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Paper No. : Quantum Mechanics-I
Module : Linear Harmonic Oscillator (Operator Method)

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Description of Module	
Subject Name	Physics
Paper Name	Quantum Mechanics-I
Module Name/Title	Linear Harmonic Oscillator (Operator Method)
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Contents of this Unit

Learning Outcomes

After studying this module, you shall be able to

- Know the important role the study of harmonic oscillator plays in diverse areas in physics
- Learn some general properties from the given form of the harmonic oscillator potential
- Learn to write the Hamiltonian in the operator form (raising and lowering operators) and to deduce the expression for the energy spectrum
- Learn to deduce the expression for the energy eigen-states of the Hamiltonian
- Show how this representation of the states can be expressed in terms of Hermite polynomials

1.Introduction

The study of the quantum mechanical properties of linear harmonic oscillator assumes its importance from the fact that it provides the basis to analyze a wide variety of physical phenomena such as the vibrations of the atoms of a molecule about their equilibrium positions, the oscillations of atoms or ions of a crystalline lattice etc. In the first module we saw that it was the study of the behavior of these oscillators at thermal equilibrium (black body radiation), which led Planck to introduce the hypothesis of quantization of energy. Whenever one has to study the behavior of a physical system in the neighborhood of a stable equilibrium position, one has to deal with the equations which, in the limit of small oscillations, are those of a harmonic oscillator In your undergraduate course on quantum mechanics you must have studied the problem of linear harmonic oscillator by solving the time independent Schrodinger's second order differential equation.

2. The Linear Harmonic Oscillator

2.1. General Properties of a Linear Harmonic Oscillator

Let us start by recapitulating some important properties of a simple harmonic oscillator. Classically, the dynamical equation which governs the motion of a harmonic oscillator is

$$m\frac{d^2x}{dt^2} = -\frac{dV}{dx} = -k\,x \qquad (17.1)$$

and the solution of this equation is given by $x = a\cos(\omega t - \varphi)$, where a denotes the amplitude and $\omega = \sqrt{k/m}$ is the angular frequency of the vibrating particle.

The kinetic energy of this particle,

$$K = \frac{1}{2}m\left(\frac{dx}{dt}\right)^2 = \frac{p^2}{2m}$$

and the total energy is

$$E = K + V = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 . \qquad (17.2)$$

In quantum mechanics, the classical quantities x and p are replaced by the corresponding operators in terms of which the Hamiltonian operator of the system is expressed as

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \tag{17.3}$$

For a time-independent Hamiltonian representing a conservative system, we have the eigenvalue equation:

$$\hat{H}|\phi\rangle = E|\phi\rangle . \tag{17.4}$$

When expressed in the {|x>} representation, this equation is written as:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2\hat{x}^2\right]\phi(x) = E\,\phi(x) \tag{17.5}$$

This is the second order differential equation, which you must have studied and solved to get the solutions for the eigenvalues and Eigen fnctions of the oscillator. Here we mention only the following general properties that can be deduced based on the form of the harmonic oscillator potential, $V(x) = kx^2$.

2.2 Eigenvalues of the Hamiltonian (Operator Method)

We have studied in the preceding module that there are many representations, connected by unitary transformations, in which the wave functions and operators can appear in quantum mechanics. In Dirac's formulation of quantum theory, the central role is played by the commutation relations between linear Hermitian operators, corresponding to the dynamical variables. Here we shall use Dirac's method which essentially consists in finding suitable operators with which one can generate all the eigen vectors of the Hamiltonian without making reference to any particular representation.

