UNIT 12

SIMPLE HARMONIC OSCILLATOR-II

Structure

12.1 INTRODUCTION

In this unit we solve the Schrödinger equation for the simple harmonic oscillator (SHO) and determine explicitly the eigenvalues and eigenfunctions using the mathematical framework developed in Units 11 and 12. The results of this unit are not new to you, however the methods used here are different from you have studied in Unit 7. You will appreciate that the mathematics presented here is simpler to execute.

In Sec. 12.2 we write the stationary state Schrödinger equation and the raising and lowering operators that you have also studied in Unit 7. We determine the minimum energy of the system and the energy eigenvalues. We show that the expectation value of the energy is always positive. Finally we write the time dependent solution for the stationary state of the SHO. In Sec. 12.3 we explain why the raising and lowering operators are called the creation and annihilation operators and in Sec 12.4 we introduce the number operator. In Sec 12.5 we determine the energy eigenfunctions. In Sec 12.6 we calculate the uncertainty product, using the generalized uncertainty principle.

Expected Learning Outcomes

After studying this unit, you should be able to:

- write the simple harmonic oscillator Hamiltonian in terms of the raising and lowering operators;
- obtain the commutator relations for the raising and lowering operators;

- ❖ determine the minimum eigenenergy and the energy eigenvalues;
- ❖ determine the action of the raising and lowering operators on the energy eigenstates;
- ❖ derive expressions for the normalized simple harmonic oscillator eigenfunctions using the raising and lowering operators; and
- ❖ determine the uncertainty product for the simple harmonic oscillator using the generalized uncertainty principle.

12.2 SOLVING THE SIMPLE HARMONIC OSCILLATOR PROBLEM

The Hamiltonian operator for the simple harmonic oscillator is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \tag{12.1}$$

In Unit 7 you have written the Schrödinger equation of stationary states:

$$\left[-\frac{\hbar^2}{m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2\hat{x}^2\right]\psi_n(x) = E_n\psi_n(x) \tag{12.2}$$

where E_n is the eigenenergy and $\psi_n(x)$ the eigenfunction of the n^{th} energy eigenstate of the simple harmonic oscillator. This is in the position representation. In Dirac notation we can express this as:

$$\hat{H}|n\rangle = E_n|n\rangle \tag{12.3}$$

This equation is of general validity and does not confine itself to any specific representation. Thus it is unlike Eq. (12.2), which is specifically when the operators and states are represented in position representation.

Here $|n\rangle$ is the eigenket for the n^{th} eigenstate having the eigenvalue E_n. In Unit 7 we have also defined the operators $\hat{a}$ and $\hat{a}^\dagger$:

$$\hat{a} = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{x} + i\hat{p}); \hat{a}^\dagger = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{x} - i\hat{p}) \tag{12.4}$$

Expressing $\hat{x}$ and $\hat{p}$ in term of $\hat{a}$ and $\hat{a}^\dagger$ from Eq. (12.4) and substituting in Eq. (12.1), the Hamiltonian operator $\hat{H}$ can be expressed in terms of $\hat{a}$ and $\hat{a}^\dagger$ as:

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) \tag{12.5}$$

Since $[\hat{x},\hat{p}] = i\hbar$, using Eq. (12.4) we get the commutator of $\hat{a}$ and $\hat{a}^\dagger$ as:

$$[\hat{a},\hat{a}^\dagger] = 1 \tag{12.6}$$

The commutator of $\hat{H}$ with $\hat{a}$ is:

$$\left[\hat{H},\hat{a}\right] = \left[\hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right),\hat{a}\right] = \hbar\omega\left[\hat{a}^\dagger\hat{a},\hat{a}\right] + \hbar\omega\left[\frac{1}{2},\hat{a}\right] \tag{12.7}$$

Since $\left[\frac{1}{2},\hat{a}\right] = 0$ and $\left[\hat{a}^\dagger\hat{a},\hat{a}\right] = \hat{a}^\dagger[\hat{a},\hat{a}] + \left[\hat{a}^\dagger,\hat{a}\right]\hat{a} = -\hat{a}$, Eq. (12.7) reduces to

$$[\hat{H},\hat{a}] = -\hbar\omega\hat{a} \tag{12.8}$$

Similarly you can show that:

$$[\hat{H},\hat{a}^{\dagger}] = \hbar\omega\hat{a}^{\dagger} \qquad (12.9)$$

SAQ 1

Show that $[\hat{H},\hat{a}^{\dagger}] = \hbar\omega\hat{a}^{\dagger}$.

We now calculate the minimum possible value of the eigenenergy of the simple harmonic oscillator.

12.2.1 Minimum Eigen Energy

Let us now consider an arbitrary eigenket $|E\rangle$ of $\hat{H}$, corresponding to the eigenvalue E $\left(\hat{H}|E\rangle = E|E\rangle\right)$. Let us consider the action of $\hat{a}$ on $|E\rangle$ which gives a ket $|\alpha\rangle$

$$|\alpha\rangle = \hat{a}|E\rangle \qquad (12.10)$$

Taking adjoint we get

$$\langle\alpha| = \langle E|\hat{a}^{\dagger} \qquad (12.11)$$

Using Eqs. (12.10) and (12.11) we can write the inner product $\langle\alpha|\alpha\rangle$ as:

$$\langle\alpha|\alpha\rangle = \langle E|\hat{a}^{\dagger}\hat{a}|E\rangle \qquad (12.12)$$

From Eq. (12.5), $\hat{a}^{\dagger}\hat{a} = \frac{\hat{H}}{\hbar\omega} - \frac{1}{2}$ and Eq. (12.12) is now:

$$\langle\alpha|\alpha\rangle = \left\langle E\left|\frac{\hat{H}}{\hbar\omega} - \frac{1}{2}\right|E\right\rangle = \left(\frac{E}{\hbar\omega} - \frac{1}{2}\right)\langle E|E\rangle$$

$$\Rightarrow \qquad \hbar\omega\langle\alpha|\alpha\rangle = \left(E - \frac{\hbar\omega}{2}\right)\langle E|E\rangle \qquad (12.13)$$

You know that the norm of a state vector is always positive, so $\langle\alpha|\alpha\rangle$ and $\langle E|E\rangle$ are positive definite quantities. Therefore Eq. (12.13) also implies:

$$E - \frac{\hbar\omega}{2} \geq 0 \Rightarrow E \geq \frac{\hbar\omega}{2} \qquad (12.14)$$

Thus we see that the **minimum possible value of the eigen energy of a linear harmonic oscillator** is $\frac{\hbar\omega}{2}$. At this stage we still cannot say that the minimum energy is $\frac{1}{2}\hbar\omega$. We can only say that the minimum energy could be $\frac{1}{2}\hbar\omega$ or anything greater than this. Further we can also see that for $E = \frac{\hbar\omega}{2}$, $\langle\alpha|\alpha\rangle = 0$ and so

$$|\alpha\rangle = \hat{a}|E\rangle = 0 \qquad (12.15)$$

We can also say that (which will become clearer in the Sec. 12.2.4).

$$\hat{a}|E\rangle = 0 \text{ iff } E = \frac{\hbar\omega}{2} \qquad (12.16)$$

It can also be shown that the expectation value of the energy of the linear harmonic oscillator is always positive.

