Harmonic Oscillator

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The problem of harmonic oscillator is an important one in Quantum Mechanics. We will consider a one-dimensional harmonic oscillator with angular frequency ω and mass m. The potential energy operator for the oscillator is

$$\hat{V} = \frac{1}{2} m \omega^2 \hat{x}^2 \quad \cdots\cdots \quad (1)$$

while the kinetic energy operator is

$$\hat{T} = \frac{\hat{p}^2}{2m} . \quad \cdots\cdots \quad (2)$$

So the Hamiltonian operator for the one-dimensional harmonic oscillator is

$$\hat{H} = \hat{T} + \hat{V}$$

or

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2 . \quad \cdots\cdots \quad (3)$$

We will now find the possible eigenvalues and the corresponding eigenstates of $\hat{H}$. The eigenstates are states of definite energy, the energy being the corresponding eigenvalue. We will use the so called ladder method, a method devised by Dirac.

Since $\hbar\omega$ has the dimensions of energy, we first isolate the factor $\hbar\omega$ in $\hat{H}$ and write

$$\hat{H} = \left(\frac{\hat{p}^2}{2m\hbar\omega} + \frac{m\omega^2}{2\hbar\omega} \hat{x}^2 \right) \hbar\omega \quad \cdots\cdots (4).$$

Each term within the brackets in this equation is dimensionless. In other words, $\sqrt{m\hbar\omega}$ has the dimensions of momentum and $\sqrt{\frac{m\omega}{\hbar}}$ has the dimensions of inverse length.

We now define the operator $\hat{a}$ as

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\, \hat{x} + i \frac{\hat{p}}{\sqrt{2m\hbar\omega}} \quad \cdots\cdots (5)$$

and its hermitian conjugate

$$\hat{a}^+ = \sqrt{\frac{m\omega}{2\hbar}}\, \hat{x} - i \frac{\hat{p}}{\sqrt{2m\hbar\omega}}. \quad \cdots\cdots (6).$$

We will express $\hat{H}$ in terms of $\hat{a}$ and $\hat{a}^+$.
To do so, let us consider

$$\hat{a}^{+}\hat{a} = \left(\sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} - i\frac{\hat{p}}{\sqrt{2m\hbar\omega}}\right)\left(\sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} + i\frac{\hat{p}}{\sqrt{2m\hbar\omega}}\right)$$

$$= \frac{m\omega}{2\hbar}\hat{x}^{2} + \frac{\hat{p}^{2}}{2m\hbar\omega} + \frac{i}{2\hbar}\left(\hat{x}\hat{p} - \hat{p}\hat{x}\right)$$

$$= \frac{\hat{H}}{\hbar\omega} + \frac{i}{2\hbar}\cdot i\hbar\,\hat{\mathbb{1}}$$

$$= \frac{\hat{H}}{\hbar\omega} - \frac{1}{2}\hat{\mathbb{1}}$$

$$\therefore \hat{H} = \left(\hat{a}^{+}\hat{a} + \tfrac{1}{2}\hat{\mathbb{1}}\right)\hbar\omega \quad \cdots\cdots\cdots (7)$$

From here on we will ~~~~ not write the identity operator $\hat{\mathbb{1}}$ that multiplies the factor $\frac{1}{2}$.

At this stage, it is convenient to define ~~~~ a hermitian operator $\hat{N}$ as follows:

$$\hat{N} = \hat{a}^{+}\hat{a} \quad \cdots\cdots\cdots (8)$$

so that

$$\hat{H} = \left(\hat{N} + \tfrac{1}{2}\right)\hbar\omega \quad \cdots\cdots\cdots (9)$$

Since $\hat{H}$ and $\hat{N}$ commute, they have simultaneous eigenvectors. Thus, if $|n\rangle$ is an eigenvector of $\hat{N}$ with eigenvalue n, i.e., if

$$\hat{N}|n\rangle = n|n\rangle, \quad \quad (10)$$

then

$$\hat{H}|n\rangle = \left(n+\tfrac{1}{2}\right)\hbar\omega\,|n\rangle, \quad \quad (11)$$

i.e., $|n\rangle$ is also an eigenvector of $\hat{H}$ with eigenvalue $\left(n+\frac{1}{2}\right)\hbar\omega$.

Eigenvalues:

Our purpose now is to find the possible values of n, i.e., we wish to find the eigenvalue spectrum of $\hat{N}$ and $\hat{H}$.

First, we note that

$$\hat{N}^{+} = \left(\hat{a}^{+}\hat{a}\right)^{+} = \hat{a}^{+}\hat{a} = \hat{N}$$

i.e., $\hat{N}$ is hermitian. Hence $\hat{H}$ is also hermitian. It follows that the eigenvalues of $\hat{N}$ and $\hat{H}$ must be real, i.e., n must be a real number.

Second, the value of n must be greater than or equal to zero, since

$$n = \langle n|\hat{N}|n\rangle = \langle n|\hat{a}^{+}\hat{a}|n\rangle = \langle\phi|\phi\rangle \geq 0 \quad \cdots (12)$$

where we have defined $|\phi\rangle = a|n\rangle$. The equality holds if $|\phi\rangle$, i.e., $\hat{a}|n\rangle$ is a null vector.

To find exactly what the possible values of n are, we will need the commutation relation between $\hat{a}$ and $\hat{a}^{+}$ which we will evaluate below.

We have

$$[\hat{a}, \hat{a}^{+}] = \frac{1}{2\hbar}\left(-i[\hat{x}, \hat{p}] + i[\hat{p}, \hat{x}]\right)$$

$$= \frac{1}{2\hbar}\left(-i(i\hbar) + i(-i\hbar)\right)$$

$$= \hat{\mathbb{1}},$$

i.e.,

$$[\hat{a}, \hat{a}^{+}] = \hat{a}\hat{a}^{+} - \hat{a}^{+}\hat{a} = \hat{\mathbb{1}} \quad \cdots\cdots (13)$$

Then we have the following commutation relations:

$$[\hat{N}, \hat{a}] = [\hat{a}^+\hat{a}, \hat{a}]$$

$$= \hat{a}^+ \underbrace{[\hat{a}, \hat{a}]}_{=0} + \underbrace{[\hat{a}^+, \hat{a}]}_{-\hat{\mathbb{1}}} \hat{a}$$

$$= -\hat{a}$$

i.e

$$[\hat{N}, \hat{a}] = -\hat{a} \quad \ldots\ldots\ldots (14)$$

and

$$[\hat{N}, \hat{a}^+] = [\hat{a}^+\hat{a}, \hat{a}^+]$$

$$= \hat{a}^+ \underbrace{[\hat{a}, \hat{a}^+]}_{\hat{\mathbb{1}}} + \underbrace{[\hat{a}^+, \hat{a}^+]}_{=0} \hat{a}$$

$$= \hat{a}^+$$

i.e

$$[\hat{N}, \hat{a}^+] = \hat{a}^+ \quad \ldots\ldots\ldots (15)$$

We can get very interesting physical interpretations of the operators $\hat{a}$ and $\hat{a}^{+}$ by allowing $[\hat{N}, \hat{a}]$ and $[\hat{N}, \hat{a}^{+}]$ act on an eigenket $|n\rangle$ of $\hat{N}$. First, we have

$$[\hat{N}, \hat{a}]|n\rangle = -\hat{a}|n\rangle \quad (\text{using Eq. (14)})$$

or $$\hat{N}\hat{a}|n\rangle + \hat{a}\hat{N}|n\rangle = -\hat{a}|n\rangle$$

i.e $$\hat{N}\hat{a}|n\rangle + \hat{a}\,n|n\rangle = -\hat{a}|n\rangle$$

or $$\hat{N}\left(\hat{a}|n\rangle\right) = (n-1)\left(\hat{a}|n\rangle\right) \qquad \text{(16)}$$

From this equation we can conclude that if $|n\rangle$ is an eigenvector of $\hat{N}$ with eigenvalue n, then $\hat{a}|n\rangle$ is an eigenvector of $\hat{N}$ with eigenvalue $(n-1)$. The operator $\hat{a}$ is therefore called the lowering operator.

In a similar manner, using Eq. (15) we can show that

$$\hat{N}\left(\hat{a}^{+}|n\rangle\right) = (n+1)\left(\hat{a}^{+}|n\rangle\right), \quad \cdots\cdots (17)$$

i.e., $a^{+}|n\rangle$ is the eigenvector of $\hat{N}$ with eigenvalue $(n+1)$. The operator $\hat{a}^{+}$ is therefore called the raising operator.