Corresponding to the Hamiltonian given by Eq.(17.3), let us introduce the operators

$$\hat{a}_{\pm} = \frac{1}{\sqrt{2m\hbar\omega}}\left[m\omega\hat{x} \mp i\,\hat{p}\right] \tag{17.6}$$

Since $\hat{x}$ *and* $\hat{p}$ are Hermitian operators, $\hat{a}_+$ *and* $\hat{a}_-$ are adjoints of each other, i.e., $\hat{a}_+ = \hat{a}_-^+$ and $\hat{a}_- = \hat{a}_+^+$. Using the commutation relation, $[\hat{x},\ \hat{p}] = i\hbar$, one can easily verify that $\hat{a}_+$ *and* $\hat{a}_-$ satisfy the commutation relation

$$[\hat{a}_+, \hat{a}_-] = \hat{1} \tag{17.7}$$

Also writing the operators $\hat{x}$ *and* $\hat{p}$ in terms of $\hat{a}_+$ *and* $\hat{a}_-$, using Eq.(17.6), we get

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\ [\hat{a}_{+} + \hat{a}_{-}] \qquad (17.8a)$$

$$\hat{p} = \frac{1}{2i}\sqrt{2m\hbar\omega}\ (\hat{a}_{-} - \hat{a}_{+}) \qquad (17.8b)$$

Substituting these expressions for $\hat{x}$ *and* $\hat{p}$ in Eq.(17.3) for the Hamiltonian, one can easily show that

$$\hat{H} = \frac{\hbar\omega}{2}(\hat{a}_{-}\hat{a}_{+} + \hat{a}_{+}\hat{a}_{-}) = \hbar\omega\ (\hat{a}_{-}\hat{a}_{+} - \frac{1}{2}) = \hbar\omega\ (\hat{a}_{+}\hat{a}_{-} + \frac{1}{2})$$
$$= \hbar\omega\ (\hat{N} + \frac{1}{2}) \qquad (17.9)$$

where $\hat{N} = \hat{a}_{+}\hat{a}_{-}$. (17.10)

In expressing the Hamiltoian, Eq,(17.9), in alternative forms we make use of the commutation relation, Eq.(17.7). Note that the adjoint of the operator $\hat{N}$, i.e.,

$$\hat{N}^{+} = (\hat{a}_{-})^{+}(\hat{a}_{+})^{+} = \hat{a}_{+}\hat{a}_{-} = \hat{N} \qquad (17.11)$$

showing that it is Hermitian. In fact, by relating the Hamiltonian to **the number operator** $\hat{N}$ through Eq.(17.9), the problem of determining the eigenvalues and eigenvectors of the Hamiltonian is essentially reduced to the problem of finding the eigenvalues and eigenvectors of the operator $\hat{N}$.

Let us calculate the commutator of $\hat{N}$ with $\hat{a}_{+}$ *and* $\hat{a}_{-}$:

$$[\hat{N},\hat{a}_{-}] = [\hat{a}_{+}\hat{a}_{-},\hat{a}_{-}] = \hat{a}_{+}[\hat{a}_{-},\hat{a}_{-}] + [\hat{a}_{+},\hat{a}_{-}]\hat{a}_{-} = -\hat{a}_{-} \qquad (17.12)$$

Similarly,

$$[\hat{N},\hat{a}_{+}] = [\hat{a}_{+}\hat{a}_{-},\hat{a}_{+}] = \hat{a}_{+}[\hat{a}_{-},\hat{a}_{+}] + [\hat{a}_{+},\hat{a}_{+}]\hat{a}_{-} = \hat{a}_{+} \qquad (17.13)$$

In simplifying the commutators in Eqs. (17.12) and (17.13) we use the commutator, Eq.(17.7) and the relations $[\hat{a}_{-},\hat{a}_{-}] = [\hat{a}_{+},\hat{a}_{+}] = 0$.

Let the ket $|\phi_n\rangle$ represent a normalized eigenvector of $\hat{N}$ belonging to the eigenvalue n, i.e.,

$$\hat{N}|\phi_n\rangle = n|\phi_n\rangle \tag{17.14}$$

Now using Eq.(17.12), we get

$$[\hat{N}, \hat{a}_-]|\phi_n\rangle = -\hat{a}_-|\phi_n\rangle$$
$$\hat{N}\,\hat{a}_-|\phi_n\rangle = \hat{a}_-\hat{N}|\phi_n\rangle - \hat{a}_-|\phi_n\rangle = (n-1)\,\hat{a}_-|\phi_n\rangle, \tag{17.15}$$