12.2.2 Expectation Value of the Hamiltonian Operator

Let us calculate the expectation value of $\hat{H}$ for the simple harmonic oscillator for any arbitrary state $|\psi\rangle$:

$$\langle\hat{H}\rangle = \langle\psi|\hat{H}|\psi\rangle = \left\langle\psi\left|\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2\right|\psi\right\rangle$$

$$= \frac{1}{2m}\langle\psi|\hat{p}^2|\psi\rangle + \frac{1}{2}m\omega^2\langle\psi|\hat{x}^2|\psi\rangle \qquad (12.17)$$

Let us define

$$|Q\rangle = \hat{x}|\psi\rangle \;;\; |P\rangle = \hat{p}|\psi\rangle \qquad (12.18)$$

Since $\hat{x}$ and $\hat{p}$ are Hermitian, we get

$$\langle Q| = \langle\psi|\hat{x}^\dagger = \langle\psi|\hat{x} \qquad (12.19a)$$

and $$\langle P| = \langle\psi|\hat{p}^\dagger = \langle\psi|\hat{p} \qquad (12.19b)$$

So $$\langle Q|Q\rangle = \langle\psi|\hat{x}^\dagger\hat{x}|\psi\rangle = \langle\psi|\hat{x}^2|\psi\rangle \qquad (12.20)$$

and $$\langle P|P\rangle = \langle\psi|\hat{p}^\dagger\hat{p}|\psi\rangle = \langle\psi|\hat{p}^2|\psi\rangle \qquad (12.21)$$

Since $\langle Q|Q\rangle \geq 0$ and $\langle P|P\rangle \geq 0$, substituting for $\langle\psi|\hat{p}^2|\psi\rangle$ and $\left\langle\psi\left|\hat{x}^2\right|\psi\right\rangle$ from Eq. (12.20) and (12.21) into Eq. (12.17) we get:

$$\langle\hat{H}\rangle = \frac{1}{2m}\langle P|P\rangle + \frac{1}{2}m\omega^2\langle Q|Q\rangle \geq 0 \qquad (12.22)$$

So the expectation value of the energy of a simple harmonic oscillator is always non-negative.

12.2.3 Energy Eigenvalues

From Eq. (12.8) we have

$$[\hat{H},\hat{a}] = -\hbar\omega\hat{a} \Rightarrow \hat{H}\hat{a} - \hat{a}\hat{H} = -\hbar\omega\hat{a} \Rightarrow \hat{H}\hat{a} = \hat{a}\hat{H} - \hbar\omega\hat{a} \qquad (12.23)$$

For the eigenket $|E\rangle$ of $\hat{H}$, corresponding to the eigenvalue E $\left(\hat{H}|E\rangle = E|E\rangle\right)$, using Eq. (12.23) we get

$$\hat{H}(\hat{a}|E\rangle) = \left(\hat{a}\hat{H} - \hbar\omega\hat{a}\right)E\rangle = \hat{a}\left(\hat{H}|E\rangle\right) - \hbar\omega(\hat{a}|E\rangle)$$

$$= (E - \hbar\omega)(\hat{a}|E\rangle) \qquad (12.24)$$

Recall that when you have an equation $\hat{A}|a\rangle = a|a\rangle, |a\rangle$ is an eigenket provided it is not a zero. Let us consider the case when $\hat{a}|E\rangle \neq 0$. In this case, for Eq. (12.24), we can draw the following conclusion:

1. If $|E\rangle$ is an eigenket, $\hat{a}|E\rangle$ is also an eigenket.
2. If $|E\rangle$ corresponds to the eigenvalue E, $\hat{a}|E\rangle$ corresponds to the eigenvalue $E - \hbar\omega$.

If however $E = E_0 = \frac{1}{2}\hbar\omega$ we necessarily should have $\hat{a}|E_0\rangle = 0$ as otherwise we will have states with energy less than $\frac{1}{2}\hbar\omega$, which is not possible as $\frac{1}{2}\hbar\omega$ is the lowest possible value of *E*.

Further, if $\hat{a}|E\rangle$ is an eigenket then $\hat{a}^2|E\rangle$ is also an eigenket corresponding to the eigenvalue $E - 2\hbar\omega$, provided $\hat{a}^2|E\rangle \neq 0$. To see this write the eigenket $(\hat{a}|E\rangle)$ as $|E'\rangle$ corresponding to the eigenvalue $E' = E - \hbar\omega$ $\left(\hat{H}|E'\rangle = E'|E'\rangle\right)$. Using Eq. (12.24) we can write

$$\hat{H}(\hat{a}^2|E\rangle) = \hat{H}(\hat{a}|E'\rangle) = (\hat{a}\hat{H} - \hbar\omega\hat{a})|E'\rangle$$
$$= (E' - \hbar\omega)(\hat{a}|E'\rangle) = (E - 2\hbar\omega)(\hat{a}^2|E\rangle) \qquad (12.25)$$

From Eq. (12.25) we can see that if $E' - \hbar\omega = E - 2\hbar\omega \neq \frac{\hbar\omega}{2}$ then $(\hat{a}^2|E\rangle)$ is an eigenket of $\hat{H}$ with the eigenvalue $(E - 2\hbar\omega)$. Thus both $E - \hbar\omega$ and $E - 2\hbar\omega$ are eigenvalues of $\hat{H}$. We can continue with this process and say that if $E \neq \frac{\hbar\omega}{2}$ is an eigenvalue of $\hat{H}$, $E - \hbar\omega, E - 2\hbar\omega, E - 3\hbar\omega, ..., E - n\hbar\omega$ are all eigenvalues of $\hat{H}$, right up until $E'' = E - n\hbar\omega = \frac{\hbar\omega}{2}$, because in that case $\hat{a}|E''\rangle = 0$. So the lowest possible energy eigenvalue of the simple harmonic oscillator is $\frac{\hbar\omega}{2}$ and the energy eigenvalues increase in units of $\hbar\omega$, so the possible energy eigenvalues are:

$$\frac{1}{2}\hbar\omega, \frac{3}{2}\hbar\omega, \frac{5}{2}\hbar\omega, \frac{7}{2}\hbar\omega, ..., \left(n + \frac{1}{2}\right)\hbar\omega, .. \qquad (12.26)$$

To show that these are the only possible eigenvalues, let us assume that $3\hbar\omega$ is an eigenvalue. Then we get that $2\hbar\omega, \hbar\omega, 0, -\hbar\omega, -2\hbar\omega$ are all eigenvalues since $\hat{a}|E\rangle$ is a null vector only for $E = \frac{\hbar\omega}{2}$. However this contradicts the result obtained in Sec. 12.2.2 that $E \geq \frac{\hbar\omega}{2}$. So the only possible eigenvalues are those in Eq. (12.26).

How many eigenvalues can you have for the simple harmonic oscillator? There can be an **infinite number of eigenvalues**. Let us see how.

From Eq. (12.9) we have:

$$[\hat{H}, \hat{a}^\dagger] = \hbar\omega\hat{a}^\dagger \Rightarrow \hat{H}\hat{a}^\dagger - \hat{a}^\dagger\hat{H} = \hbar\omega\hat{a}^\dagger \Rightarrow \hat{H}\hat{a}^\dagger = \hat{a}^\dagger\hat{H} + \hbar\omega\hat{a}^\dagger \qquad (12.27)$$

For the eigenket $|E\rangle$ of $\hat{H}$, corresponding to the eigenvalue E $\left(\hat{H}|E\rangle = E|E\rangle\right)$,

$$\hat{H}(\hat{a}^\dagger|E\rangle) = (\hat{a}^\dagger\hat{H} + \hbar\omega\hat{a}^\dagger)|E\rangle = \hat{a}^\dagger(\hat{H}|E\rangle) + \hbar\omega(\hat{a}^\dagger|E\rangle)$$
$$= E(\hat{a}^\dagger|E\rangle) + \hbar\omega(\hat{a}^\dagger|E\rangle) = (E + \hbar\omega)(\hat{a}^\dagger|E\rangle) \qquad (12.28)$$

So for every eigenket $|E\rangle$, $(\hat{a}^\dagger|E\rangle)$ is also an eigenket of the Hamiltonian with an eigenenergy $(E + \hbar\omega)$. Let us now check if $(\hat{a}^\dagger|E\rangle)$ can be a null vector.

