2)e^{-\rho^2/2}\nu(\rho) = 0. \quad (3.14)$$



Simplifying this equation gives

$$[\ddot{\nu}(\rho) - 2\rho\dot{\nu}(\rho) + (\lambda - 1)\nu(\rho)] = 0. \quad (3.15)$$

Let us assume the series solution of the Eq. (3.15) and its first order and second order derivatives with respect to  $\rho$  as

$$\nu(\rho) = \sum_{s=\sigma}^{\infty} c_s \rho^s, \quad (3.16)$$

$$\dot{\nu}(\rho) = \sum_{s=\sigma}^{\infty} c_s s \rho^{s-1}, \quad (3.17)$$

$$\ddot{\nu}(\rho) = \sum_{s=\sigma}^{\infty} c_s s(s-1) \rho^{s-2}, \quad (3.18)$$

Substituting these, Eq. (3.15) becomes

$$\sum_{s=\sigma}^{\infty} c_s [s(s-1) \rho^{s-2} - 2\rho s \rho^{s-1} + (\lambda - 1)\rho^s] = 0. \quad (3.19)$$

If Eq. (3.19) is to hold good, then the individual terms in the sum should be equal to zero. Hence taking the coefficients of  $\rho^s$  for any  $s \geq 0$  and equating them to zero  $\Rightarrow$

$$c_{s+2}(s+2)(s+1) - c_s [2s - (\lambda - 1)] = 0. \quad (3.20)$$

From the above equation, Eq. (3.20), the recursion relation can be obtained as

$$\frac{c_{s+2}}{c_s} = \frac{[2s - (\lambda - 1)]}{(s+2)(s+1)}. \quad (3.21)$$

This Eq. (3.21) determines the behaviour of an infinite series. However what we require is that the equation should be a finite degree polynomial. Hence to convert the Eq. (3.15) to a finite degree polynomial, we truncate the series at some finite term, say  $n^{\text{th}}$  term, by assuming

$$s = n \quad (3.22)$$

$$\lambda = 2n + 1. \quad (3.23)$$

This will cause Eq. (3.21) to become

$$\frac{c_{s+2}}{c_s} = 0. \quad (3.24)$$

This means the coefficient  $c_n \neq 0$ , but the coefficients  $c_{n+1}, c_{n+2}, c_{n+3}, \dots$  and all the succeeding values are zero. Under this condition, Eq. (3.15) when multiplied by a

constant factor, say  $N_n$  gets converted into the **Hermite Differential Equation**

$$\ddot{H}_n(\rho) - 2\rho \dot{H}_n(\rho) + 2n H_n(\rho) = 0. \quad (3.25)$$

The solutions of this equation are the familiar **Hermite polynomial function**  $H_n(\rho)$ . In terms of these Hermite Polynomial Function, the wave function  $u_n(\rho)$  for the LHO can be given as

$$u_n(\rho) = N_n e^{-\rho^2/2} H_n(\rho), \quad (3.26)$$

where,  $N_n$ =Normalization constant.

### 3.3 To find the Normalization Constant ( $N_n$ )

We know the orthonormal property of the wavefunctions is given as

$$\int_{-\infty}^{+\infty} u_m^* u_n dx = \delta_{m,n}. \quad (3.27)$$

Substituting Eq. (3.26) in Eq. (3.27) gives

$$\int_{-\infty}^{+\infty} N_m e^{-\rho^2/2} H_m(\rho) N_n e^{-\rho^2/2} H_n(\rho) \left( \frac{d\rho}{\alpha} \right) = \delta_{m,n}, \quad \because dx = \frac{d\rho}{\alpha},$$

or

$$\frac{N_m N_n}{\alpha} \int_{-\infty}^{+\infty} e^{-\rho^2} H_m(\rho) H_n(\rho) d\rho = \delta_{m,n}. \quad (3.28)$$

We know that the orthonormal property of the Hermite polynomial functions is given as

$$\int_{-\infty}^{+\infty} e^{-\rho^2} H_m(\rho) H_n(\rho) d\rho = \sqrt{\pi} 2^n n! \quad (3.29)$$

Substituting Eq. (3.29) in Eq. (3.28) gives

$$\frac{N_m N_n}{\alpha} \sqrt{\pi} 2^n n! = \delta_{m,n}. \quad (3.30)$$

If  $m = n$ , then  $N_m N_n = N_n^2$  and  $\delta_{m,n} = 1$ . Under such conditions Eq. (3.30) becomes

$$\frac{N_n^2}{\alpha} \sqrt{\pi} 2^n n! = 1$$

or

$$N_n = \left[ \frac{\alpha}{\sqrt{\pi} 2^n n!} \right]^{\frac{1}{2}}. \quad (3.31)$$

The Eq. (3.31) gives the expression for the normalization constant of the wavefunction.