which shows that $\hat{a}_-|\phi_n\rangle$ is an eigenvector of $\hat{N}$ belonging to the eigenvalue (n-1). In the same way, $\hat{a}_-^2|\phi_n\rangle$ can be shown to be an eigenvector of $\hat{N}$ having the eigenvalue (n-2). In general, $(\hat{a})_-^r|\phi_n\rangle$ is an eigenvector of $\hat{N}$ with eigenvalue (n-r). Also note that the eigenvalue

$$n = \langle\phi_n|\hat{N}|\phi_n\rangle = \langle\phi_n|\hat{a}_+\hat{a}_-|\phi_n\rangle$$
$$= \|\hat{a}_-|\phi_n\rangle\|^2 \geq 0, \tag{17.16}$$

as the norm of a vector is always positive definite. In this case,($\hat{a}_-|\phi_n\rangle$) can not be negative. Thus it follows that the series

$$|\phi_n\rangle, \hat{a}_-|\phi_n\rangle, (\hat{a}_-)^2|\phi_n\rangle, \ldots\ldots\ldots\ldots\ldots\ldots, (\hat{a}_-)^r|\phi_n\rangle, \ldots\ldots \tag{17.17}$$

must terminate, as otherwise it would lead to a state for which $(\hat{a})_-^s|\phi_n\rangle$ would give the eigenvalue, (n-s), which is negative. As a general property of a linear harmonic oscillator having a potential V(x)$\geq \boldsymbol{V_0}$, we have also noted in the earlier subsection that the eigenvalues are always positive.

Let the last term in the series (9.17) generate the state $|\phi_0\rangle$ such that

$$\hat{a}_-|\phi_0\rangle = 0 \tag{17.18}$$

It, therefore, implies that states given in the series (9.17) correspond to the eigenvalues

n, (n-1), (n-2),……………,2, 1, 0. (17.19)

Similarly, starting from the commutation relation, Eq.(9.13), it is straight forward to show that

$$[\hat{N},\hat{a}_+]|\phi_n\rangle = \hat{a}_+|\phi_n\rangle$$
$$\hat{N}\hat{a}_+|\phi_n\rangle = \hat{a}_+\hat{N}|\phi_n\rangle + \hat{a}_+|\phi_n\rangle = (n+1)\hat{a}_+|\phi_n\rangle \tag{17.20}$$

In general,
$$\hat{N}(\hat{a}_+)^r|\phi_n\rangle = (n+r)(\hat{a}_+)^r|\phi_n\rangle \tag{17.21}$$

We thus have the series representing the states

$$\hat{a}_+|\phi_n\rangle,\ (\hat{a}_+)^2|\phi_n\rangle,\ldots\ldots\ldots\ldots\ldots\ldots\ldots,(\hat{a}_+)^r|\phi_n\rangle,\ldots\ldots \tag{17.22}$$

corresponding to the eigenvalues

(n + 1), (n + 2),……….,(n + r),…….+∞

Thus the eigenvalue spectrum of the operator $\hat{N}$ is given by

n = 0, 1, 2,…………..+∞

Referring back to the expression Eq.(9.9), for the Hamiltonian, $\hat{H} = (\hat{N} + \frac{1}{2})\hbar\omega$, and operating on the ket $|\phi_n\rangle$, we get

$$\hat{H}|\phi_n\rangle = \hbar\omega(\hat{N}+1/2)|\phi_n\rangle = \hbar\omega(n+1/2)|\phi_n\rangle = E_n|\phi_n\rangle, \tag{17.23}$$

where the energy eigenvalues**,**

$$E_n = (n+1/2)\hbar\omega\ \text{, n=0,1,2…..}\infty \tag{17.24}$$

2.2.1 Interpretation of the operators $\hat{a}_-$ and $\hat{a}_+$:

By now, it must be clear that if we start with an eigenstate $|\phi_n\rangle$ of $\hat{H}$ corresponding to the eigenvalue $E_n = (n+1/2)\hbar\omega$**,** application of the operator $\hat{a}_-$ gives an eigenvector associated with the eigenvalue $E_{n-1} = (n+1/2)\hbar\omega - \hbar\omega$, and similarly application of $\hat{a}_+$ gives the energy, $E_{n+1} = (n+1/2)\hbar\omega + \hbar\omega$.