Now, starting with the eigenvector $|n\rangle$ we can successively apply the lowering operator $\hat{a}$ reducing the value of n in steps of 1. However, Eq. (12), which states that n must be greater than or equal to zero, limits the number of times the lowering operator may be applied. When by successive downward steps an eigenvalue between 0 and 1 $(0 \leq n < 1)$ has been reached, by applying the lowering operator again we do not get a new eigenvector, because that would be an eigenvector violating the restriction given in Eq. (12). Denoting the eigenvalue in the lowest step of the ladder by n_0, we must have:

$$\hat{a}^{+}\hat{a}\,|n_0\rangle = n_0\,|n_0\rangle\,, \qquad 1 > n_0 \geq 0$$

and
$$\hat{a}\,|n_0\rangle = \phi \text{ (null)}.$$

Consequently
$$n_0\,|n_0\rangle = \phi \text{ (null)}$$

i.e., $n_0 = 0$. In other words, the lowest eigenvalue of $\hat{N}$ is zero. Now, starting from $n_0 = 0$, we may obtain all other eigenvalues and eigenvectors by repeated application of the raising operator $\hat{a}^{+}$. The eigenvalues increase in unit steps. Hence, the possible values of n are zero and the positive integers, i.e.,

$$\boxed{n = 0, 1, 2, 3, \ldots .} \qquad \text{- - - - -} \qquad (18)$$

There is no upper limit to the value of n. For, if an upper limit n' did exist, we would have

$$\hat{a}^{+}\,|n'\rangle = 0$$

i.e
$$\langle n'|\hat{a}\hat{a}^{+}\,|n'\rangle = 0.$$

But this condition cannot be fulfilled since

$$\langle n' | \hat{a}\hat{a}^{+} | n' \rangle = \langle n' | \hat{a}^{+}\hat{a} + \hat{\mathbb{1}} | n' \rangle = (n'+1)\langle n' | n' \rangle > 0.$$

In summary, the eigenvalue spectrum of $\hat{N}$ consists of zero and the denumerable infinity of all positive integers. Hence, from Eq. (11), the eigenvalues of $\hat{H}$ are given by

$$\boxed{E_n = \left(n + \tfrac{1}{2}\right)\hbar\omega,} \qquad \text{(19)}$$

with

$$n = 0, 1, 2, \ldots .$$

- Construction of the eigenstates of $\hat{H}$ for a harmonic oscillator.

We have seen that if $|n\rangle$ is an eigenvector of $\hat{N}$ with eigenvalue n, then $\hat{a}|n\rangle$ is an eigenvector of $\hat{N}$ with eigenvalue $n-1$, and $\hat{a}^{+}|n\rangle$ is an eigenvector of $\hat{N}$ with eigenvalue $|n+1\rangle$. Therefore, we can write

$$\hat{a}|n\rangle = c_{-}|n-1\rangle \quad \text{------} \quad (20)$$

and

$$\hat{a}^{+}|n\rangle = c_{+}|n+1\rangle \qquad (21)$$

where c_{-} and c_{+} are constants chosen such that all states $|n\rangle$, $|n-1\rangle$ and $|n+1\rangle$ are normalized.

From Eq. (20) we obtain

$$|c_{-}|^{2}\langle n-1|n-1\rangle = \langle n|\hat{a}^{+}\hat{a}|n\rangle$$

or $$|c_{-}|^{2} = n\langle n|n\rangle = n$$

or $$\boxed{c_{-} = \sqrt{n}} \quad \text{..........} \quad (22)$$

Similarly from Eq. (21) we have

$$|C_+|^2 \langle n+1|n+1\rangle = \langle n|\hat{a}\hat{a}^+|n\rangle$$

$$= \langle n|\hat{a}^+\hat{a}+1|n\rangle$$

$$= (n+1)\langle n|n\rangle$$

or $$|C_+|^2 = (n+1)$$

i.e. $$\boxed{C_+ = \sqrt{n+1}.} \qquad \text{------} \quad (23)$$

Thus we have

$$\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle \qquad \text{------} \quad (24)$$

$$\hat{a}^+|n\rangle = \sqrt{n+1}\,|n+1\rangle. \qquad \text{------} \quad (25)$$

Using Eq. (25) we can construct all the normalized eigenstates of $\hat{N}$ & $\hat{H}$ starting from the ground state $|0\rangle$. Let assume that $\langle 0|0\rangle = 1$. Then the normalized excited states are:

$$|1\rangle = \hat{a}^{+}|0\rangle$$

$$|2\rangle = \frac{1}{\sqrt{2}}\hat{a}^{+}|1\rangle = \frac{1}{\sqrt{2!}}(\hat{a}^{+})^{2}|0\rangle$$

$$|3\rangle = \frac{1}{\sqrt{3}}\hat{a}^{+}|2\rangle = \frac{1}{\sqrt{3!}}(\hat{a}^{+})^{3}|0\rangle$$

etc.

In general,

$$|n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^{+})^{n}|0\rangle \quad \text{- - - - - -} \quad (26)$$

where $\langle n|n\rangle = 1$. We can think of an excited state $|n\rangle$ of the oscillator as containing n quanta of energy $\hbar\omega$ in addition to the zero-point energy $\frac{1}{2}\hbar\omega$. The operator $\hat{a}^{+}$ creates a quantum of energy; therefore, $\hat{a}^{+}$ is called the creation operator. Similarly, the operator $\hat{a}$ annihilates a quantum of energy and is therefore called the annihilation operator or the destruction operator. Further, since $\hat{N}|n\rangle = n|n\rangle$, the operator $\hat{N}$ acting on an eigenstate $|n\rangle$ simply gives the number of quanta times $|n\rangle$. Therefore, $\hat{N}$ is called the number operator.

- Connection with coordinate representation.

We will now find the wavefunctions in the coordinate representation of the different stationary states of the harmonic oscillator, i.e., we will evaluate

$$\psi_0(x) \equiv \langle x|0\rangle$$
$$\psi_1(x) \equiv \langle x|1\rangle$$
$$\vdots \qquad \vdots$$
$$\psi_n(x) \equiv \langle x|n\rangle$$

etc. First we consider the ~~gs~~ ground state $|0\rangle$. For the ground state we have

$$\hat{a}\,|0\rangle = 0 \qquad \text{- - - - - - - (26)}$$

where
$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} + \frac{i}{\sqrt{2m\hbar\omega}}\,\hat{p}.$$

In the coordinate representation Eq. (26) is is written as

$$\langle x|\hat{a}|0\rangle = 0 \quad \cdots\cdots\cdots (27)$$

In coordinate representation

$$\hat{x} \rightarrow x \longrightarrow \text{i.e., } \langle x|\hat{x} = x\langle x|$$
$$\hat{p} \rightarrow -i\hbar\frac{\partial}{\partial x} \longrightarrow \text{i.e., } \langle x|\hat{p} = -i\hbar\frac{\partial}{\partial x}\langle x|$$

Therefore

$$\langle x|\hat{a} = \langle x|\left(\sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} + \frac{i}{\sqrt{2m\hbar\omega}}\,\hat{p}\right)$$

$$= \sqrt{\frac{m\omega}{2\hbar}}\,x\langle x| + \frac{i}{\sqrt{2m\hbar\omega}}\left(-i\hbar\frac{\partial}{\partial x}\right)\langle x|$$

$$= \left(\sqrt{\frac{m\omega}{2\hbar}}\,x + \sqrt{\frac{\hbar}{2m\omega}}\,\frac{\partial}{\partial x}\right)\langle x| \quad \cdots\cdots (28)$$

Using Eq. (28) in Eq. (27) we have

$$\left(\sqrt{\frac{m\omega}{2\hbar}}\,x + \sqrt{\frac{\hbar}{2m\omega}}\,\frac{\partial}{\partial x}\right)\langle x|0\rangle = 0$$

or $$\left(\sqrt{\frac{m\omega}{2\hbar}}\,x + \sqrt{\frac{\hbar}{2m\omega}}\,\frac{\partial}{\partial x}\right)\psi_0(x) = 0 \quad \cdots\cdots (29)$$

where $\psi_0(x) \equiv \langle x|0\rangle$ is the ground state wavefunction. Here it is convenient to introduce the dimensionless variable

$$\xi = \sqrt{\frac{m\omega}{\hbar}}\, x. \quad \text{------------} (30)$$

Eq. (29) then becomes

$$2^{-1/2}\left(\xi + \frac{d}{d\xi}\right)\psi_0 = 0, \quad \text{------------} (31)$$

where ψ_0 can now be considered a function of ξ.

Eq. (31) has the solution

$$\psi_0 = c\, e^{-\frac{1}{2}\xi^2} = c\, e^{-m\omega x^2/2\hbar}.$$

Normalizing ψ_0, we have

$$\boxed{\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}} \quad \text{------} (32)$$

The ground state wave function is Gaussian and symmetric about the origin.