Now $\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) \Rightarrow \hat{a}^\dagger\hat{a} = \frac{\hat{H}}{\hbar\omega} - \frac{1}{2}$ and since the commutator of $\hat{a}$ and $\hat{a}^\dagger$ is 1:

$$\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = 1 \Rightarrow \hat{a}\hat{a}^\dagger = \hat{a}^\dagger\hat{a} + 1 \Rightarrow \hat{a}\hat{a}^\dagger = \frac{\hat{H}}{\hbar\omega} + \frac{1}{2} \qquad (12.29)$$

And

$$\hat{a}\left(\hat{a}^\dagger|E\rangle\right) = \left(\frac{\hat{H}}{\hbar\omega} + \frac{1}{2}\right)|E\rangle$$

$$\Rightarrow \qquad \hat{a}\left(\hat{a}^\dagger|E\rangle\right) = \left(\frac{E}{\hbar\omega} + \frac{1}{2}\right)|E\rangle \Rightarrow \hbar\omega\hat{a}\left(\hat{a}^\dagger|E\rangle\right) = \left(E + \frac{\hbar\omega}{2}\right)|E\rangle \qquad (12.30)$$

If $\hat{a}^\dagger|E\rangle = 0$, we get in Eq.(12.30)

$$\left(E + \frac{\hbar\omega}{2}\right)|E\rangle = 0 \qquad (12.31)$$

Since $|E\rangle$ is not a null vector, for Eq. (12.31) to hold, $E = -\frac{\hbar\omega}{2}$, which is clearly a contradiction. Thus $\hat{a}^\dagger|E\rangle \neq 0$ and from Eq. (12.28), for every eigenvalue E, $E + \hbar\omega$ is also an eigenvalue. So the simple harmonic oscillator has an infinite number of energy eigenvalues. The energy eigenvalues are given by:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \quad \text{for } n = 0,1,2,3,... \qquad (12.32)$$

We will henceforth follow the nomenclature that the eigenket corresponding to $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$ is $|n\rangle$. The eigenkets form a bases for a denumerable infinite dimensional Hilbert space, since the energy eigenvalues are non-degenerate and the energy eigenkets are orthogonal, as $\hat{H}$ is Hermitian. We can always construct normalized eigenkets, which then satisfy the following orthonormality condition:

$$\langle n|m\rangle = \delta_{nm} \qquad (12.33)$$

And we can write:

$$\sum_{n=0,1,2..} |n\rangle\langle n| = \hat{\mathbf{I}} \qquad (12.34)$$

The lowest possible energy is $\frac{\hbar\omega}{2}$, which is the ground state energy or the zero point energy. The ground state is labelled $|0\rangle$. Since $|0\rangle$ (corresponding to $E_n = \frac{1}{2}\hbar\omega$) is the ket with lowest energy, $\hat{a}|E\rangle = 0$ for $E = \frac{\hbar\omega}{2}$ and so we must have $\hat{a}|0\rangle = 0$. So

$$\hat{H}|0\rangle = \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2})|0\rangle = \frac{1}{2}\hbar\omega|0\rangle \qquad (12.35a)$$

And $$\hat{H}|n\rangle = E_n|n\rangle = \left(n + \frac{1}{2}\right)\hbar\omega|n\rangle \qquad (12.35b)$$

Since Hamiltonian is an observable, it eigenstates $|n\rangle$ from a complete set.

The general state of the simple harmonic oscillator can be written as a simple superposition of the eigenkets of $\hat{H}$:

$$|\psi\rangle = \sum_{n=0}^{\infty} c_n |n\rangle \tag{12.36}$$

12.2.4 Time Evolution of the State Vector

The time dependent Schrödinger equation for the simple harmonic oscillator is

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle = \left(\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2\right)|\psi(t)\rangle \tag{12.37}$$

Using Eq. (11.41) of Unit 11, we can write the general solution $|\psi(t)\rangle$ of this equation as: $|\psi(t)\rangle = e^{-\frac{i\hat{H}t}{\hbar}}|\psi(0)\rangle$. Since $|\psi(0)\rangle = \sum_n c_n(0)|n\rangle$, (where $c_n(0) = \langle n|\psi(0)\rangle$), we have:

$$|\psi(t)\rangle = \sum_{n=0,1,2..} \langle n|\psi(0)\rangle e^{-\frac{iE_n t}{\hbar}}|n\rangle$$

$$= \sum_{n=0,1,2..} a_n(0) e^{-i\omega\left(n+\frac{1}{2}\right)t}|n\rangle \tag{12.38}$$

12.3 CREATION AND ANNIHILATION OPERATORS

Using the notation introduced in Sec. 12.2.4, with $|E\rangle = |n\rangle$, we can write

$$\hat{H}(\hat{a}|n\rangle) = (E_n - \hbar\omega)(\hat{a}|n\rangle) = \left[\left(n+\frac{1}{2}\right)\hbar\omega - \hbar\omega\right](\hat{a}|n\rangle)$$

$$= \left[\left(n-\frac{1}{2}\right)\hbar\omega\right](\hat{a}|n\rangle) \tag{12.39}$$

Notice also that from Eq. (12.32) we can determine the energy eigenvalue of the $(n-1)^{th}$ state

$$\hat{H}|n-1\rangle = E_{n-1}|n-1\rangle = \left[\left(n-1+\frac{1}{2}\right)\hbar\omega\right]|n-1\rangle$$

$$= \left[\left(n-\frac{1}{2}\right)\hbar\omega\right]|n-1\rangle \tag{12.40a}$$

And: $$\hat{H}|n-1\rangle = (E_n - \hbar\omega)|n-1\rangle \tag{12.40b}$$

Comparing the RHS of Eqs. (12.39) and (12.40b), we can say that $(\hat{a}|n\rangle)$ is an eigenket of $\hat{H}$ with the energy eigenvalue corresponding to the eigenstate $|n-1\rangle$. This still does not fix the normalization as any multiple of an eigenstate, is also an eigenstate with the same eigenvalue. Therefore $\hat{a}|n\rangle$ has to be some multiple of $|n-1\rangle$, so let us say that:

$$\hat{a}|n\rangle = b_n|n-1\rangle \tag{12.41}$$

which implies:

$$\langle n|\hat{a}^{\dagger} = \langle n-1|b_n{}^* \tag{12.42}$$

Taking the inner product of $\langle n|\hat{a}^\dagger$ and $\hat{a}|n\rangle$ we get:

$$\langle n|\hat{a}^\dagger\hat{a}|n\rangle = \langle n-1|b_n^* b_n|n-1\rangle = b_n^* b_n\langle n-1|n-1\rangle$$

$$= b_n^* b_n = |b_n|^2 \qquad (12.43)$$

From Eq. (12.5) we have $\hat{a}^\dagger\hat{a} = \frac{\hat{H}}{\hbar\omega} - \frac{1}{2}$ and so:

$$\langle n|\hat{a}^\dagger\hat{a}|n\rangle = \left\langle n\left|\frac{\hat{H}}{\hbar\omega} - \frac{1}{2}\right|n\right\rangle = \left[\frac{1}{\hbar\omega}\left(n+\frac{1}{2}\right)\hbar\omega - \frac{1}{2}\right]\langle n|n\rangle = n \qquad (12.44)$$

Comparing Eqs. (12.43) and (12.44) we get

$$|b_n|^2 = n \Rightarrow b_n = \sqrt{n} \qquad (12.45)$$

Substituting for b_n from Eq. (12.45) into Eq. (12.41) we get:

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle \qquad (12.46)$$

Notes that there can always be a phase factor $e^{i\theta}$ multiplying the RHS of Eq.(12.46). Thus if $|n\rangle$ is normalized eigenket, then the normalized eigenket corresponding to $|n-1\rangle$ is $\sqrt{n}|n-1\rangle$.

The operator $\hat{a}$ is therefore called the **lowering** operator, the action of the operator $\hat{a}$ on an energy eigenstate $|n\rangle$ is to turn the state into another energy eigenstate, which has a lower energy, $|n-1\rangle$. Since $\hat{H}|n-1\rangle = (E_n - \hbar\omega)|n-1\rangle$, the energy is reduced by one quantum ($\hbar\omega$), so we can say that $\hat{a}$ effectively annihilates one quantum of energy. This is why $\hat{a}$ is also called the **annihilation** operator.

We can do a similar analysis for the operator $\hat{a}^\dagger$ and show that:

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \qquad (12.47)$$

Thus if $|n=0\rangle$ is the ground state, the normalised states are $|1\rangle, \sqrt{2}|2\rangle, \sqrt{6}|3\rangle, 2\sqrt{6}|4\rangle$, etc.

The operator $\hat{a}^\dagger$ is called the **raising** operator. The action of the $\hat{a}^\dagger$ on an energy eigenket $|n\rangle$ is to turn it into another energy eigenket which has a higher energy, $|n+1\rangle$. Since

$$\hat{H}|n+1\rangle = E_{n+1}|n+1\rangle = \left[\left(n+1+\frac{1}{2}\right)\hbar\omega\right]|n+1\rangle$$

$$= (E_n + \hbar\omega)|n+1\rangle \qquad (12.48)$$

Since the energy increases by one quantum ($\hbar\omega$), we can say $\hat{a}^\dagger$ effectively creates one quantum of energy, hence $\hat{a}^\dagger$ is also called the **creation** operator.