For this reason the operator $\hat{a}_-$ is said to be a **lowering (or destruction) operator** and $\hat{a}_+$ is called a **raising (or construction) operator**.

2.3 Eigenstates of the Hamiltonian; the basis vectors $|\phi_n\rangle$:

The vector $|\phi_0\rangle$ associated with n=0 satisfies the property, Eq.(17.18),

$$\hat{a}_-|\phi_0\rangle = 0$$

Let us assume the state $|\phi_0\rangle$ to be normalized. Now the state $|\phi_1\rangle$, which corresponds to n=1, is proportional to $\hat{a}_+|\phi_0\rangle$. Writing

$$|\phi_1\rangle = c_1\,\hat{a}_+|\phi_0\rangle \qquad (17.25)$$

To determine c_1, we require the vector $|\phi_1\rangle$ to be normalized, so that

$$\langle\phi_1|\phi_1\rangle = |c_1|^2\langle\phi_0|\hat{a}_-\hat{a}_+|\phi_0\rangle = |c_1|^2\langle\phi_0|(\hat{a}_+\hat{a}_- + 1)|\phi_0\rangle \qquad (17.26)$$

Since $|\phi_0\rangle$ is a normalized eigenstate of $\hat{N} = \hat{a}_+\hat{a}_-$ with the eigenvalue zero, we get

$$\langle\phi_1|\phi_1\rangle = |c_1|^2 = 1 \qquad (17.27)$$

Choosing the phase of $|\phi_1\rangle$ relative to $|\phi_0\rangle$ such that c_1 is real and positive, we have c_1=1. As a result

$$|\phi_1\rangle = \hat{a}_+|\phi_0\rangle \qquad (17.28)$$

In a similar fashion, we can construct $|\phi_2\rangle$ from $|\phi_1\rangle$:

$$|\phi_2\rangle = c_2\,\hat{a}_+|\phi_1\rangle \qquad (17.29)$$

Requiring $|\phi_2\rangle$ to be normalized and choosing the phase such that c_2 is real and positive, we have:

$$\langle\phi_2|\phi_2\rangle = |c_2|^2\langle\phi_1|\hat{a}_-\hat{a}_+|\phi_1\rangle = |c_2|^2\langle\phi_1|(\hat{a}_+\hat{a}_- + 1)|\phi_1\rangle$$
$$= 2|c_2|^2 = 1 \qquad (17.30)$$

Thus
$$|\phi_2\rangle = \frac{1}{\sqrt{2}}\hat{a}_+|\phi_1\rangle = \frac{1}{\sqrt{2}}(\hat{a}_+)^2|\phi_0\rangle \qquad (17.31)$$

This procedure can be easily extended. Thus the normalized state vector $|\phi_n\rangle$ is obtained if we know the state $|\phi_{n-1}\rangle$ (which is normalized):

$$|\phi_n\rangle = c_n\,\hat{a}_+|\phi_{n-1}\rangle \qquad (17.32)$$

Since
$$\langle\phi_n|\phi_n\rangle = |c_n|^2\langle\phi_{n-1}|\hat{a}_-\hat{a}_+|\phi_{n-1}\rangle$$
$$= n\,|c_n|^2 = 1 \qquad (17.33)$$