All other functions can be found by repeated application of $\hat{a}^+$. In the coordinate representation

$$\langle x|\hat{a}^+ = \langle x|\left(\sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} - \frac{i}{\sqrt{2m\hbar\omega}}\,\hat{p}\right)$$

$$= \left(\sqrt{\frac{m\omega}{2\hbar}}\,x - \sqrt{\frac{\hbar}{2m\omega}}\,\frac{\partial}{\partial x}\right)\langle x| \,. \quad \text{- - - - (33)}$$

The wave function for the first excited state is

Then

$$\langle x|1\rangle = \langle x|\hat{a}^+|0\rangle$$

or $$\psi_1(x) = \left(\sqrt{\frac{m\omega}{2\hbar}}\,x - \sqrt{\frac{\hbar}{2m\omega}}\,\frac{d}{dx}\right)\langle x|0\rangle$$

or $$\psi_1(x) = \left(\sqrt{\frac{m\omega}{2\hbar}}\,x - \sqrt{\frac{\hbar}{2m\omega}}\,\frac{d}{dx}\right)\psi_0(x)\,.$$

In terms of the variable ξ we have

$$\psi_1(x) = 2^{-1/2}\left(\xi - \frac{d}{d\xi}\right)\psi_0(\xi)$$

or,

$$\psi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2}} \left(\xi - \frac{d}{d\xi}\right) e^{-\frac{1}{2}\xi^2}$$

or

$$\psi_1 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2}}\, 2\xi\, e^{-\frac{1}{2}\xi^2}$$

Noting that, the Hermite polynomial $H_1(\xi) = 2\xi$, we have

$$\boxed{\psi_1 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2}} H_1(\xi)\, e^{-\frac{1}{2}\xi^2}} \quad \text{- - - - - (34)}.$$

Next, let us find the wave function for the second excited state $|2\rangle$. We have

$$|2\rangle = \frac{1}{\sqrt{2!}} \hat{a}^{+} |1\rangle = \frac{1}{\sqrt{2!}} \left(\hat{a}^{+}\right)^2 |0\rangle \quad \text{- - - - (35)}$$

Noting that in the coordinate representation

$$\hat{a}^{+} = \sqrt{\frac{m\omega}{2\hbar}}\, x - \sqrt{\frac{\hbar}{2m\omega}} \frac{d}{dx}$$

$$= \frac{1}{\sqrt{2}} \left(\xi - \frac{d}{d\xi}\right),$$

the coordinate representation of Eq. (35) becomes

$$\psi_2(x) = \frac{1}{\sqrt{2!}}\frac{1}{(\sqrt{2})^2}\left(\xi - \frac{d}{d\xi}\right)^2 \psi_0(\xi)$$

$$= \frac{1}{\sqrt{2^2 2!}}\left(\xi - \frac{d}{d\xi}\right)^2 \psi_0(\xi)$$

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

The Hermite polynomial of second order, $H_2(\xi)$ is defined as

$$\left(\xi - \frac{d}{d\xi}\right)^2 e^{-\frac{1}{2}\xi^2} = H_2(\xi)\, e^{-\frac{1}{2}\xi^2}.$$

We find

$$H_2(\xi) = 4\xi^2 - 2.$$

Hence

$$\boxed{\psi_2 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^2 2!}}\, H_2(\xi)\, e^{-\frac{1}{2}\xi^2}.} \quad \cdots\cdots (36)$$

In general, for the state $|n\rangle$ we have

$$|n\rangle = \frac{1}{\sqrt{n!}} (\hat{a}^{+})^{n} |0\rangle$$

In coordinate representation

$$\langle x|n\rangle = \frac{1}{\sqrt{n!}} \langle x|(\hat{a}^{+})^{n}|0\rangle .$$

$$= \frac{1}{\sqrt{n!}} \left[\frac{1}{\sqrt{2}}\left(\xi - \frac{d}{d\xi}\right)\right]^{n} \langle x|0\rangle$$

or

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\xi - \frac{d}{d\xi}\right)^{n} \psi_0(x)$$

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

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

We define the n^{th} order Hermite polynomial $H_n(\xi)$ as

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

Thus, the wave function for the state $|n\rangle$ is

$$\boxed{\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi)\, e^{-\frac{1}{2}\xi^2}. \qquad \xi = \sqrt{\frac{m\omega}{\hbar}}\, x.} \quad \cdots (37)$$

The first few Hermite polynomials are

$$H_0(\xi) = 1$$
$$H_1(\xi) = 2\xi$$
$$H_2(\xi) = 4\xi^2 - 2$$
$$H_3(\xi) = 8\xi^3 - 12\xi.$$

Note that the Hermite polynomials $H_n(x)$ are even or odd functions of x (or ξ) according as n is even or odd. Therefore $\psi_n(x)$ are even or odd functions of x according as n is even $(0, 2, 4, \cdots)$ or odd $(n = 1, 3, 5, \cdots)$.

At this stage we will make some comments about the eigenvalues and eigenvectors of the Hamiltonian operator for a one-dimensional harmonic oscillator. First, none of the eigenvalues $(n+1/2)\hbar\omega$ of $\hat{H}$ are degenerate. In other words, there is only one linearly independent eigenvector corresponding to each eigenvalue. This follows from the ~~...~~ general theorem that in a one-dimensional problem, each eigenvalue of $\hat{H}$ corresponding to bound states is nongenerate (see later). In the specific example of a one-dimensional harmonic oscillator we can also prove the assertion as follows:

First we show that if the eigenvalue n of the number operator $\hat{N}$ is non-degenerate so is the eigenvalue $n+1$. Assume, on the contrary that there are two linearly independent eigenvectors $|\phi_{n+1}\rangle$ and $|\psi_{n+1}\rangle$ corresponding to $(n+1)$. Let

$$|\phi_n\rangle = \hat{a}\,|\phi_{n+1}\rangle$$

$$|\psi_n\rangle = \hat{a}\,|\psi_{n+1}\rangle$$

Since $\hat{a}$ is the lowering operator, both $|\phi_n\rangle$ and $|\psi_n\rangle$ must be eigenvectors with the same eigenvalue n. Further, since we have assumed that n is non-degenerate, the vectors $|\phi_n\rangle$ and $|\psi_n\rangle$ must be linearly dependent,

i.e.,

$$|\phi_n\rangle = \lambda\,|\psi_n\rangle,$$

where λ is a constant. Now, operating by $\hat{a}^+$ on both sides of this equation we get

$$\text{LHS} = \hat{a}^+|\phi_n\rangle = \hat{a}^+\hat{a}\,|\phi_{n+1}\rangle = \hat{N}\,|\phi_{n+1}\rangle = (n+1)\,|\phi_{n+1}\rangle$$

$$= \text{RHS} = \lambda\,\hat{a}|\psi_n\rangle = \lambda\,\hat{a}^+\hat{a}\,|\psi_{n+1}\rangle = \lambda\,\hat{N}\,|\psi_{n+1}\rangle = \lambda\,(n+1)\,|\psi_{n+1}\rangle.$$

Hence

$$|\phi_{n+1}\rangle = \lambda\,|\psi_{n+1}\rangle,$$

i.e., $|\phi_{n+1}\rangle$ and $|\psi_{n+1}\rangle$ are linearly dependent, a contradiction to our initial assumption. Thus, there is only one linearly independent eigenvector corresponding to the eigenvalue $n+1$.

The proof will be completed if the lowest eigenvalue $n=0$, i.e., the eigenvalue corresponding to the ground state, is nondegenerate. To show this consider the fact that the ground state eigenvector of $\hat{H}$ satisfies the equation

$$\hat{a}\,|0\rangle = \phi .$$

There is only one linearly independent eigenvector that satisfies this equation. Hence, $n=0$ is non-degenerate.