SAQ 2

Show that $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$.

12.4 THE NUMBER OPERATOR

We define $\hat{a}^\dagger\hat{a}$ as the number operator $\hat{N}$. Notice that from Eq. (12.5)

$$\hat{N}|n\rangle = \hat{a}^\dagger\hat{a}|n\rangle = \left(\frac{\hat{H}}{\hbar\omega} - \frac{1}{2}\right)|n\rangle = \left[\frac{1}{\hbar\omega}\left(n+\frac{1}{2}\right)\hbar\omega - \frac{1}{2}\right]|n\rangle \Rightarrow n|n\rangle \tag{12.49}$$

So the energy eigenkets are also eigenkets of $\hat{N}$, with eigenvalues 0,1,2,...,*n*,.... The Hamiltonian can be rewritten as:

$$\hat{H} = \hbar\omega\left(\hat{N} + \frac{1}{2}\right) \text{ with } \hat{H}|n\rangle = \hbar\omega\left(n+\frac{1}{2}\right)|n\rangle \tag{12.50}$$

And for any two eigenkets $|m\rangle$ and $|l\rangle$, we get

$$\langle m|\hat{N}|l\rangle = m\delta_{ml} \tag{12.51}$$

SAQ 3

Show that $\langle n|\hat{a}\hat{a}^\dagger|n\rangle = n+1$.

12.5 EIGENFUNCTIONS OF THE SIMPLE HARMONIC OSCILLATOR

We first determine the wave function for the ground state of the simple harmonic oscillator. For the ground state, we know that:

$$\hat{a}|0\rangle = 0 \Rightarrow \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{x} + i\hat{p})|0\rangle = 0 \tag{12.52}$$

Taking the inner product of $\hat{a}|0\rangle$ with $\langle x|$ we get:

$$\langle x|\hat{a}|0\rangle = 0 \Rightarrow \left\langle x\left|\left[\frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{x} + i\hat{p})\right]\right|0\right\rangle = 0 \tag{12.53}$$

which is

$$\sqrt{\frac{m\omega}{2\hbar}}\langle x|\hat{x}|0\rangle + \frac{i}{\sqrt{2m\omega\hbar}}\langle x|\hat{p}|0\rangle = 0 \tag{12.54}$$

Using $\langle x|\hat{x}|0\rangle = x\langle x|0\rangle$, $\langle x|\hat{p}|0\rangle = \left(-i\hbar\frac{d}{dx}\right)\langle x|0\rangle$ and $\psi_0(x) = \langle x|0\rangle$ (the eigenfunction for the ground state) we can write

$$\left[\sqrt{\frac{m\omega}{2\hbar}}\,x + \frac{i}{\sqrt{2m\omega\hbar}}\left(-i\hbar\frac{d}{dx}\right)\right]\psi_0(x) = 0 \tag{12.55}$$

And we get the following ODE

$$\left[\sqrt{\frac{m\omega}{2\hbar}}\,x + \sqrt{\frac{\hbar}{2m\omega}}\,\frac{d}{dx}\right]\psi_0(x) = 0 \tag{12.56}$$

which is

$$\frac{d}{dx}\psi_0(x) = -\left(\frac{m\omega}{\hbar}\right)x\psi_0(x) \tag{12.57}$$

Defining $a^2 = \frac{m\omega}{\hbar}$ as in Unit 7, Eq. (12.57) reduces to

$$\frac{d}{dx}\psi_0(x) = -a^2 x\psi_0(x) \tag{12.58}$$

With the solution

$$\psi_0(x) = A\exp\left(-\frac{a^2x^2}{2}\right) \tag{12.59}$$

Where A is a constant which can be determined upto a phase factor using the normalization condition $\int_{-\infty}^{\infty}\psi_0{}^*(x)\psi_0(x)dx = 1$. The normalized wavefunction, as you have determined in Unit 7 is:

$$\psi_0(x) = \left(\frac{a}{\sqrt{\pi}}\right)^{1/2}\exp\left(-\frac{a^2x^2}{2}\right) \tag{12.60}$$

Once again, as in Unit 7, defining $\xi = ax$, we can write:

$$\psi_0(x) = \left(\frac{a}{\sqrt{\pi}}\right)^{1/2}\exp\left(-\frac{\xi^2}{2}\right) \tag{12.61}$$

To derive the wave functions for the remaining eigenstates, we use Eq. (12.49)

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \Rightarrow |n+1\rangle = \frac{1}{\sqrt{n+1}}\left(\hat{a}^\dagger|n\rangle\right) \tag{12.62}$$

Therefore, for the first excited state of the simple harmonic oscillator we can write (with n = 0) and using the definition of $\hat{a}^\dagger$ from Eq. (12.4),

$$|1\rangle = \hat{a}^\dagger|0\rangle = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{x} - i\hat{p})|0\rangle \tag{12.63}$$

which can be written as:

$$\langle x|1\rangle = \left\langle x\left|\left[\frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{x} - i\hat{p})\right]\right|0\right\rangle \tag{12.64}$$

with $\psi_1(x) = \langle x|1\rangle$ being the eigenfunction for the first excited state of the simple harmonic oscillator. We get

$$\psi_1(x) = \left[\sqrt{\frac{m\omega}{2\hbar}}\,x - \sqrt{\frac{\hbar}{2m\omega}}\,\frac{d}{dx}\right]\psi_0(x) \tag{12.65}$$

Note that:

$$\frac{d}{dx}\psi_0(x) = \left(\frac{a}{\sqrt{\pi}}\right)^{1/2}\frac{d}{dx}\left[\exp\left(-\frac{a^2x^2}{2}\right)\right]$$

$$= \left(\frac{a}{\sqrt{\pi}}\right)^{1/2}\left(-a^2x\right)\exp\left(-\frac{a^2x^2}{2}\right) = \left(-a^2x\right)\psi_0(x) \tag{12.66}$$

Substituting for $\psi_0(x), \frac{d}{dx}\psi_0(x)$ and using $a^2 = \frac{m\omega}{\hbar}$ in Eq. (12.65), we get:

$$\psi_1(x) = \left[\sqrt{\frac{a^2}{2}}\, x - \sqrt{\frac{1}{2a^2}}\left(-a^2 x\right)\right]\psi_0(x)$$

$$= \left(\frac{a}{\sqrt{\pi}}\right)^{1/2}\left[\sqrt{\frac{1}{2}}\, a\, x + \sqrt{\frac{1}{2}}\, ax\right]\exp\left(-\frac{a^2x^2}{2}\right)$$

$$= \left(\frac{a}{2\sqrt{\pi}}\right)^{1/2} 2ax \exp\left(-\frac{a^2x^2}{2}\right) \qquad (12.67)$$

With $\xi = ax$, the wave function is just:

$$\psi_1(x) = \left(\frac{a}{2\sqrt{\pi}}\right)^{1/2} 2\xi \exp\left(-\frac{\xi^2}{2}\right) \qquad (12.68)$$

You can check for yourself that the wave function derived in Eq. (12.67) is normalized.

From Eq. (12.62) we get:

$$|n\rangle = \frac{1}{\sqrt{n}}\left(\hat{a}^\dagger |n-1\rangle\right) = \frac{1}{\sqrt{n(n-1)}}\left[\left(\hat{a}^\dagger\right)^2 |n-2\rangle\right]$$

$$= \frac{1}{\sqrt{n(n-1)(n-2)}}\left[\left(\hat{a}^\dagger\right)^3 |n-3\rangle\right] = .. \qquad (12.69)$$

Continuing in this fashion, we get

$$|n\rangle = \frac{1}{\sqrt{n!}}\left[\left(\hat{a}^\dagger\right)^n |0\rangle\right] \qquad (12.70)$$

And

$$|1\rangle = \left(\hat{a}^\dagger |0\rangle\right);\ |2\rangle = \frac{1}{\sqrt{2}}\left(\hat{a}^\dagger |1\rangle\right);.|3\rangle = \frac{1}{\sqrt{3}}\left(\hat{a}^\dagger |2\rangle\right)..... \qquad (12.71)$$

Eq. (12.71) is used to determine all the eigenfunctions for the simple harmonic oscillator.