### 3.4 Energy Eigen Functions $u_n(\rho)$ and Probability Densities $P_n(\rho)$

Substituting Eq. (3.31) in Eq. (3.26) gives the energy eigen functions of the Linear Harmonic Oscillator as

$$u_n(\rho) = \left[ \frac{\alpha}{\sqrt{\pi} 2^n n!} \right]^{\frac{1}{2}} e^{-\rho^2/2} H_n(\rho) \quad (3.32)$$

Here  $H_n(\rho)$  is the Hermite Polynomial function of degree  $n$ . The expressions for  $H_n(\rho)$  for some values of  $n$  are given in the table 3.1.

TABLE 3.1: First few values of the Hermite Polynomials

Order $n$	Hermite Polynomial $H_n(\rho)$
0	$H_0(\rho) = 1$
1	$H_1(\rho) = 2\rho$
2	$H_2(\rho) = 4\rho^2 - 2$
3	$H_3(\rho) = 8\rho^3 - 12\rho$
4	$H_4(\rho) = 16\rho^4 - 48\rho^2 + 12$
5	$H_5(\rho) = 2\rho^5 - 160\rho^3 + 120\rho$

The eigenfunctions  $u_n(\rho)$  of the LHO for different values of  $n$  are evaluated numerically using the analytical expressions for the Hermite polynomial functions. Then the plots of  $u_n(\rho)$  as function of  $\rho$  give the wavefunction profiles of the LHO for different quantum states. From these the probability densities  $|u(\rho)|^2$  are also evaluated. The wavefunction profiles so obtained for even-state wavefunctions ( $n = 0, 2, 4, \dots$ ) and their probability densities are shown in Figs. (3.1) respectively. Similarly the wavefunction profiles for odd-state wavefunctions ( $n = 1, 3, 5, \dots$ ) and their probability densities are shown in Figs. (3.2) respectively.

From the profiles of the wave functions  $u_n(\rho)$ , we find that for the  $n^{\text{th}}$  eigen state, there are  $n$ -nodes, that is, there are  $n$  finite values of  $\rho$  for which  $u_n(\rho)$  vanishes. Thus we find greater the number of nodes that a wave function has, greater will be its energy.