The second comment we would like to make is that for a harmonic oscillator the eigenfunctions of $\hat{H}$ have definite parity, i.e., eigenfunctions are either even or odd. This follows from the general principle that for a symmetric potential (the harmonic oscillator potential $V(x)=\frac{1}{2}m\omega^2x^2$ is symmetric), the eigenvectors of $\hat{H}$ corresponding to non-degenerate eigenvalues are either even or odd. This is easy to prove. Consider the Schrödinger equation for a particle moving in one-dimension under the potential $V(x)$:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi(x)=E\,\psi(x).$$

Now, make the coordinate transformation

$$x \to -x.$$

The Schrödinger equation then becomes

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(-x)\right]\psi(-x)=E\,\psi(-x).$$

If $V(x)$ is symmetric, i.e., if $V(-x)=V(x)$, then the Hamiltonian operator remains unchanged under the transformation $x \to -x$. We then have

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi(-x)=E\,\psi(-x),$$

i.e., $\psi(-x)$ is also an eigenfunction of $\hat{H}$ with eigenvalue E just like $\psi(x)$. Since we have assumed that the eigenvalue E is non-degenerate, the two wavefunctions $\psi(-x)$ and $\psi(x)$ must be linearly dependent, i.e., they can differ by at most a multiplicative constant, i.e.,

$$\psi(-x) = \pi\, \psi(x)$$

where π is a constant. The above equation can also be written as

$$\psi(x) = \pi\, \psi(-x).$$

Combining these two equations we have

$$\pi^2 = 1$$

i.e., $\pi = 1$ or -1.

If $\pi = 1$, we have

$$\psi(-x) = \psi(x),$$

i.e., the wavefunction is even and is said to have even parity. If, on the other hand $\pi = -1$, then

$$\psi(-x) = -\psi(x)$$

i.e., the wavefunction is odd and is said to have odd parity.

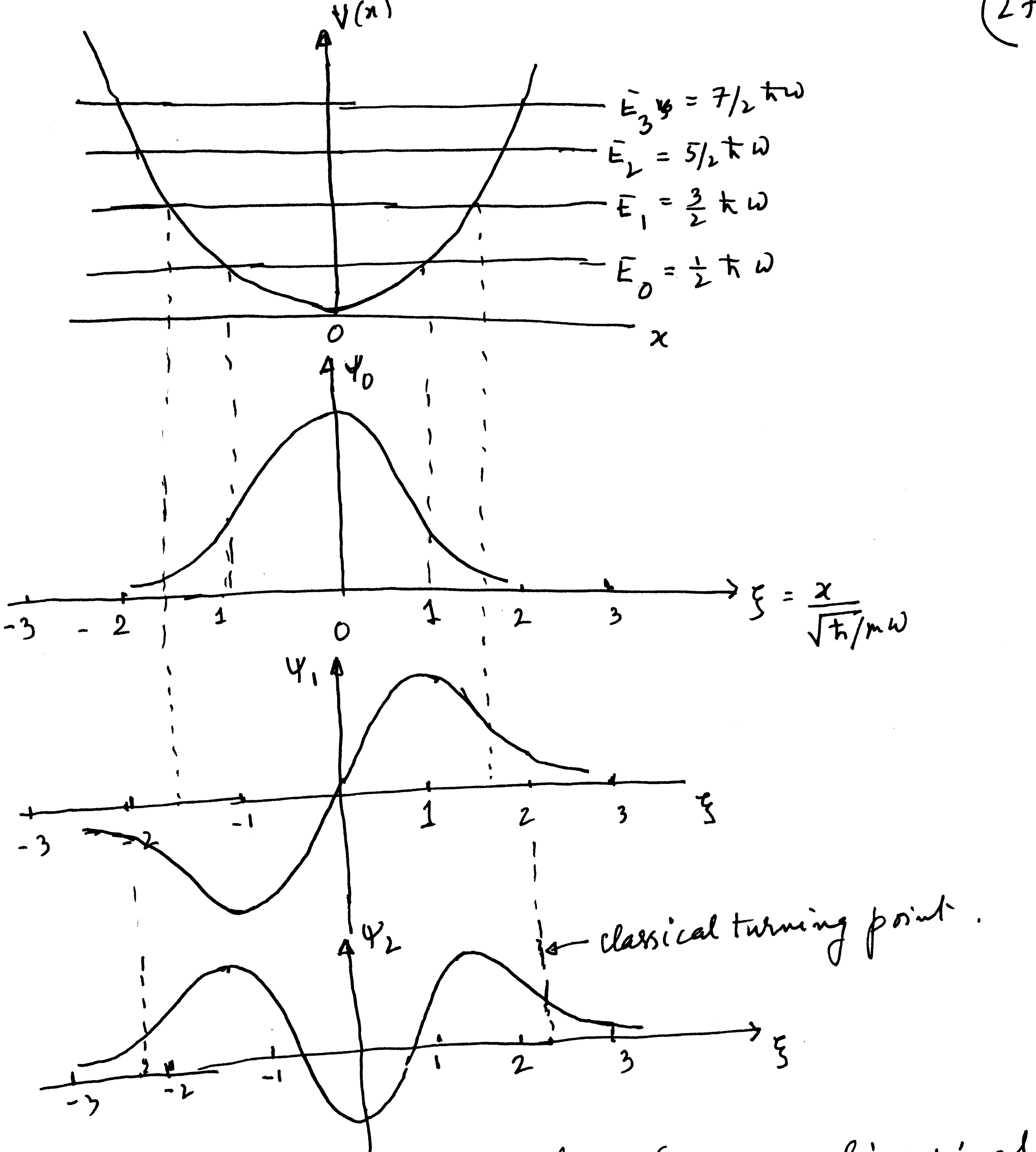


Fig: The first three wave functions for a one-dimensional harmonic oscillator. Note that ψ_0 and ψ_2 are even functions of x while ψ_1 is an odd function of x.

The ground state is even and does not have any node. The first excited state, $|1\rangle$, is odd and has one node, namely at the origin. The second excited state is even with two nodes. In this way, the parity of the states ~~beco~~ is alternatively even or odd starting with even parity for the ground state.

The fact that the ground state is always even can be understood from the Schrödinger equation which we write as

$$\frac{d^2\psi(x)}{dx^2} + k^2(x)\,\psi(x) = 0$$

where

$$k(x) = \sqrt{\frac{2m}{\hbar^2}\left(E - V(x)\right)}$$

If E is large, as for excited states, then k would be large. Within the classically allowed region $k(x)$ is +ve, and the wave function $\psi(x)$ is oscillatory. If $k(x)$ is larger, spatial oscillation frequency is larger too (i.e., there are more oscillations per unit distance). So there will be more nodes in the wave function.

In the classically forbidden region ($V(x) > E$), k becomes imaginary and wave function decays exponentially.

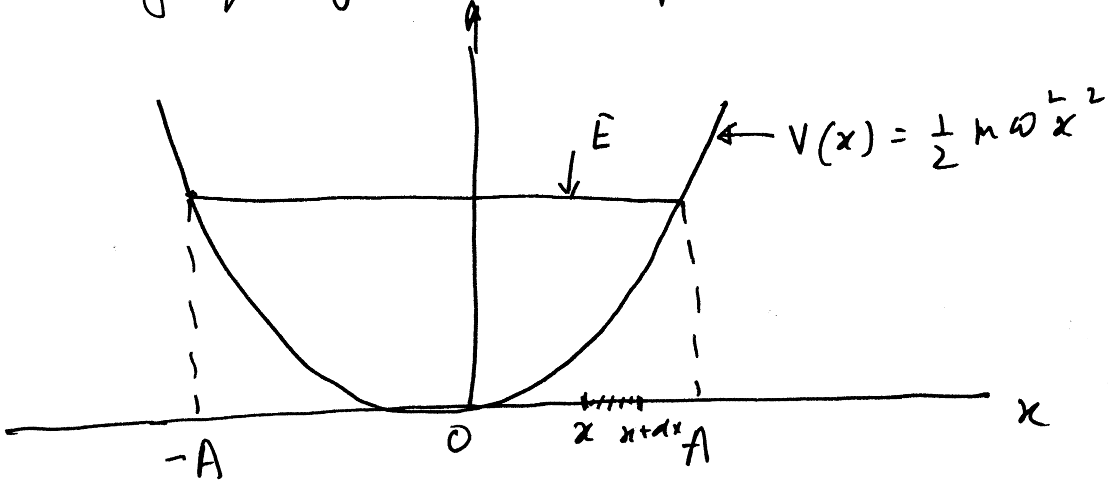
For the ground state, E has the least value, so that there are no nodes at all. The wave function then must be even, because for an odd function there must be at least one node at $x = 0$.

~~For a classically har~~

For a classical harmonic oscillator there is no possibility at all for finding the oscillator in the forbidden region. But a quantum oscillator tunnels into the classically forbidden region so that there is a finite probability for finding the oscillator in the forbidden region.

Position probability density.

First, we consider a classical harmonic oscillator with a frequency ω and amplitude A.



The points $x = +A$ and $x = -A$ are the turning points of motion. The amplitude is found in terms of energy by noting that at $x = \pm A$, the entire energy is potential. Therefore

$$\frac{1}{2} m\omega^2 A^2 = E$$

$$A = \sqrt{\frac{2E}{m\omega^2}} .$$

The regions $x > A$ and $x < -A$ are totally forbidden to the classical oscillator, since in these regions $V(x) > E$ so that kinetic energy formally becomes negative.