SAQ 4

a) Show that for $\psi_1(x) = \left(\frac{a}{2\sqrt{\pi}}\right)^{1/2} 2\xi \exp\left(-\frac{\xi^2}{2}\right)$, $\int_{-\infty}^{\infty} \psi_1^*(x)\psi_1(x)dx = 1$.

b) Show that: $\psi_{n+1}(x) = \frac{1}{\sqrt{2(n+1)}}\left[\xi - \frac{d}{d\xi}\right]\psi_n(x)$.

12.6 UNCERTAINTY PRODUCT

We determine the uncertainty product $\Delta x \Delta p$ for the eigenket $|n\rangle$ of the simple harmonic oscillator. Following Eq. (11.7) of Unit 11, we can define the uncertainty as the root mean square deviation and so Δx and Δp can be written as:

$$\Delta x = \sqrt{\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2} \qquad (12.72a)$$

where

$$\langle \hat{x} \rangle = \langle n | \hat{x} | n \rangle; \langle \hat{x}^2 \rangle = \langle n | \hat{x}^2 | n \rangle \quad (12.72b)$$

Using the definition of the creation and annihilation operators in Eq.(12.4) we can write:

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^\dagger); \ \hat{p} = i\sqrt{\frac{\hbar m\omega}{2}} (\hat{a}^\dagger - \hat{a}) \quad (12.73)$$

So,

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

$$= \sqrt{\frac{\hbar}{2m\omega}} \left[\sqrt{n} \langle n | n-1 \rangle + \sqrt{n+1} \langle n | n+1 \rangle \right] = 0 \quad (12.74)$$

And,

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

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

$$= \frac{\hbar}{2m\omega} \left[\sqrt{n(n-1)} \langle n | n-2 \rangle + \sqrt{(n+1)(n+2)} \langle n | n+2 \rangle \right.$$

$$\left. + (n+1) \langle n | n \rangle + n \langle n | n \rangle \right]$$

$$= \frac{\hbar}{2m\omega} (2n+1) = \frac{\hbar}{m\omega} \left(n + \frac{1}{2} \right) \quad (12.75)$$

Similarly, it can be shown that (SAQ 5):

$$\langle \hat{p} \rangle = 0 \quad (12.76)$$

And $$\langle \hat{p}^2 \rangle = \hbar m\omega \left(n + \frac{1}{2} \right) \quad (12.77)$$

SAQ 5

Show that for the eigenket $|n\rangle$ of the simple harmonic oscillator $\langle \hat{p} \rangle = 0$ and $\langle \hat{p}^2 \rangle = \hbar m\omega \left(n + \frac{1}{2} \right)$.

Using Eqs. (12.74 to 12.77), the uncertainty in the observable *x* is:

$$\Delta x = \sqrt{\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2} = \sqrt{\frac{\hbar}{m\omega} \left(n + \frac{1}{2} \right) - 0} = \sqrt{\frac{\hbar}{m\omega} \left(n + \frac{1}{2} \right)} \quad (12.78)$$

And the uncertainty in the observable *p* is:

$$\Delta p = \sqrt{\langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2} = \sqrt{\hbar m\omega \left(n + \frac{1}{2} \right) - 0} = \sqrt{\hbar m\omega \left(n + \frac{1}{2} \right)} \quad (12.79)$$

The uncertainty product is:

$$\Delta x \Delta p = \left[\sqrt{\frac{\hbar}{m\omega} \left(n + \frac{1}{2} \right)} \right] \left[\sqrt{\hbar m\omega \left(n + \frac{1}{2} \right)} \right] = \hbar \left(n + \frac{1}{2} \right) \quad (12.80)$$

We can use the results derived in this section to, answer the following SAQ.

SAQ 6

Calculate the expectation value of $\hat{H}$ in the n^{th} eigenstate of the simple harmonic oscillator.

12.7 SUMMARY

- The Hamiltonian operator for the simple harmonic oscillator is $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$ can be written in terms of the ladder operators(Unit 7) $\hat{a}$ and $\hat{a}^\dagger$ given by

$$\hat{a} = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{x} + i\hat{p}); \quad \hat{a}^\dagger = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{x} - i\hat{p})$$

as $\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$. The stationary state Schrödinger equation is:

$$\hat{H}|n\rangle = E_n|n\rangle$$

$\hat{a}$ and $\hat{a}^\dagger$ satisfy the following commutator algebra:

$$[\hat{a},\hat{a}^\dagger] = 1; \quad [\hat{H},\hat{a}] = -\hbar\omega\hat{a}; [\hat{H},\hat{a}^\dagger] = \hbar\omega\hat{a}^\dagger$$

- The **minimum possible value of the eigenenergy *E* of a linear harmonic oscillator** is $\frac{\hbar\omega}{2}$ and $\hat{a}\left|E = \frac{\hbar\omega}{2}\right\rangle = 0$.
- The expectation value of $\hat{H}$ for the simple harmonic oscillator for any arbitrary state $|\psi\rangle$ is always greater than or equal to zero:

$$\langle\hat{H}\rangle = \left\langle\psi\left|\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2\right|\psi\right\rangle \geq 0$$

- If $|E\rangle$ is an eigenket of $\hat{H}$ with the energy eigenvalue E then
  - $\hat{a}|E\rangle$ is also an eigenket of $\hat{H}$ with the eigenenergy $(E - \hbar\omega)$, provided that $E \neq \frac{\hbar\omega}{2}$, because in that case $\hat{a}|E\rangle = 0$.
  - $\left(\hat{a}^\dagger|E\rangle\right)$ is also an eigenket of the Hamiltonian with an eigenenergy $(E + \hbar\omega)$.
- The energy eigenvalues of the simple harmonic oscillator are given by:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \quad \text{for } n = 0,1,2,3,...$$

There can be an **infinite number of eigenvalues**. The corresponding energy eigenkets are labelled by $|n\rangle$. The ground state is labelled by $|0\rangle$ which has the energy $\frac{\hbar\omega}{2}$.

- The eigenkets form a bases for a denumerable infinite dimensional Hilbert space.

The energy eigenvalues are non-degenerate and the energy eigenkets are orthogonal, since $\hat{H}$ is Hermitian.

We can always construct normalized eigenkets, which then satisfy orthonormality condition:

$$\langle n|m\rangle = \delta_{nm}$$

The Identity operator in this basis is

$$\sum_{n=0,1,2..} |n\rangle\langle n| = \hat{\mathbf{I}}.$$

A general state of the simple harmonic oscillator can be written as a simple superposition of the eigenkets of $\hat{H}$:

$$|\psi\rangle = \sum_{n=0,1,2..} c_n |n\rangle$$

- The general time dependent solution $|\psi(t)\rangle$ for the simple harmonic oscillator is:

$$|\psi(t)\rangle = \sum_{n=0,1,2..} \langle n|\psi(0)\rangle e^{-\frac{iE_n t}{\hbar}} |n\rangle$$

- For any eigenstate $|n\rangle$, $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$ and $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$. The operator $\hat{a}$ is called the **lowering or annihilation** operator, since the action of the operator $\hat{a}$ on an energy eigenstate $|n\rangle$ is to turn the state into another energy eigenstate with a lower energy, reducing the energy by one quantum $(\hbar\omega)$. The operator $\hat{a}^\dagger$ is called the **raising or creation** operator, the action of the $\hat{a}^\dagger$ on an energy eigenket $|n\rangle$ is to turn it into another energy eigenket which has a higher energy, $|n+1\rangle$ increasing the energy by one quantum.
- We define the number operator $\hat{N} = \hat{a}^\dagger\hat{a}$ and $\hat{N}|n\rangle = n|n\rangle$.
- The ground state wave function $\psi_0(x)$ is derived from the relation: $\hat{a}|0\rangle = 0$ by taking the inner product of $\hat{a}|0\rangle$ with $\langle x|$. The higher order eigenfunctions $\psi_0(x)$ are derived in the same way using the relation:

$$|n\rangle = \frac{1}{\sqrt{n!}}\left[\left(\hat{a}^\dagger\right)^n|0\rangle\right]$$

- The uncertainty product for the simple harmonic operator is:

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

12.8 TERMINAL QUESTIONS

1. Evaluate: i) $\langle m|\hat{x}|n\rangle$ ii) $\langle m|\hat{p}|n\rangle$.
2. Determine $\langle m|[\hat{x},\hat{p}]|n\rangle$.
3. Determine: i) $\langle m|\hat{x}^2|n\rangle$ ii) $\langle m|\hat{p}^2|n\rangle$.