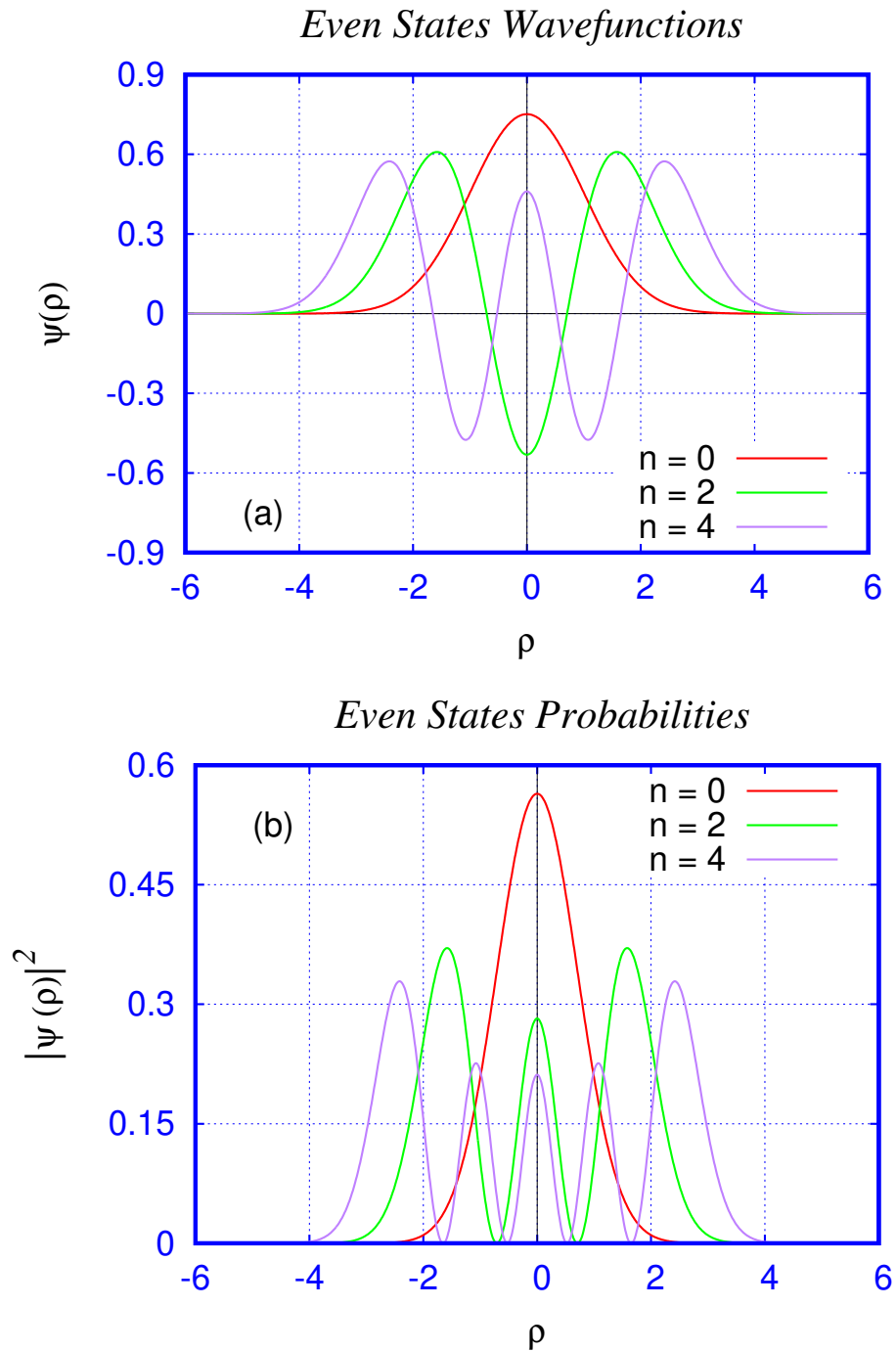


FIGURE 3.1: (a) The wavefunction profiles for the first three even eigen states namely  $n = 0$ ,  $n = 2$  and  $n = 4$  plotted as a function of  $\rho$ . It can be clearly seen that the wavefunctions have  $n$ -nodes, that is they cross the  $\rho$ -axis  $n$  number of times. Thus  $u_0(\rho)$  has no node,  $u_2(\rho)$  has 2 nodes and  $u_4(\rho)$  has 4 nodes and (b) the probability densities  $P_n(\rho)$  corresponding to these wavefunctions.