The probability that the oscillating particle would be found in a small spatial interval x to $x+dx$, within the accessible region is equal to the fraction of the time the particle spends in traversing this spatial interval during one cycle. Thus

$$dP = \frac{2\,dt}{T},$$

where T is the time period and dt is the time taken to traverse the distance dx at x. The particle traverses this distance interval twice in a cycle. This accounts for the factor 2 in the above formula.

Now,

$$dt = \frac{dx}{|v(x)|}$$

where $v(x)$ is the velocity of the particle at x. We can find $v(x)$ from conservation of energy:

$$\frac{1}{2} m v^2(x) + \frac{1}{2} m \omega^2 x^2 = E = \frac{1}{2} m \omega^2 A^2$$

or

$$v^2(x) = \omega^2 (A^2 - x^2)$$

i.e

$$|v(x)| = \omega \sqrt{A^2 - x^2}$$

Also,

$$T = \frac{2\pi}{\omega}.$$

$$\therefore\ dP = \frac{2\,dt}{T} = \frac{2}{\frac{2\pi}{\cancel{\omega}}} \cdot \frac{dx}{\cancel{\omega}\sqrt{A^2-x^2}}$$

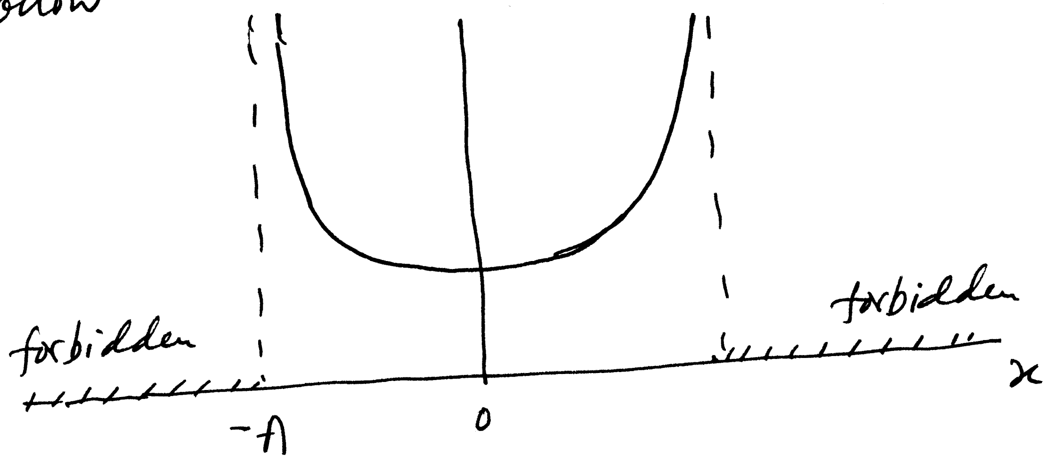
or

$$dP = \frac{dx}{\pi\sqrt{A^2-x^2}} = P(x)\,dx$$

where

$$P(x) = \frac{1}{\pi\sqrt{A^2-x^2}} \qquad (-A \le x \le A)$$

is the position probability density for the classical oscillator. We plot $P(x)$ vs x in the figure below



Note that the regions $x > A$ and $x < -A$ are totally forbidden to the classical oscillator. So $P(x) = 0$ in these regions.

Also, $P(x) \to \infty$ as $x \to -A$ & $x \to A$ from the inside, since $v = 0$ at $x = \pm A$. However

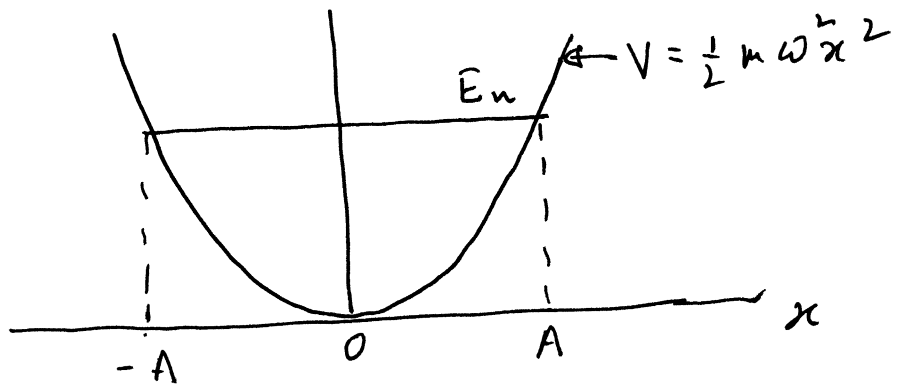
$$\int_{-A}^{A} P(x)\,dx = 1 .$$

Position probability density for the quantum oscillator.

Let us find the position probability density of the one-dimensional quantum oscillator in the state $|n\rangle$ with energy

$$E_n = \left(n + \tfrac{1}{2}\right)\hbar\omega .$$

The classical turning points of the oscillator are the points of intersection of E_n and $V(x)$



The turning points are at $x = \pm A$ given by

$$\frac{1}{2} m\omega^2 A^2 = E_n$$

or $x = A = \sqrt{\dfrac{2E_n}{m\omega^2}} = \sqrt{\dfrac{2(n+\frac{1}{2})\hbar\omega}{m\omega^2}}$

or $x = A = \sqrt{2n+1}\sqrt{\dfrac{\hbar}{m\omega}}$

We define the dimensionless variable ξ as

$$\xi = \frac{x}{\sqrt{\frac{\hbar}{m\omega}}}$$

Then the turnings are at

$\xi = 1$ for $|0\rangle$ $n=0$

$\xi = \sqrt{3}$ for $|1\rangle$ $n=1$

$\xi = \sqrt{5}$ for $|2\rangle$ $n=2$

etc.

$\sqrt{3} = 1.67$
$\sqrt{5} = 2.2$

In the next diagram we will plot the wave function in the ground state and the corresponding position probability density. Note that position probability density in the state $|n\rangle$ is

$$P(x) = |\psi_n(x)|^2$$

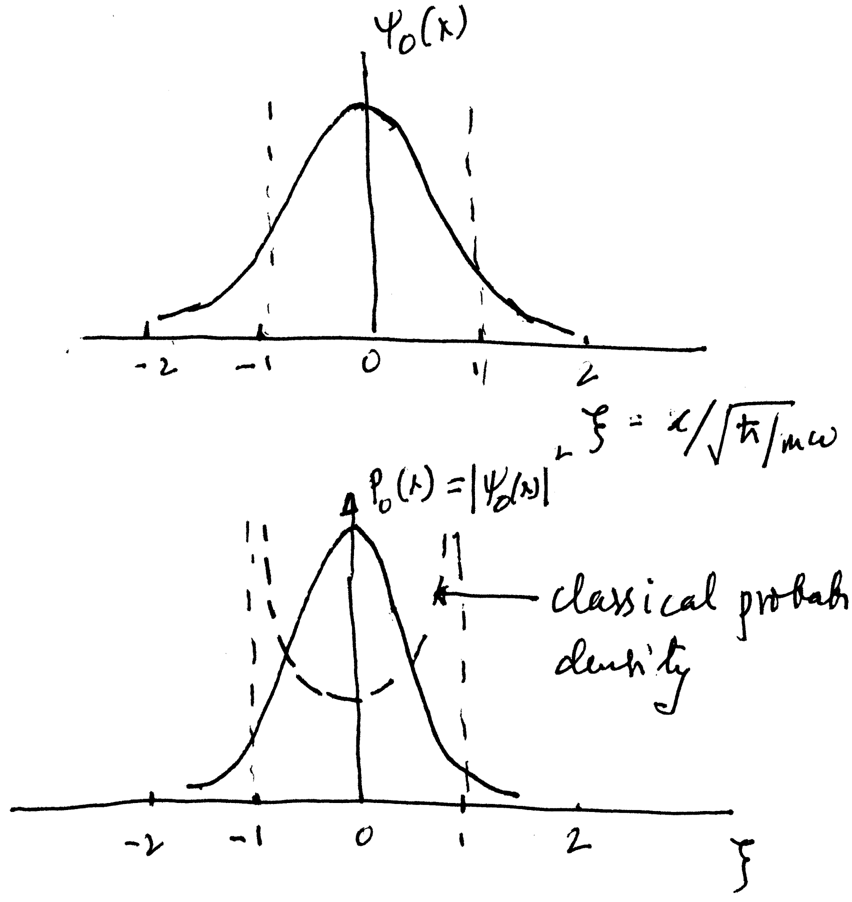


Fig: The wave function $\psi_0(x)$ and the position probability density $P_0(x) = |\psi_0(x)|^2$. Also shown is the classical probability density with dashed line.