4. Derive the wave functions $\psi_2(x)$ and $\psi_3(x)$ for the simple harmonic oscillator.

5. Derive the equations of motion for the operators $\hat{a}$ and $\hat{a}^\dagger$. Solve the equations to determine their time dependence.

6. Show that, for the function $f(\hat{a}^\dagger)$: $\hat{a}f(\hat{a}^\dagger)|0\rangle = \dfrac{df(\hat{a}^\dagger)}{d\hat{a}^\dagger}|0\rangle$.

7. An eigenstate $|A\rangle$ of the operator $\hat{a}$ defined by the relation: $\hat{a}|A\rangle = \alpha|A\rangle$, is called a coherent state of the simple harmonic oscillator. Show that $|A\rangle$ can be written as: $|A\rangle = N_0 e^{\alpha\hat{a}^\dagger}|0\rangle$ where $N_0 = e^{-\frac{|\alpha|^2}{2}}$. Show also that $\langle A|\hat{N}|A\rangle = \alpha^2$ where $\hat{N}$ is the number operator.

12.9 SOLUTIONS AND ANSWERS

Self-Assessment Questions

1. $$[\hat{H},\hat{a}^\dagger] = \left[\hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right),\hat{a}^\dagger\right] = \hbar\omega[\hat{a}^\dagger\hat{a},\hat{a}^\dagger] + \hbar\omega\left[\frac{1}{2},\hat{a}^\dagger\right]$$

$$[\frac{1}{2},\hat{a}^\dagger] = 0 \text{ and } [\hat{a}^\dagger\hat{a},\hat{a}^\dagger] = \hat{a}^\dagger[\hat{a},\hat{a}^\dagger] + [\hat{a}^\dagger,\hat{a}^\dagger]\hat{a} = \hat{a}^\dagger$$

Therefore $[\hat{H},\hat{a}^\dagger] = \hbar\omega\hat{a}^\dagger$

2. From Eq. (12.28)

$$\hat{H}(\hat{a}^\dagger|n\rangle) = (E_n + \hbar\omega)(\hat{a}^\dagger|n\rangle) = \left[\left(n + \frac{1}{2}\right)\hbar\omega + \hbar\omega\right](\hat{a}^\dagger|n\rangle)$$

$$= \left[\left(n + \frac{3}{2}\right)\hbar\omega\right](\hat{a}^\dagger|n\rangle) \qquad \text{(i)}$$

Notice also that from Eq. (12.35b) we can say

$$\hat{H}|n+1\rangle = \left[\left(n + 1 + \frac{1}{2}\right)\hbar\omega\right]|n+1\rangle = \left[\left(n + \frac{3}{2}\right)\hbar\omega\right]|n+1\rangle \qquad \text{(ii)}$$

Comparing Eqs. (i) and (ii) we can say that since $(\hat{a}^\dagger|n\rangle)$ is an eigenket of $\hat{H}$ with the eigen energy corresponding to the eigenstate $|n+1\rangle$, $\hat{a}^\dagger|n\rangle$ has to be some multiple of $|n+1\rangle$, so let us say that

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

which also gives us $\langle n|\hat{a} = \langle n+1|b_n{}^*$

Taking the inner product of $\langle n|\hat{a}$ and $\hat{a}^\dagger|n\rangle$ we get:

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

$$= b_n{}^* b_n = |b_n|^2 \qquad \text{(iii)}$$

From Eq. (12.5)

$$\hat{a}\hat{a}^\dagger|n\rangle = \left(\frac{\hat{H}}{\hbar\omega} + \frac{1}{2}\right)|n\rangle \Rightarrow \hat{a}\hat{a}^\dagger|n\rangle = (n+1)|n\rangle \qquad \text{(iv)}$$

And $$\left\langle n\middle|\hat{a}\hat{a}^\dagger\middle|n\right\rangle = (n+1)\langle n|n\rangle = (n+1) \qquad \text{(v)}$$

So from Eqs. (iii) and (v) we get $|b_n|^2 = n+1 \Rightarrow b_n = \sqrt{n+1}$.

And therefore: $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$

3. We know that $\left[\hat{a},\hat{a}^\dagger\right] = 1 \Rightarrow \hat{a}\hat{a}^\dagger = \hat{a}^\dagger\hat{a} + 1 = \hat{N} + 1$

$$\left\langle n\middle|\hat{a}\hat{a}^\dagger\middle|n\right\rangle = \left\langle n\middle|\hat{N}+1\middle|n\right\rangle = \left\langle n\middle|\hat{N}\middle|n\right\rangle + \langle n|n\rangle = n+1 \text{ (since } \langle n|n\rangle = 0)$$

4. a) $$I = \int_{-\infty}^{\infty} \psi_1^*(x)\psi_1(x)dx = \int_{-\infty}^{\infty} \left(\frac{a}{2\sqrt{\pi}}\right) 4\xi^2 e^{-\xi^2} dx, \text{ with } \xi = ax$$

$\because$ $d\xi = a\,dx$, we have

$$I = \frac{2a}{\sqrt{\pi}} \int_{-\infty}^{\infty} \xi^2 e^{-\xi^2}\left(\frac{d\xi}{a}\right) = \frac{2}{\sqrt{\pi}} \int_{-\infty}^{\infty} \xi^2 e^{-\xi^2} d\xi = \frac{2}{\sqrt{\pi}}\left(\frac{1}{2}\sqrt{\pi}\right) = 1$$

(using Integral 5 of Table 3.1)

b) From Eq. (12.69) $|n+1\rangle = \frac{1}{\sqrt{n+1}}\left(\hat{a}^\dagger|n\rangle\right)$

$\therefore$ $$\psi_{n+1}(x) = \frac{1}{\sqrt{n+1}}\left[\sqrt{\frac{m\omega}{2\hbar}}x - \sqrt{\frac{\hbar}{2m\omega}}\frac{d}{dx}\right]\psi_n(x) \qquad \text{(i)}$$

$$\xi = ax = \sqrt{\frac{m\omega}{\hbar}}x \qquad \text{(ii)}$$

$$\frac{d\psi_n}{dx} = \frac{d\psi_n}{d\xi}\frac{d\xi}{dx} = a\frac{d\psi_n}{d\xi} \qquad \text{(iii)}$$

Substituting from Eqs. (ii) and (iii) into Eq. (i) we get (with $\xi = ax$):

$$\psi_{n+1}(x) = \frac{1}{\sqrt{n+1}}\left[\frac{ax}{\sqrt{2}} - \frac{1}{a\sqrt{2}}\left(a\frac{d}{d\xi}\right)\right]\psi_n(x)$$

$$= \frac{1}{\sqrt{2(n+1)}}\left[\xi - \frac{d}{d\xi}\right]\psi_n(x) \qquad \text{(i)}$$

5. From Eq. (12.73) $\hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}\left(\hat{a}^\dagger - \hat{a}\right)$

$$\therefore \quad \langle n|\hat{p}|n\rangle = i\sqrt{\frac{\hbar m\omega}{2}}\left[\langle n|\hat{a}^\dagger|n\rangle - \langle n|\hat{a}|n\rangle\right]$$

$$= i\sqrt{\frac{\hbar m\omega}{2}}\left[\sqrt{n+1}\langle n|n+1\rangle - \sqrt{n}\langle n|n-1\rangle\right]$$

$$= 0 \ (\because \langle n|n+1\rangle = \langle n|n-1\rangle = 0)$$

$$\langle n|\hat{p}^2|n\rangle = -\frac{\hbar m\omega}{2}\left[\left\langle n\left|(\hat{a}^\dagger - \hat{a})^2\right|n\right\rangle\right]$$

$$= -\frac{\hbar m\omega}{2}\left[\left\langle n\left|\hat{a}^{\dagger 2}\right|n\right\rangle + \langle n|\hat{a}^2|n\rangle - \langle n|\hat{a}^\dagger\hat{a}|n\rangle - \langle n|\hat{a}\hat{a}^\dagger|n\rangle\right]$$