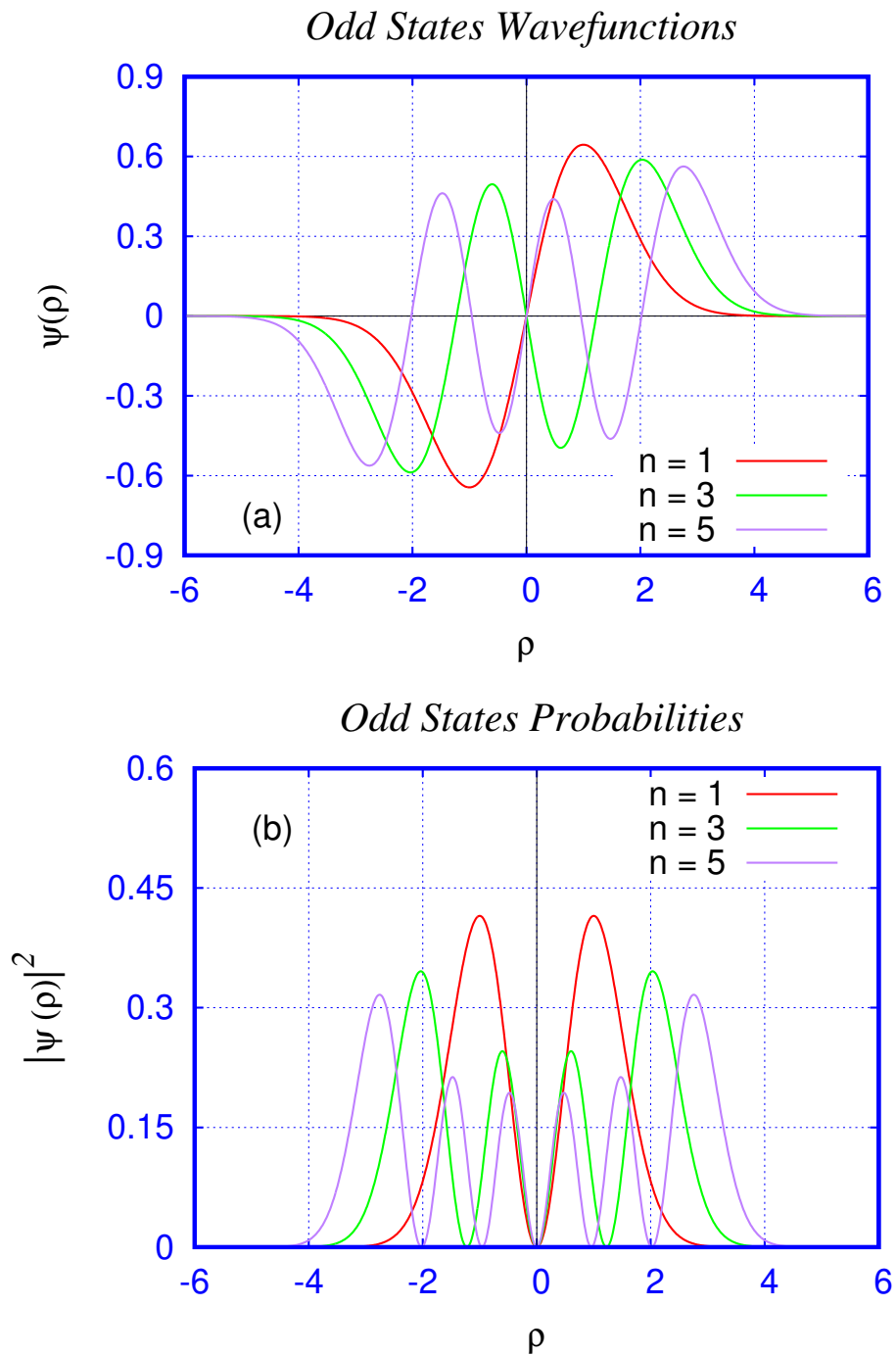


FIGURE 3.2: (a) The wavefunction profiles for the first three odd eigen states namely  $n = 1$ ,  $n = 3$  and  $n = 5$  plotted as a function of  $\rho$ . Here also it can be seen that the wavefunctions have  $n$ -nodes, that is they cross the  $\rho$ -axis  $n$  number of times. Thus  $u_1(\rho)$  has 1 node,  $u_3(\rho)$  has 3 nodes and  $u_5(\rho)$  has 5 nodes and (b) the probability densities  $P_n(\rho)$  corresponding to these wavefunctions.

*Note*

Greater the number of nodes that a wave function has, greater will be energy of the particle.

### 3.5 Energy Eigen values

From Eq. (3.9) we have

$$\begin{aligned}\lambda &= \left(\frac{2E}{\hbar\omega}\right) \quad \text{or} \\ E &= \frac{1}{2}\lambda\hbar\omega_c.\end{aligned}\tag{3.33}$$

However from Eq. (3.23) we have

$$\lambda = 2n + 1.\tag{3.34}$$

Substituting Eq. (3.34) in Eq. (3.33) gives

$$E = \frac{1}{2}(2n + 1)\hbar\omega_c$$

Or, on rearranging it gives

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega_c.\tag{3.35}$$

Equation(3.35) gives the expression for the energy levels of LHO for various quantum states defined by  $n = 1, 2, 3, \dots$  etc., It tells that

- *Quantization of Energy Levels:* The energy levels of a LHO are quantized,(i.e) they are discrete.
- *Even Spacing of Energy Levels:* The energy levels are evenly spaced,(i.e) the difference between any two consecutive quantum states is  $\Delta E = \hbar\omega$ .
- *Zero Point Energy:* The energy of the LHO, even for its ground state, is not zero but a finite non-zero value given by  $E_0 = \frac{1}{2}\hbar\omega_c$ . This energy is called as the *zero-point energy*. The zero point energy is a characteristic feature of a Linear Harmonic Oscillator and is not possessed by any other system.

