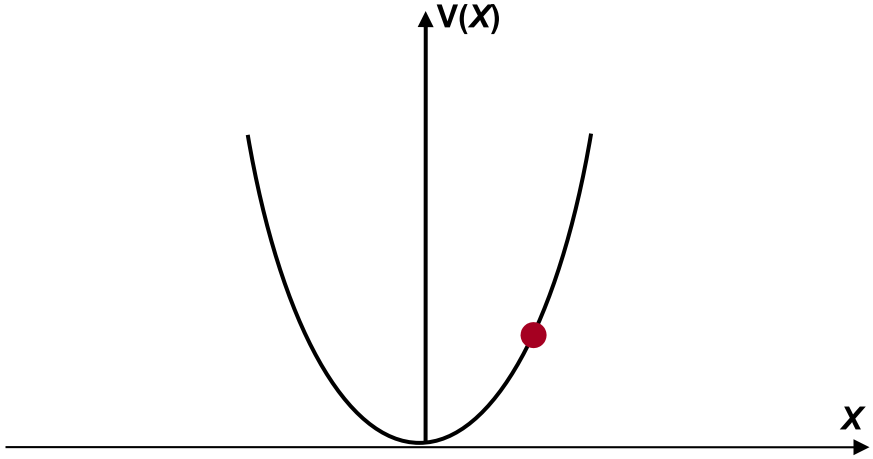
Chapter 4: Quantum Mechanics of a Simple Harmonic Oscillator

4.1 Quantum Mechanics of a Simple Harmonic Oscillator



Consider the Hamiltonian of a simple harmonic oscillator (a particle in a quadratic potential well),

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

Define normalized operators as,

$$\hat{p} = \frac{\hat{P}}{\sqrt{m}} \qquad \hat{x} = \sqrt{m}\hat{X} \qquad \left\{ [\hat{x},\hat{p}] = [\hat{X},\hat{P}] = i\hbar \right.$$

In terms of these operators, the Hamiltonian $\hat{H}$ becomes,

$$\hat{H} = \frac{\hat{p}^2}{2} + \frac{\omega_o^2 \hat{x}^2}{2}$$

In the Heisenberg picture, the equation for the momentum operators is,

$$\frac{d\hat{p}(t)}{dt} = \frac{-i}{\hbar}\left[\hat{p}(t),\hat{H}(t)\right] = -\omega_o^2\, \hat{x}(t)$$

and,

$$\frac{d\hat{x}(t)}{dt} = \frac{-i}{\hbar}\left[\hat{x}(t),\hat{H}(t)\right] = \hat{p}(t)$$

We can write these as,

$$\frac{d}{dt}\begin{bmatrix} \hat{p}(t) \\ \hat{x}(t) \end{bmatrix} = \begin{bmatrix} 0 & -\omega_o^2 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} \hat{p}(t) \\ \hat{x}(t) \end{bmatrix}$$

The matrix in the above equation has off-diagonal terms. We need to diagonalize it in order to solve it. The eigenvalues of the matrix are,

$$\lambda_1 = -i\omega_o$$

$$\lambda_2 = +i\omega_o$$

and the corresponding eigenvectors are,

$$v_1 \propto \begin{bmatrix} \omega_o \\ i \end{bmatrix} \quad \text{and } v_2 \propto \begin{bmatrix} \omega_o \\ -i \end{bmatrix}$$

We define a new operator $\hat{a}$ as proportional to the first eigenvector,

$$\hat{a} = \frac{1}{\sqrt{2\hbar\omega_o}}(\omega_o \hat{x} + i\hat{p})$$

The Heisenberg equation for $\hat{a}$ is,

$$\frac{d\hat{a}(t)}{dt} = \lambda_1 \hat{a}(t) = -i\omega_o \hat{a}(t)$$

The operator $\hat{a}$ is not Hermitian. The corresponding adjoint operator $\hat{a}^+$ is,

$$\hat{a}^+ = \frac{1}{\sqrt{2\hbar\omega_o}}(\omega_o \hat{x} - i\hat{p})$$

The adjoint operator is proportional to the second eigenvector of the matrix above. It follows that the Heisenberg equation for $\hat{a}^+$ is,

$$\frac{d\hat{a}^+(t)}{dt} = \lambda_2 \hat{a}^+(t) = i\omega_o \hat{a}^+(t)$$

4.1.1 Canonical Form of the Hamiltonian

Note that,

$$\hat{a}^+\hat{a} = \frac{1}{\sqrt{2\hbar\omega_o}}(\omega_o \hat{x} - i\hat{p})\frac{1}{\sqrt{2\hbar\omega_o}}(\omega_o \hat{x} + i\hat{p})$$

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

$$= \frac{1}{2\hbar\omega_o}\left(\omega_o^2 \hat{x}^2 + \hat{p}^2 - \hbar\omega_o\right)$$

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

$$\Rightarrow \frac{1}{2}\hat{p}^2 + \frac{1}{2}\omega_o^2 \hat{x}^2 = \hbar\omega_o\left(\hat{a}^+\hat{a} + \frac{1}{2}\right)$$

So the Hamiltonian $\hat{H}$ can be written as,

$$\hat{H} = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\omega_o^2 \hat{x}^2 = h\omega_o\left(\hat{a}^+\hat{a} + \frac{1}{2}\right)$$