Since $\left\langle n\left|\hat{a}^{\dagger 2}\right|n\right\rangle = \langle n|\hat{a}^2|n\rangle = 0$

And $\langle n|\hat{a}\hat{a}^\dagger|n\rangle + \langle n|\hat{a}^\dagger\hat{a}|n\rangle = (2n+1)\langle n|n\rangle = 2n+1$

$$\therefore \quad \langle n|\hat{p}^2|n\rangle = -\frac{\hbar m\omega}{2}[-(2n+1)] = m\hbar\omega\left(n+\frac{1}{2}\right)$$

6. $$\langle\hat{H}\rangle = \langle n|\hat{H}|n\rangle = \left\langle n\left|\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2\right|n\right\rangle$$

$$= \frac{1}{2m}\langle n|\hat{p}^2|n\rangle + \frac{1}{2}m\omega^2\langle n|\hat{x}^2|n\rangle$$

Using the results of Sec. 12.6, we can write:

$$\langle\hat{H}\rangle = \frac{1}{2m}\left[\hbar m\omega\left(n+\frac{1}{2}\right)\right] + \frac{1}{2}m\omega^2\left[\frac{\hbar}{m\omega}\left(n+\frac{1}{2}\right)\right] = \hbar\omega\left(n+\frac{1}{2}\right)$$

Notice further that $\left\langle n\left|\frac{\hat{p}^2}{2m}\right|n\right\rangle = \left\langle n\left|\frac{1}{2}m\omega^2\hat{x}^2\right|n\right\rangle = \frac{\hbar\omega}{2}\left(n+\frac{1}{2}\right)$

Terminal Questions

1. i) $$\langle m|\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\langle m|(\hat{a}+\hat{a}^\dagger)|n\rangle$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left[\langle m|\hat{a}|n\rangle + \langle m|\hat{a}^\dagger|n\rangle\right]$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n}\langle m|n-1\rangle + \sqrt{n+1}\langle m|n+1\rangle\right]$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\,\delta_{m,n+1}\right]$$

ii) $\langle m|\hat{p}|n\rangle = i\sqrt{\frac{\hbar m\omega}{2}}\langle m|(\hat{a}^\dagger - \hat{a})|n\rangle$

$= i\sqrt{\frac{\hbar m\omega}{2}}[\langle m|\hat{a}^\dagger|n\rangle - \langle m|\hat{a}|n\rangle]$

$= i\sqrt{\frac{\hbar m\omega}{2}}[\sqrt{n+1}\,\delta_{m,n+1} - \sqrt{n}\,\delta_{m,n-1}]$

2. $[\hat{x},\hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x}$

$= i\sqrt{\frac{\hbar}{2m\omega}}\sqrt{\frac{\hbar m\omega}{2}}[(\hat{a}^\dagger + \hat{a})(\hat{a}^\dagger - \hat{a}) - (\hat{a}^\dagger - \hat{a})(\hat{a}^\dagger + \hat{a})]$

$= \frac{i\hbar}{2}[\hat{a}^{\dagger 2} - \hat{a}^2 + \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} - \hat{a}^{\dagger 2} + \hat{a}^2 - \hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger]$

$= \frac{i\hbar}{2}2[\hat{a},\hat{a}^\dagger] = i\hbar$

$\therefore \quad \langle m|[\hat{x},\hat{p}]|n\rangle = i\hbar\langle m|n\rangle = i\hbar\delta_{mn}$

3. i) $\langle \hat{x}^2\rangle = \left\langle m\left|\left[\sqrt{\frac{\hbar}{2m\omega}}(\hat{a}+\hat{a}^\dagger)\right]^2\right|n\right\rangle$

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

$= \frac{\hbar}{2m\omega}[\sqrt{n(n-1)}\langle m|n-2\rangle + \sqrt{(n+1)(n+2)}\langle m|n+2\rangle$

$+ (n+1)\langle m|n\rangle + n\langle m|n\rangle]$

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

$+ (n+1)\delta_{m,n} + n\langle m|n\rangle\delta_{m,n}]$

$= \frac{\hbar}{2m\omega}[\sqrt{n(n-1)}\delta_{m,n-2} + \sqrt{(n+1)(n+2)}\delta_{m,n+2} + (2n+1)\delta_{m,n}]$

ii) $\langle m|\hat{p}^2|n\rangle = -\frac{\hbar m\omega}{2}\left[\left\langle m\left|(\hat{a}^\dagger - \hat{a})^2\right|n\right\rangle\right]$

$= -\frac{\hbar m\omega}{2}\left[\left\langle m\left|\hat{a}^{\dagger 2}\right|n\right\rangle + \langle m|\hat{a}^2|n\rangle - \langle m|\hat{a}^\dagger\hat{a}|n\rangle - \langle m|\hat{a}\hat{a}^\dagger|n\rangle\right]$

$= -\frac{\hbar m\omega}{2}[\sqrt{(n+1)(n+2)}\langle m|n+2\rangle + \sqrt{n(n-1)}\langle m|n-2\rangle$

$- n\langle m|n\rangle - (n+1)\langle m|n\rangle]$

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

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

4. From SAQ 4b and Eq. (12.68)

$$\psi_2(x) = \frac{1}{\sqrt{2.2}}\left[\xi - \frac{d}{d\xi}\right]\psi_1(x) = \frac{1}{2}\left[\xi - \frac{d}{d\xi}\right]\left[\left(\frac{a}{2\sqrt{\pi}}\right)^{\frac{1}{2}} 2\xi\, e^{-\frac{\xi^2}{2}}\right]$$

$$= \left(\frac{a}{2\sqrt{\pi}}\right)^{\frac{1}{2}} \xi^2 e^{-\frac{\xi^2}{2}} - \left(\frac{a}{2\sqrt{\pi}}\right)^{\frac{1}{2}} \frac{d}{d\xi}\left(\xi e^{-\frac{\xi^2}{2}}\right)$$

$$= \left(\frac{a}{2\sqrt{\pi}}\right)^{\frac{1}{2}} \left[2\xi^2 - 1\right] e^{-\frac{\xi^2}{2}}$$

$$\psi_3(x) = \frac{1}{\sqrt{6}}\left(\xi - \frac{d}{d\xi}\right)\psi_2(x)$$

$$= \left(\frac{a}{2\sqrt{\pi}}\right)^{\frac{1}{2}} \frac{1}{\sqrt{6}}\left(\xi - \frac{d}{d\xi}\right)\left[\left(2\xi^2 - 1\right)e^{-\frac{\xi^2}{2}}\right]$$

$$= \left(\frac{a}{48\sqrt{\pi}}\right)^{\frac{1}{2}} \left[8\xi^3 - 12\xi\right] e^{-\frac{\xi^2}{2}}$$

5. From Eq. (11.59) of Unit 11: $i\hbar\frac{\partial \hat{a}}{\partial t} = \left[\hat{a}, \hat{H}\right]$; $\quad i\hbar\frac{\partial \hat{a}^\dagger}{\partial t} = \left[\hat{a}^\dagger, \hat{H}\right]$

With $\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$ we get,

$$i\hbar\frac{\partial}{\partial t}\hat{a} = \left[\hat{a}, \hat{a}^\dagger\hat{a} + \frac{1}{2}\right]\hbar\omega = \hbar\omega\left[\hat{a}, \hat{a}^\dagger\right]\hat{a}^\dagger + \hbar\omega\hat{a}^\dagger\left[\hat{a}, \hat{a}\right] = \hat{a}\,\hbar\omega$$

$$\Rightarrow \qquad \frac{d\hat{a}}{dt} = -i\hbar\omega\ \hat{a} \qquad \text{(i)}$$

Similarly: $i\hbar\frac{\partial \hat{a}^\dagger}{\partial t} = \hbar\omega\left[\hat{a}^\dagger, \hat{a}^\dagger\hat{a} + \frac{1}{2}\right] = \hbar\omega\left[\hat{a}^\dagger, \hat{a}^\dagger\right]\hat{a} + \hbar\omega\left[\hat{a}^\dagger, \hat{a}\right]\hat{a}^\dagger = -\hbar\omega\hat{a}^\dagger$

$$\Rightarrow \qquad \frac{d\hat{a}^\dagger}{dt} = i\hbar\omega\hat{a}^\dagger \qquad \text{(ii)}$$

Eqs. (i) and (ii) can be solved to get

$$\hat{a}(t) = e^{-i\hbar\omega t}\hat{a}(0) \quad ; \hat{a}^\dagger(t) = e^{i\hbar\omega t}\hat{a}^\dagger(0)$$

6. We can write the function $f(\hat{a}^\dagger)$ as

$$f(\hat{a}^\dagger) = \sum_n C_n(\hat{a}^\dagger)^n = C_0 + C_1\hat{a}^\dagger + C_2\hat{a}^{\dagger 2} + C_3\hat{a}^{\dagger 3} + \ldots$$

where $C_0, C_1, C_2 \ldots$ are arbitrary coefficients.