**Reason for Zero Point Energy:**

The reason for the arising of the zero point energy can be explained as due to the Heisenberg's uncertainty principle. In the ground state, the particle executing harmonic motions is confined to a finite region of space due to the action of the potential  $V(x) = \frac{1}{2}m\omega_c^2 x^2$ . Therefore by the principle of uncertainty  $(\Delta p \Delta x) \geq \hbar$ , as  $\Delta x \simeq 0$  the particle cannot have a finite value of momentum or energy, that is  $\Delta p \rightarrow \infty$ . Hence the momentum or energy cannot have a finite value, much less a zero value. Hence the *zero point energy* will always be a non-zero value.

### 3.6 Probability Inside and Outside Classically Allowed Region

The wavefunction profile and the probability density for the tenth eigen state are shown in Figs. 3.3(a) and (b) respectively. The quantum mechanical probability of finding of the particle in a particular region  $P = \int u_0(\rho)^2 d\rho$ . Let  $\rho_0 = \alpha x_0$  be the maximum amplitude of oscillation for a given energy of LHO. Then the amount of time it spends between  $\rho$  and  $\rho + d\rho$  is propotional to  $\frac{1}{\sqrt{(\rho_0^2 - \rho^2)}}$ . Thus the classical probability

density for finding the oscillator in the neighbourhood of  $\rho$  is propotional to  $\frac{1}{\sqrt{(\rho_0^2 - \rho^2)}}$ .

This means that at classical boundaries, the probability should tend to infinity at the maximum amplitude points ( $\pm\rho_0$ ). This is clearly seen in Fig. 3.3(b) for  $n = 10$ . Quantum mechanically, the probability curve has  $n = 10$  nodes and all these 10 nodes lie in the classically allowed regions only. However we find a finite quantum probability of finding the oscillator in the classically forbidden region. This can also be seen from Fig. 3.3(b). Though the quantum probability behaves much differently because of the wave nature of the partilce, a good agreement of the quantum probability and the classical probability curvs are observed. This agreement of classical and averaged quantum probabilities holds good only for higher energies of Linear Harmonic Oscillator.

### 3.7 Ground State Probabality of Finding the Particle in the Classical Limits

Quantum mechanically, the energy of an oscillating particle in the ground state is