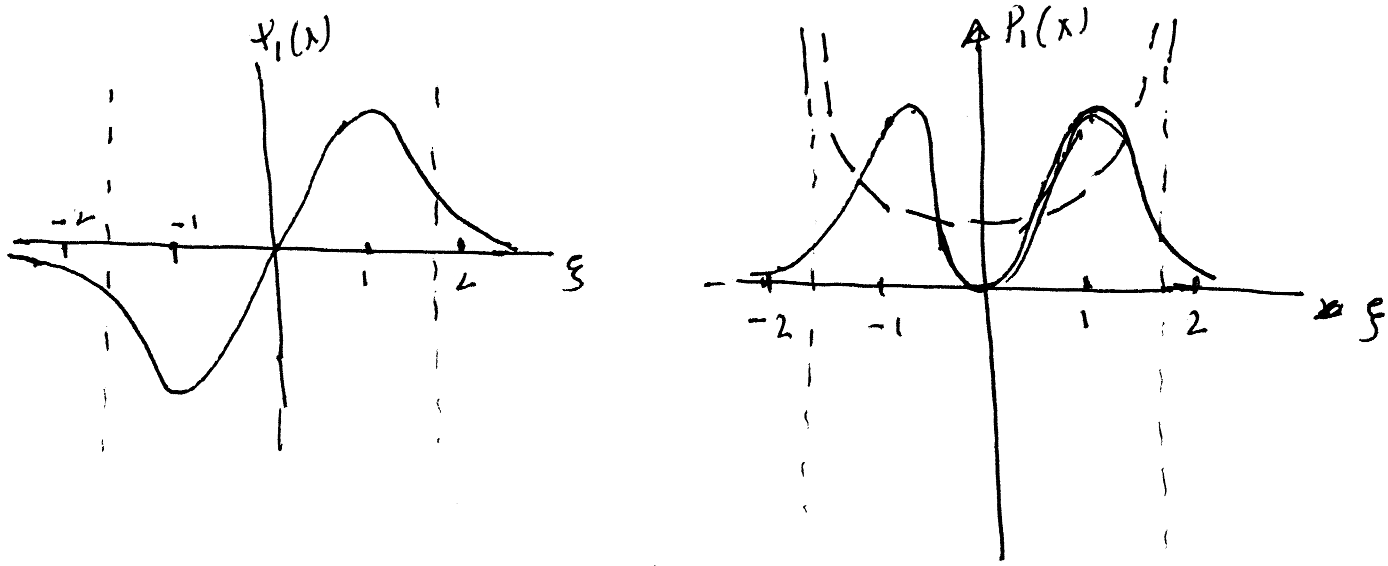


Fig: Position probability density $P_1(x)$.