We get
$$c_n = \frac{1}{\sqrt{n}}. \qquad (17.34)$$

We can thus obtain $|\phi_n\rangle$ in terms of $|\phi_0\rangle$ by successively relating the eigen vectors to the lower states, i.e.,

$$|\phi_n\rangle = \frac{1}{\sqrt{n}}\hat{a}_+|\phi_{n-1}\rangle = \frac{1}{\sqrt{n}}\frac{1}{\sqrt{n-1}}(\hat{a}_+)^2|\phi_{n-2}\rangle = \ldots\ldots\ldots$$
$$= \frac{1}{\sqrt{n}}\frac{1}{\sqrt{n-1}}\ldots\ldots\ldots\ldots\frac{1}{\sqrt{2}}(\hat{a}_+)^n|\phi_0\rangle$$
$$= \frac{1}{\sqrt{n!}}(\hat{a}_+)^n|\phi_0\rangle \qquad (17.35)$$

Since the Hamiltonian $\hat{H}$ is Hermitian, the set of eigen vectors $|\phi_n\rangle$ corresponding to n varying from 0 to $+\infty$ constitute a complete orthonormal set and thus defines a representation, called the occupation number representation. The operator $\hat{N}$ is diagonal in this representation.

$$\langle \phi_{n'} | \hat{N} | \phi_n \rangle = n\delta_{n,n'} \tag{17.36}$$

$$\hat{a}_-|\phi_n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}_-)(\hat{a}_+)^n|\phi_0\rangle = \frac{1}{\sqrt{n!}}(\hat{a}_-\hat{a}_+)(\hat{a}_+)^{n-1}|\phi_0\rangle$$
$$= \frac{1}{\sqrt{n!}}(\hat{a}_+\hat{a}_- + 1)(\hat{a}_+)^{n-1}|\phi_0\rangle = \frac{1}{\sqrt{n!}}(\hat{a}_+\hat{a}_- + 1)\sqrt{(n-1)!}|\phi_{n-1}\rangle$$
$$= \sqrt{n}|\phi_{n-1}\rangle$$

Also, (17.37)

So that $\langle \phi_{n'} | \hat{a}_- | \phi_n \rangle = \sqrt{n}\ \delta_{n',n-1}$ (17.38)

$$\hat{a}_+|\phi_n\rangle = \sqrt{(n+1)}|\phi_{n+1}\rangle$$

In a similar way, *and* $\langle \phi_{n'} | \hat{a}_+ | \phi_n \rangle = \sqrt{(n+1)}\,\delta_{n',n+1}$ (17.39)

2.3.1 Matrix Representation of the operators $(\hat{a}_-)$, $(\hat{a}_+)$ *and* $(\hat{N})$

The operators, $(\hat{a}_-)$, $(\hat{a}_+)$ *and* $(\hat{N})$ can thus be written in the matrix forms as:

$$(\hat{a}_-) = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0\ldots\ldots\ldots\ldots \\ 0 & 0 & \sqrt{2} & 0 & 0\ldots\ldots\ldots\ldots \\ 0 & 0 & 0 & \sqrt{3} & 0\ldots\ldots\ldots\ldots \\ 0 & 0 & 0 & 0 & \sqrt{4}\ldots\ldots\ldots\ldots \\ . & . & . & . & . \quad . \quad . \end{pmatrix} \qquad (\hat{a}_+) = \begin{pmatrix} 0 & 0 & 0 & 0\ldots\ldots\ldots\ldots \\ \sqrt{1} & 0 & 0 & 0\ldots\ldots\ldots\ldots \\ 0 & \sqrt{2} & 0 & 0\ldots\ldots\ldots\ldots \\ 0 & 0 & \sqrt{3} & 0\ldots\ldots\ldots\ldots \\ 0 & 0 & 0 & \sqrt{4}\ldots\ldots\ldots\ldots \\ . & . & . & . \quad \ldots\ldots\ldots\ldots \end{pmatrix} \tag{17.40}$$

$$(\hat{N}) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0\ldots\ldots\ldots\ldots \\ 0 & 1 & 0 & 0 & 0\ldots\ldots\ldots\ldots \\ 0 & 0 & 2 & 0 & 0\ldots\ldots\ldots\ldots \\ 0 & 0 & 0 & 3 & 0\ldots\ldots\ldots \\ 0 & 0 & 0 & 0 & 4\ldots\ldots\ldots\ldots \\ . & . & . & . & \end{pmatrix} \tag{17.41}$$

2.4 Wave functions associated with the stationary states

We now show how the linear harmonic oscillator eigenfunctions in the position representations can be obtained by using the operators $\hat{a}_+$ *and* $\hat{a}_-$.