$$E_0 = \frac{1}{2} \hbar \omega_c. \quad (3.36)$$

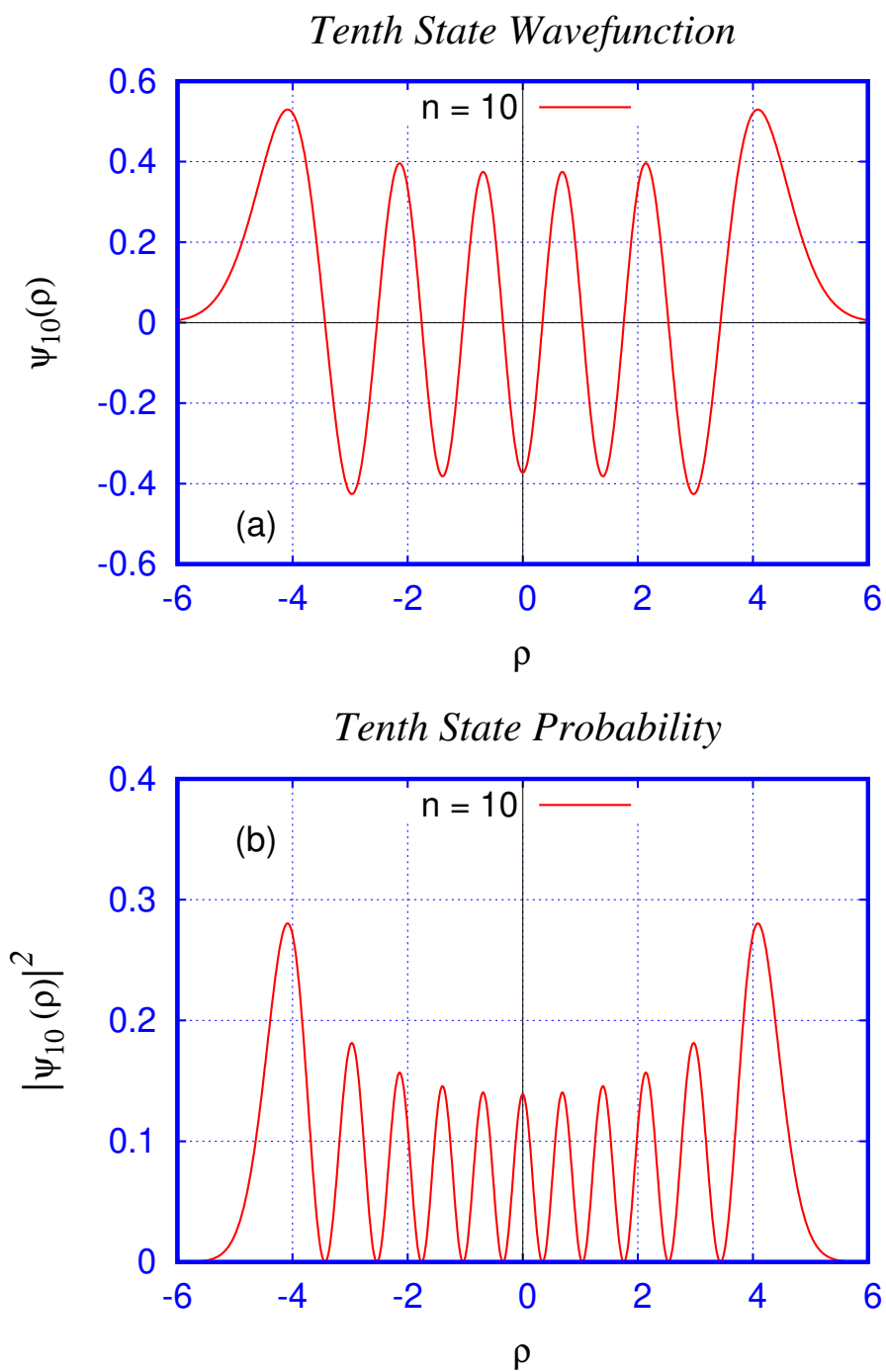


FIGURE 3.3: (a) The eigenfunction profile and (b) the probability density for tenth eigen state of the LHO,  $n = 10$



If  $a$  is the amplitude, then the total energy of the particle according to classical mechanics is given as

$$\epsilon_0 = \frac{1}{2}m\omega_c^2 a^2. \quad (3.37)$$

Equating the Eqs. (3.36) and (3.37), we get

$$\begin{aligned} \frac{1}{2}m\omega_c^2 a^2 &= \frac{1}{2}\hbar\omega_c \\ \text{or } a &= \sqrt{\frac{\hbar}{m\omega_c}}. \end{aligned} \quad (3.38)$$

The Eq. (3.38) gives the expression for the classical amplitude of the particle. Then the probability of finding the particle in classical limits is

$$P = \int_{-a}^{+a} |u_0(\rho)|^2 dx \quad (3.39)$$

If  $x \rightarrow -a$ , then  $\rho \rightarrow -\alpha a$ , that is  $\rho \rightarrow -\sqrt{\frac{m\omega}{\hbar}}\sqrt{\frac{\hbar}{m\omega}} = -1$ ,  
 $\therefore \alpha = \sqrt{\frac{m\omega}{\hbar}}$  and  $a = \sqrt{\frac{\hbar}{m\omega}}$ .  
 Similarly if  $x \rightarrow +a$ , then  $\rho \rightarrow +1$ .

Hence

$$P = \int_{-1}^{+1} |u_0(\rho)|^2 \frac{d\rho}{\alpha}$$

or

$$P = \frac{2}{\alpha} \int_0^{+1} |u_0(\rho)|^2 d\rho. \quad (3.40)$$

We know that the wavefunction  $u_0(\rho)$  is given as

$$u_0 = \left[ \frac{\alpha}{\sqrt{\pi}} \right]^{\frac{1}{2}} e^{-\left(\frac{\rho^2}{2}\right)}. \quad (3.41)$$