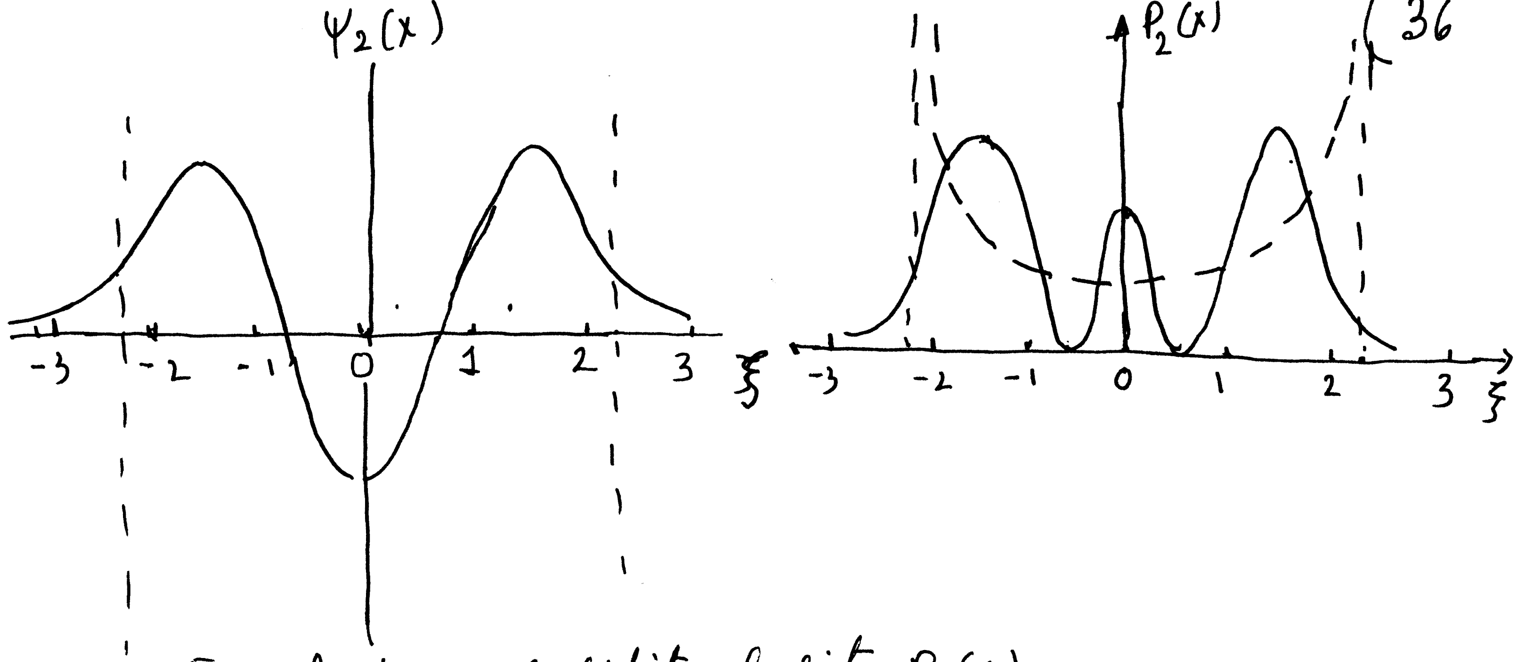


Fig: Position probability density $P_2(x)$

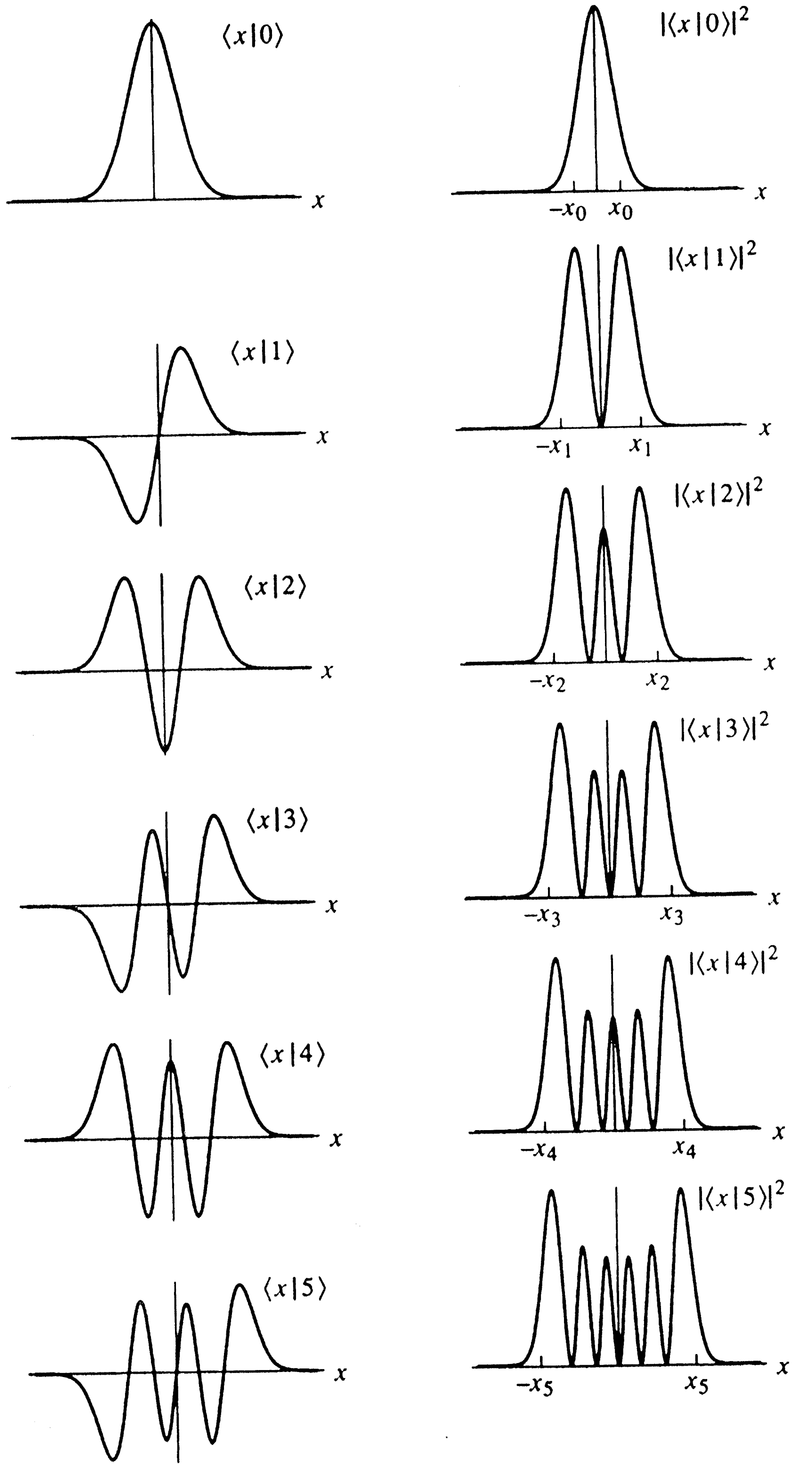


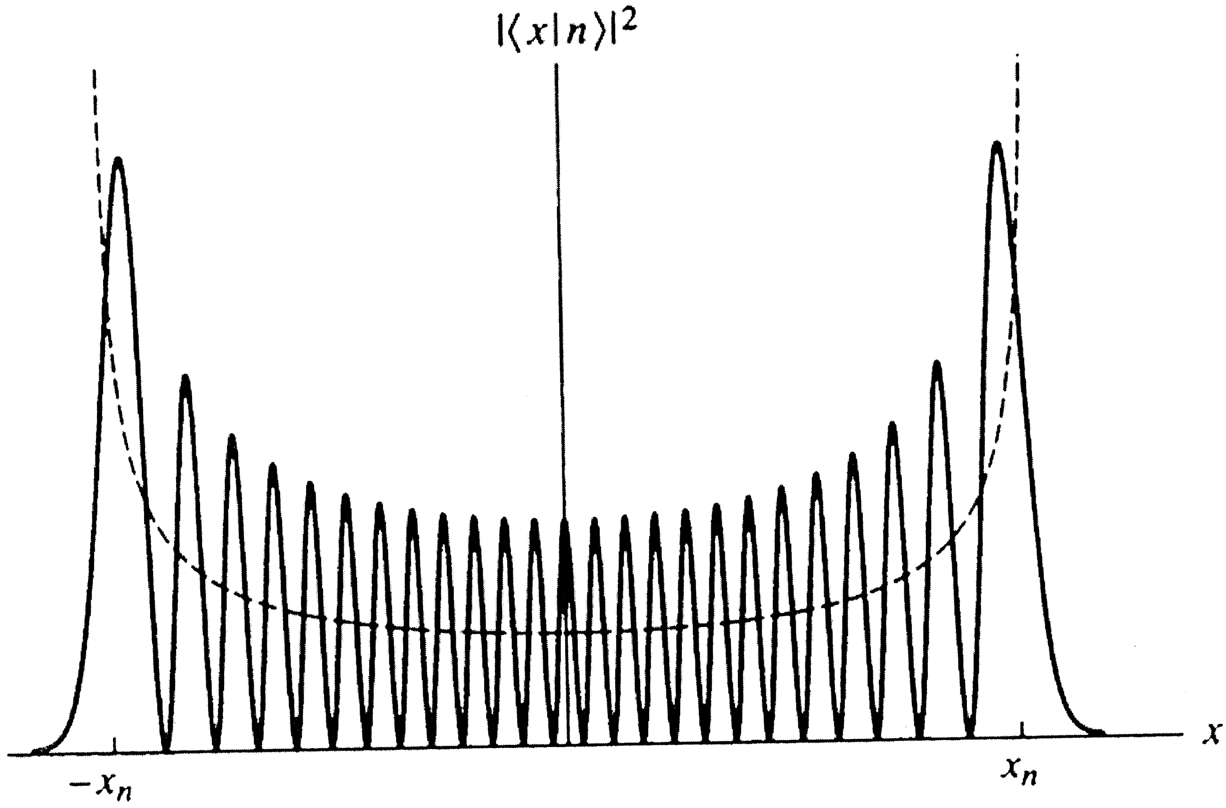
FIGURE 7.7
The wave functions $\langle x|n\rangle$ and the probability densities $|\langle x|n\rangle|^2$ plotted for the first six energy eigenstates of the harmonic oscillator. The classical turning points at $x_n = \sqrt{(2n+1)(\hbar/m\omega)}$ are determined from (7.59).

We see that when n is small, the position probality density $P_n(x) = |\psi_n(x)|^2$ doesn't at all match with the classical probability density. However when n is large, $P_n(x)$ oscillates very rapidly over spatial distance and the mean of $P_n(x)$ becomes equal to the classical position probability density. This is an example of 'correspondence principle' which states that if the quantum number n is large, then the predictions of quantum theory becomes the same as the prediction from classical theory.

The quantization of the energy levels of bound states, which is the hallmark of the quantum theory, also becomes inapparent as n becomes very large. For the one dimesinal harmonic oscillator, the energy levels are equispaced in energy, the energy spacing being $\frac{1}{2}\hbar\omega$. The ratio of this spacing to the energy for the state $|n\rangle$ is

$$\frac{\frac{1}{2}\hbar\omega}{(n+\frac{1}{2})\hbar\omega} = \frac{1}{2n+1} \to 0 \text{ as } n \to \infty$$

So for large quantum numbers, the discreteness of the energy levels do not show and it seems that the energy of the oscillator can be made to change in a continuous manner as is predicted in the classical theory of the harmonic oscillator.



A plot of the probability density $|\langle x|n\rangle|^2$ for large n. The dashed line is a plot of the classical probability density ~~function~~. x_n and $-x_n$ are the classical turning points.

Matrix elements in the energy representation.

We will now write down the matrix elements of the various operators — $\hat{a}$, $\hat{a}^+$, $\hat{x}$, $\hat{p}$, $\hat{H}$ and $\hat{N}$ — in the energy representation. By energy representation we mean that the eigenvectors of Hamiltonian operator $\hat{H}$ are chosen as the basis vectors. The basis vectors are $|n\rangle$; $n = 0, 1, 2, \cdots$, where

$$\hat{H}|n\rangle = E_n|n\rangle \quad \cdots \cdots \quad (38)$$

with

$$E_n = \left(n + \tfrac{1}{2}\right)\hbar\omega. \qquad (39).$$

• Matrix elements of $\hat{H}$

The matrix of $\hat{H}$ in the energy representation is of course diagonal.

$$H_{nn'} \equiv \langle n|\hat{H}|n'\rangle = E_n \delta_{nn'} \quad \cdots \quad (40).$$

Explicitly,

$$\underline{H} = \begin{pmatrix} \frac{1}{2}\hbar\omega & 0 & 0 & 0 & \cdot & \cdot \\ 0 & \frac{3}{2}\hbar\omega & 0 & 0 & \cdot & \cdot \\ 0 & 0 & \frac{5}{2}\hbar\omega & 0 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} \qquad (41)$$

• <u>Matrix elements of $\hat{a}$</u>

$$a_{nn'} = \langle n|\hat{a}|n'\rangle = \sqrt{n'}\,\langle n|n'-1\rangle = \sqrt{n'}\,\delta_{n\,n'-1}.$$

$$\underline{a} = \begin{pmatrix} \langle 0|\hat{a}|0\rangle & \langle 0|\hat{a}|1\rangle & \langle 0|\hat{a}|2\rangle & \cdot & \cdot & \cdot \\ \langle 1|\hat{a}|0\rangle & \langle 1|\hat{a}|1\rangle & \langle 1|\hat{a}|2\rangle & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

or,

$$\underline{a} = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdot & \cdot \\ 0 & 0 & \sqrt{2} & 0 & 0 & \cdot & \cdot \\ 0 & 0 & 0 & \sqrt{3} & 0 & & \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

• Matrix elements of $\hat{a}^+$

$$a^+_{nn'} = \langle n|\hat{a}^+|n'\rangle = \sqrt{n'+1}\,\langle n|n'+1\rangle = \sqrt{n'+1}\,\delta_{n\,n'+1}$$

$$\underline{a}^+ = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdot & \cdot \\ \sqrt{1} & 0 & 0 & 0 & \cdot & \cdot \\ 0 & \sqrt{2} & 0 & 0 & \cdot & \cdot \\ 0 & 0 & \sqrt{3} & 0 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

Note that the matrix $\underline{\hat{a}}^+$ is adjoint of the matrix $\underline{\hat{a}}$.