According to Eq.(9.18), $\hat{a}_-|\phi_0\rangle = 0$

Using the definition of $\hat{a}_-$, cf., Eq.(9.6), we write

$$\frac{1}{\sqrt{2m\hbar\omega}}\left[m\omega\hat{x} + i\,\hat{p}\right]|\phi_0\rangle = 0$$

In the $\{|x\rangle\}$ representation, where $\phi_0(x) = \langle x|\phi_0\rangle$, the above equation is written as

$$\frac{1}{\sqrt{2m\hbar\omega}}\left[m\omega x + \hbar\frac{d}{dx}\right]\phi_0(x) = 0 \tag{17.42}$$

Or
$$\left(\frac{m\omega}{\hbar}x + \frac{d}{dx}\right)\phi_0(x) = 0 \tag{17.43}$$

Eq.(17.43) is the first order differential equation. Its general solution is

$$\begin{aligned}\phi_0(x) &= N_0 \exp\left(-\frac{m\omega}{2\hbar}x^2\right) \\ &= N_0 \exp\left(-\alpha^2 x^2/2\right)\end{aligned} \tag{17.44}$$

where the symbol $\alpha = \sqrt{m\omega/\hbar}$ *and* N_0 is a normalization constant chosen to be real and such that $\phi_0(x)$ is normalizd to unity :

$$N_0 = \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \tag{17.45}$$

The other eigenfunctions can be obtained by using the operator $\hat{a}_+$, given in Eq.(17.6):

$$\phi_n(x) = \langle x|\phi_n\rangle = \frac{1}{\sqrt{n!}}\langle x|(\hat{a}_+)^n|\phi_0\rangle$$

$$= \frac{1}{\sqrt{n!}}\frac{1}{\sqrt{2^n}}\left[\sqrt{\frac{m\omega}{\hbar}}x - \sqrt{\frac{\hbar}{m\omega}}\frac{d}{dx}\right]^n \phi_0(x) \quad , \qquad (17.46)$$

2.4.1 Identifying the eigenfunctions with Hermite polynomials

In order to identify that the eigenfunctions obtained in Eq.(17.46), are indeed related to the Hermite polynomials which we obtain by solving the second order differential equation for the linear harmonic oscillator, we have to go back to the representation of Hermite polynomials:

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

$$= \exp(\rho^2/2)\left[\rho - \frac{d}{d\rho}\right]^n \exp\left(-\rho^2/2\right) \qquad (17.47)$$

Now defining the variable, $\rho = \alpha x = \sqrt{\frac{m\omega}{\hbar}}\, x \quad so \quad that \quad \frac{d}{d\rho} = \sqrt{\frac{\hbar}{m\omega}}\frac{d}{dx}$ and writing the ground state $\phi_0(\rho) = N_0 \exp(-\rho^2/2) = \left(\frac{\alpha}{\sqrt{\pi}}\right)\exp(-\rho^2/2)$, we re-express Eq.(17.46) as

$$\phi_n(\rho) = \left(\frac{\alpha}{\sqrt{\pi}\, 2^n\, n!}\right)^{1/2} \exp(-\rho^2/2)\; H_n(\rho) \qquad (17.48)$$

This equation, which gives the normalized linear harmonic oscillator eigenfunctions, is identical to the one which one gets on solving the second order differential equation.

4. Summary

After studying this module you should be able to

- Explain the important role the study of harmonic oscillator plays in diverse areas in physics
- Learn some general properties from the given form of the harmonic oscillator potential
- Learn to write the Hamiltonian in the operator form (raising and lowering operators) and to deduce the expression for the energy spectrum

- Learn to deduce the expression for the energy eigen-states of the Hamiltonian
- Show how this representation of the states can be expressed in terms of Hermite polynomials