Substituting Eqn. (3.41) in Eqn. (3.40), gives

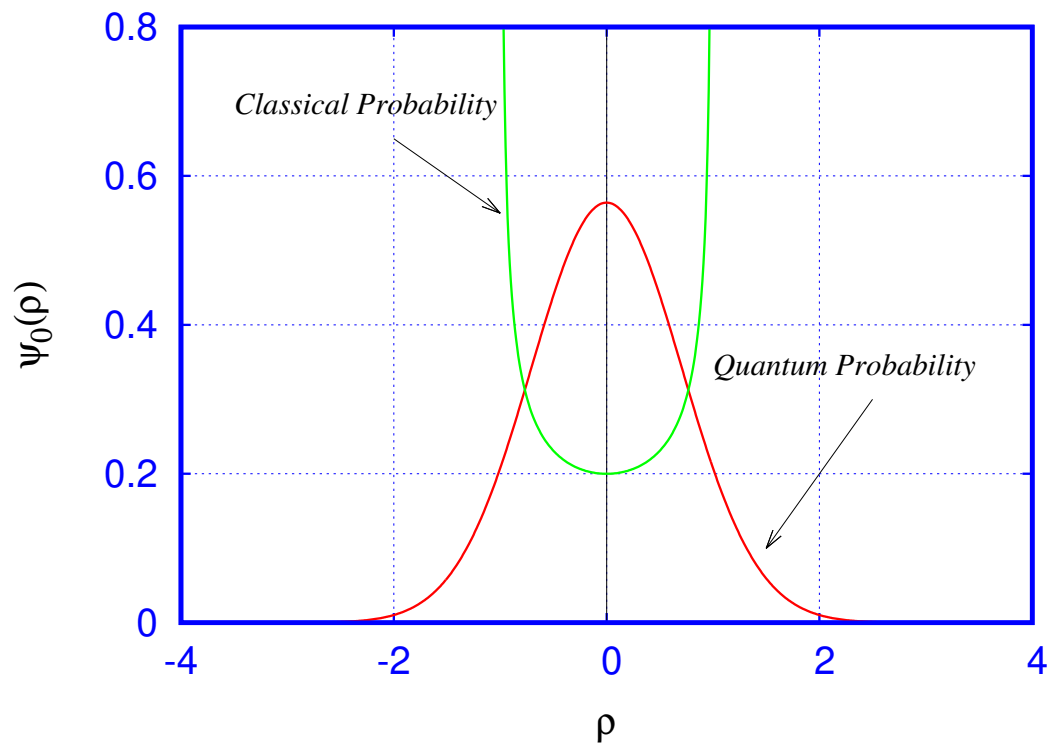


FIGURE 3.4: The classical (green online) and the quantum mechanical (red online) probability densities for the LHO in ground state. It can be clearly seen that the quantum probability density extends well beyond the classical limits into the classically forbidden regions  $|\rho| > 1.0$ .

$$P = \frac{\alpha}{\sqrt{\pi}} \frac{2}{\alpha} \int_0^{+1} e^{-\rho^2} d\rho$$

or

$$P = \frac{2}{\sqrt{\pi}} \int_0^{+1} e^{-\rho^2} d\rho. \quad (3.42)$$

We know that

$$e^{-x} = \left\{ 1 - x + \frac{x^2}{2!} - \frac{x^3}{3!} + \frac{x^4}{4!} + \dots \right\}$$

Hence if we assume  $x = \rho^2$ , then 3.42 becomes

$$\begin{aligned}
 P &= \frac{2}{\sqrt{\pi}} \int_0^{+1} \left\{ 1 - \rho^2 + \frac{\rho^4}{2!} - \frac{\rho^6}{3!} + \frac{\rho^8}{4!} - \dots \right\} d\rho, \\
 P &= \frac{2}{\sqrt{\pi}} \left\{ \rho - \frac{\rho^3}{3} + \frac{\rho^5}{5 \times 2!} - \frac{\rho^7}{7 \times 3!} + \frac{\rho^9}{9 \times 4!} - \dots \right\}_0^1, \\
 P &= \frac{2}{\sqrt{\pi}} \left\{ 1 - \frac{1}{3} + \frac{1}{5 \times 2!} - \frac{1}{7 \times 3!} + \frac{1}{9 \times 4!} - \dots \right\}. \tag{3.43}
 \end{aligned}$$

Evaluating the above Eqn. 3.43 the probability of finding the particle within the classical limits is  $P = 0.843$  or if expressed as a percentage,  $P = 84.3\%$ . This means that the probability of finding the particle beyond the classical limits well into the classically forbidden region is not zero but is a finite value given as

$$\begin{aligned}
 P &= (100 - 84.3) \%, \\
 &\text{or} \\
 P &= 15.7\%. \tag{3.44}
 \end{aligned}$$

This is shown graphically in Fig. (3.4).