• Matrix elements of $\hat{x}$ and $\hat{p}$

We have

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} + \frac{i}{\sqrt{2m\hbar\omega}}\,\hat{p}$$

$$\hat{a}^{+} = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} - \frac{i}{\sqrt{2m\hbar\omega}}\,\hat{p}$$

Solving for $\hat{x}$ and $\hat{p}$ we obtain

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\,(\hat{a} + \hat{a}^{+})$$

$$\hat{p} = \frac{1}{i}\sqrt{\frac{m\hbar\omega}{2}}\,(\hat{a} - \hat{a}^{+}).$$

Therefore

$$x_{nn'} = \langle n|\hat{x}|n'\rangle$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\,\langle n|\hat{a} + \hat{a}^{+}|n'\rangle$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left(\langle n|\hat{a}|n'\rangle + \langle n|\hat{a}^{+}|n'\rangle\right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n'}\,\delta_{n\,n'-1} + \sqrt{n'+1}\,\delta_{n,\,n'+1}\right)$$

and

$$p_{nn'} = \langle n|\hat{p}|n'\rangle$$

$$= \sqrt{\frac{m\hbar\omega}{2}}\,\frac{1}{i}\left(\langle n|\hat{a}|n'\rangle - \langle n|\hat{a}^{+}|n'\rangle\right)$$

$$= \sqrt{\frac{m\hbar\omega}{2}}\,\frac{1}{i}\left(\sqrt{n'}\,\delta_{n\,n'-1} - \sqrt{n'+1}\,\delta_{n,\,n'+1}\right)$$

Explicitly

$$\underline{x} = \left(\frac{\hbar}{2m\omega}\right)^{1/2}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdot \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \cdot \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \cdot \\ \cdot & \cdot & \cdot & \vdots & \cdot \end{pmatrix}$$

and

$$\underline{p} = \left(\frac{m\hbar\omega}{2}\right)^{1/2}\frac{1}{i}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdot \\ -\sqrt{1} & 0 & \sqrt{2} & 0 & \cdot \\ 0 & -\sqrt{2} & 0 & \sqrt{3} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

Home work

1. Calculate the uncertainty product $\Delta x \Delta p$ for a one-dimensional harmonic oscillator when the oscillator is in the energy state $|n\rangle$.

Ans: We have

$$(\Delta x)^2 = \langle n|(\hat{x} - \langle x\rangle)^2|n\rangle$$
$$= \langle n|\hat{x}^2|n\rangle - \langle x\rangle^2$$

Similarly

$$(\Delta p)^2 = \langle n|\hat{p}^2|n\rangle - \langle p\rangle^2$$

We can express $\hat{x}$ and $\hat{p}$ in terms of the lowering and raising operators $\hat{a}$ and $\hat{a}^+$. We have

$$\hat{x} = \left(\frac{\hbar}{2m\omega}\right)^{1/2}(\hat{a} + \hat{a}^+)$$
$$\hat{p} = \left(\frac{\hbar m\omega}{2}\right)^{1/2}\frac{1}{i}(\hat{a} - \hat{a}^+)$$

Therefore

$$\langle x\rangle = \langle n|\hat{x}|n\rangle = \left(\frac{\hbar}{2m\omega}\right)^{1/2}\left(\langle n|\hat{a}|n\rangle + \langle n|\hat{a}^+|n\rangle\right)$$
$$= \left(\frac{\hbar}{2m\omega}\right)^{1/2}\left(\sqrt{n}\,\underbrace{\langle n|n-1\rangle}_{=0} + \sqrt{n+1}\,\underbrace{\langle n|n+1\rangle}_{=0}\right)$$
$$= 0.$$

Similarly

$$\langle p \rangle = 0 .$$

Next, let us calculate $\langle x^2 \rangle$.

$$\langle x^2 \rangle = \langle n | \hat{x}^2 | n \rangle$$

$$= \left(\frac{\hbar}{2m\omega}\right) \langle n | (\hat{a} + \hat{a}^+)(\hat{a} + \hat{a}^+) | n \rangle$$

$$= \left(\frac{\hbar}{2m\omega}\right) \Big(\underbrace{\langle n | \hat{a}\hat{a} | n \rangle}_{=0} + \underbrace{\langle n | \hat{a}\hat{a}^+ | n \rangle}_{(n+1)} + \underbrace{\langle n | \hat{a}^+\hat{a} | n \rangle}_{n} + \underbrace{\langle n | \hat{a}^+\hat{a}^+ | n \rangle}_{=0} \Big)$$

$$= \left(\frac{\hbar}{2m\omega}\right) \left(0 + (n+1) + n + 0 \right)$$

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

$$= \left(n + \frac{1}{2}\right) \frac{\hbar}{m\omega} ,$$

$$= \frac{E_n}{m\omega^2}$$

where

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

$$\therefore \boxed{\Delta x = \sqrt{\frac{E_n}{m\omega^2}}} .$$

The expectation value $\langle n|\hat{p}^2|n\rangle$ can also be calculated in a similar manner.

$$\langle p^2\rangle = \langle n|\hat{p}^2|n\rangle$$

$$= -\frac{m\hbar\omega}{2}\langle n|(\hat{a}-\hat{a}^+)(\hat{a}-\hat{a}^+)|n\rangle$$

$$= -\frac{m\hbar\omega}{2}\Big(\langle n|\hat{a}\hat{a}|n\rangle - \langle n|\hat{a}\hat{a}^+|n\rangle - \langle n|\hat{a}^+\hat{a}|n\rangle + \langle n|\hat{a}^+\hat{a}^+|n\rangle\Big)$$

$$= -\frac{m\hbar\omega}{2}\big(0 - (n+1) - n + 0\big)$$

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

$$= m\left(n+\tfrac{1}{2}\right)\hbar\omega$$

$$= mE_n$$

$$\therefore \Delta p = \sqrt{mE_n}.$$

The uncertainty product is

$$\Delta x\,\Delta p = \sqrt{\frac{E_n}{m\omega^2}\cdot E_n m} = \frac{E_n}{\omega} = \left(n+\tfrac{1}{2}\right)\hbar$$

$$\boxed{\Delta x\,\Delta p = \left(n+\tfrac{1}{2}\right)\hbar}$$

For the ground state, $n=0$, and the uncertainty product is minimum.

Ex Show that in a one-dimensional bound state problem, the energy spectrum of the bound states is always non-degenerate.

Ans Suppose the contrary is true. Let us assume that there are two linearly independent eigenvectors with wave functions $\psi_1(x)$ and $\psi_2(x)$ corresponding to a particular eigenvalue E of the Hamiltonian. The wave functions $\psi_1(x)$ and $\psi_2(x)$ satisfy the following differential equations:

$$\psi_1''(x) + \frac{2m}{\hbar^2}\left[E - V(x)\right]\psi_1(x) = 0 \quad \text{--- (1)}$$

$$\psi_2''(x) + \frac{2m}{\hbar^2}\left[E - V(x)\right]\psi_2(x) = 0, \quad \text{--- (2)}$$

i.e., they satisfy the same differential equation. For bound states E is -ve, and more importantly for the present problem, $\psi_1(x)$ and $\psi_2(x)$ must tend to zero as $x \to \pm\infty$.

Now, from Eqs. (1) and (2) we find

$$\frac{\psi_1''}{\psi_1} = \frac{\psi_2''}{\psi_2} = \frac{2m}{\hbar^2}\left[-E + V(x)\right]$$

$$\therefore \quad \psi_1''\psi_2 - \psi_1\psi_2'' = 0$$

or $$(\psi_1'\psi_2)' - (\psi_2'\psi_1)' = 0$$

Integrating

$$\psi_1'\psi_2 - \psi_2'\psi_1 = \text{constant.} \qquad \text{------ (3)}$$

This equation holds for all x including $x \to \pm\infty$.

Now

$$\psi_1(x),\ \psi_2(x) \longrightarrow 0 \quad \text{as} \quad x \to \pm\infty .$$

Therefore

$$\text{Constant} = 0$$

Hence

$$\psi_1'\psi_2 - \psi_2'\psi_1 = 0$$

or $$\frac{\psi_1'}{\psi_1} = \frac{\psi_2'}{\psi_2}$$

or $$\ln \psi_1 = \ln \psi_2 + \ln C$$

or $$\psi_1 = C\psi_2$$

i.e., the two states are linearly dependent contrary to our assumption.