Now

$$\hat{a}(\hat{a}^\dagger)^n|0\rangle = \hat{a}\sqrt{n!}\,|n\rangle = \sqrt{n!}\,\hat{a}\,|n\rangle = \sqrt{n!}\sqrt{n}\,|n-1\rangle$$

$$= n\sqrt{(n-1)!}\,|n-1\rangle = n(\hat{a}^\dagger)^{n-1}|0\rangle$$

$$\therefore \qquad \hat{a}\,f(\hat{a}^\dagger)|0\rangle = \sum_n C_n\hat{a}(\hat{a}^\dagger)^n|0\rangle = \sum_n C_n n(\hat{a}^\dagger)^{n-1}|0\rangle = \frac{df(\hat{a}^\dagger)}{d\hat{a}^\dagger}|0\rangle$$

7. Using the results of TQ 6, we can write for a coherent state:

$$\hat{a}|A\rangle = \alpha|A\rangle \qquad \text{(i)}$$

$$|A\rangle = f(\hat{a}^\dagger)|0\rangle \qquad \text{(ii)}$$

Substituting from Eq. (ii) into Eq. (i) we get

$$\hat{a}f(\hat{a}^\dagger)|0\rangle = \alpha f(\hat{a}^\dagger)|0\rangle \Rightarrow \frac{df(\hat{a}^\dagger)}{d\hat{a}^\dagger}|0\rangle = \alpha f(\hat{a}^\dagger)|0\rangle \qquad \text{(iii)}$$

$$\Rightarrow \qquad \left[\frac{df(\hat{a}^\dagger)}{d\hat{a}^\dagger} - \alpha f(\hat{a}^\dagger)\right]|0\rangle = 0 \qquad \text{(iv)}$$

Solving the differential equation in the bracket we can write

$$f(\hat{a}^\dagger) = N_0\, e^{\alpha\hat{a}^\dagger} \qquad \text{(v)}$$

$$\therefore \qquad |A\rangle = N_0\, e^{\alpha\hat{a}^\dagger}\,|0\rangle \qquad \text{(vi)}$$

To determine N_0 we calculate the inner product $\langle A|A\rangle$. From (vi) we get

$$\langle A| = N_0^*\langle 0|e^{\alpha^*(\hat{a}^\dagger)^\dagger} = N_0^*\langle 0|e^{\alpha^*\hat{a}} \qquad \left(\because (\hat{a}^\dagger)^\dagger = \hat{a}\right) \qquad \text{(vii)}$$

$$\therefore \qquad \langle A|A\rangle = |N_0|^2 \left\langle 0\left| e^{\alpha^* \hat{a}} e^{\alpha \hat{a}^\dagger} \right| 0 \right\rangle \qquad \text{(viii)}$$

We can write:

$$e^{\alpha^* \hat{a}} = \sum_{m=0}^{\infty} \frac{(\alpha^* \hat{a})^m}{m!} \qquad \text{(ix)}$$

Now from TQ 6 , we know that

$$\hat{a} f(\hat{a}^\dagger)|0\rangle = \frac{df(\hat{a}^*)}{d\hat{a}^\dagger}|0\rangle \,;\; \hat{a}^2 f(\hat{a}^\dagger)|0\rangle = \frac{d^2}{d\hat{a}^{\dagger 2}}[f(\hat{a}^\dagger)]|0\rangle; \text{ and so on.}$$

Hence:

$$\hat{a}^m f(\hat{a}^\dagger)|0\rangle = \frac{d^m}{d\hat{a}^{\dagger m}} f(\hat{a}^\dagger)|0\rangle \qquad \text{(x)}$$

Taking $f(\hat{a}^\dagger) = e^{\alpha \hat{a}^\dagger}$ in Eq. (x) we get:

We can write

$$\hat{a}^m e^{\alpha \hat{a}^\dagger}|0\rangle = \left(\frac{d}{d\hat{a}^\dagger}\right)^m e^{\alpha \hat{a}^\dagger}|0\rangle \qquad \text{(xi)}$$

Using Eqs. (ix) and (xi) in Eq. (viii) we get:

$$\therefore \qquad e^{\alpha^* \hat{a}} e^{\alpha \hat{a}^\dagger}|0\rangle = \sum_{m=0}^{\infty} \frac{(\alpha^* \hat{a})^m}{m!} e^{\alpha \hat{a}^\dagger}|0\rangle$$

$$= \sum_{m=0}^{\infty} \frac{(\alpha^*)^m}{m!} \left(\frac{d}{d\hat{a}^\dagger}\right)^m e^{\alpha \hat{a}^\dagger}|0\rangle \qquad \text{(xii)}$$

Thus

$$\left\langle 0\left| e^{\alpha^* \hat{a}} e^{\alpha \hat{a}^\dagger} \right| 0 \right\rangle = \sum_{m=0}^{\infty} \frac{(\alpha^* \alpha)^m}{m!} \langle 0| e^{\alpha \hat{a}^\dagger}|0\rangle \qquad \text{(xiii)}$$

$$e^{\alpha \hat{a}^\dagger}|0\rangle = \sum_{n=0}^{\infty} \left\langle 0\left| \frac{(\alpha \hat{a}^\dagger)^n}{n!} \right| 0 \right\rangle$$

And

$$\langle 0| e^{\alpha \hat{a}^\dagger}|0\rangle = \sum_{n=0}^{\infty} \left\langle 0\left| I + (\alpha \hat{a}^\dagger) + \frac{(\alpha \hat{a}^\dagger)^2}{2!} + \ldots \right| 0 \right\rangle = I \qquad \text{(xiv)}$$

To obtain the results of Eq. (xiv) we have used Eq. (12.47):

$$\langle 0|I|0\rangle = I\langle 0|0\rangle = I \; ; \; \left\langle 0\left|\alpha\hat{a}^{\dagger}\right|0\right\rangle = \alpha\langle 0|1\rangle = 0 \; ;$$

$$\left\langle 0\left|\left(\alpha\hat{a}^{\dagger}\right)^2\right|0\right\rangle = \alpha^2\sqrt{2}\langle 0|2\rangle = 0 \; ; \text{ etc.}$$

Substituting in Eq. (xiii) we get

$$\left\langle 0\left|e^{\alpha^*\hat{a}}e^{\alpha\hat{a}^{\dagger}}\right|0\right\rangle = \sum_{m=0}^{\infty}\frac{\left(\alpha^*\alpha\right)^n}{m!} = e^{|\alpha|^2} \qquad \text{(xv)}$$

Therefore: $|N_0|^2 = e^{-|\alpha|^2} \Rightarrow No = e^{-|\alpha|^2/2}$

Also $\left\langle A\left|\hat{N}\right|A\right\rangle = \left\langle A\left|\hat{a}^{\dagger}\hat{a}\right|A\right\rangle$

So:

$\therefore$ $\left\langle A\left|\hat{N}\right|A\right\rangle = \alpha\alpha^* = |\alpha|^2 \qquad \left(\because \hat{a}|A\rangle = \alpha|A\rangle \; ; \langle A|a^{\dagger} = \alpha^*\langle A|\right)$