4.1.2 Commutation Relations

The commutation relation between operators $\hat{a}$ and $\hat{a}^+$ can be found from those between $\hat{x}$ and $\hat{p}$,

$$\hat{a} = \frac{1}{\sqrt{2\hbar\omega_o}}(\omega_o \hat{x} + i\hat{p}) \qquad \hat{a}^+ = \frac{1}{\sqrt{2\hbar\omega_o}}(\omega_o \hat{x} - i\hat{p})$$

$$\left[\hat{a},\hat{a}^+\right] = \frac{1}{2\hbar\omega_0}\left(-i\omega_o[\hat{x},\hat{p}] + i\omega_o[\hat{p},\hat{x}]\right)$$

$$= 1$$

$$\left[\hat{a}\ ,\hat{a}\ \right] = \left[\hat{a}^+,\hat{a}^+\right] = 0$$

4.1.3 Time Dependence and Heisenberg Equations

The time evolution equation for the operator $\hat{a}$ can be found directly using the Heisenberg equation and the commutation relations found in Section 4.1.2. A useful identity to remember is,

$$\left[\hat{A},\hat{B}\hat{C}\right]=\left[\hat{A},\hat{B}\right]\hat{C}+\hat{B}\left[\hat{A},\hat{C}\right]$$

Using the identity above we get,

$$i\hbar\frac{d\hat{a}(t)}{dt}=\left[\hat{a}(t),\hat{H}(t)\right]=\left[\hat{a}(t),\hbar\omega_o\left(\hat{a}^+(t)\hat{a}(t)+\frac{1}{2}\right)\right]$$

$$=\hbar\omega_o\,\hat{a}(t)$$

$$\Rightarrow\frac{d\hat{a}(t)}{dt}=-i\omega_o\hat{a}(t)$$

$$\Rightarrow\hat{a}(t)\;=\hat{a}(t=0)e^{-i\omega_o t}=\hat{a}\;e^{-i\omega_o t}$$

Also,

$$\frac{d\hat{a}^+(t)}{dt}=-\frac{i}{\hbar}\left[\hat{a}^+(t),\hat{H}(t)\right]=i\omega_o\hat{a}^+(t)$$

$$\Rightarrow\hat{a}^+(t)\;=\hat{a}^+(t=0)\,e^{i\omega_o t}=\hat{a}^+\;e^{i\omega_o t}$$

4.1.4 Eigenvectors and Eigenvalues of the Hamiltonian

We need to find all the eigenvalues of the Hamiltonian,

$$\hat{H}=\hbar\omega_o\left(\hat{a}^+\hat{a}+\frac{1}{2}\right)$$

Consider the operator $\hat{a}^+\hat{a}$. Let,

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

Let $|\,\lambda\rangle$ be an eigenstate of $\hat{n}$ with eigenvalue λ.,

$$\hat{n}\,|\,\lambda\rangle=\lambda\,|\,\lambda\rangle$$

The operator $\hat{n}=\hat{a}^+\hat{a}$ is semi-positive definite which means it has eigenvalues that are all greater than or equal to zero. To see this consider the state,

$$\left|\psi\right\rangle=\hat{a}\,|\,\lambda\rangle$$

Since,

$$\left\langle\psi\middle|\psi\right\rangle\geq 0$$

we have,

$$\left\langle\lambda\right|\hat{a}^+\hat{a}\,|\,\lambda\rangle\geq 0$$

$$\Rightarrow\lambda\geq 0$$

Now consider the state $\hat{a}\left|\lambda\right\rangle$. The action of the operator $\hat{n}$ on this state is,

$$\hat{n}\left\{\hat{a}\left|\lambda\right\rangle\right\}=\hat{n}\hat{a}\left|\lambda\right\rangle=\left(\hat{a}\hat{n}+\left[\hat{n},\hat{a}\right]\right)\,\left|\lambda\right\rangle$$

$$=\left\{\hat{a}\hat{n}+\left[\hat{a}^+\hat{a},\hat{a}\right]\right\}\left|\lambda\right\rangle=(\hat{a}\hat{n}-\hat{a})\left|\lambda\right\rangle$$

$$=(\lambda-1)\hat{a}\left|\lambda\right\rangle$$

$$=(\lambda-1)\left\{\hat{a}\left|\lambda\right\rangle\right\}$$

Therefore, $\hat{a}\left|\lambda\right\rangle$ is an eigenstate of $\hat{n}$ with eigenvalue $(\lambda-1)$. Repeating the above procedure yields that $\hat{a}\left(\hat{a}\left|\lambda\right\rangle\right)$ is also an eigenstate of $\hat{n}$ with eiganvalve $(\lambda\,-\,2)$. Therefore, $\hat{a}^2\left|\lambda\right\rangle$ is an eigenvalue of $\hat{n}$

with eigenvalue $(\lambda-2)$. Similarly, it can be shown that $\hat{a}^m|\lambda\rangle$ is an eigenstate of $\hat{n}$ with eigenvalue $(\lambda-m)$.

Now consider that state $\hat{a}^+|\lambda\rangle$. We have,

$$\hat{n}\hat{a}^+|\lambda\rangle = \left(\hat{a}^+\hat{n} + \left[\hat{n},\hat{a}^+\right]\right)|\lambda\rangle$$
$$= \left(\hat{a}^+\lambda + \hat{a}^+\right)|\lambda\rangle$$
$$= (\lambda+1)\hat{a}^+|\lambda\rangle$$

Therefore, $\hat{a}^+|\lambda\rangle$ is an eigenstate of $\hat{n}$ with eigenvalue $(\lambda+1)$. Similarly, $(\hat{a}^+)^m|\lambda\rangle$ is also an eigenstate of $\hat{n}$ with eigenvalue $(\lambda+m)$.

In summary, starting from an arbitrary eigenstate $|\lambda\rangle$ of $\hat{n}$, with eigenvalue λ, we were able to generate eigenstates with eiganvalues greater than and less than λ by integers. If we keep doing this, then for some integer p, $\hat{a}^p|\lambda\rangle$ must be a state with eigenvalue $(\lambda-p)$ that is negative. This cannot happen because the operator $\hat{a}^+\hat{a}$ is positive semi-definite and must only have non-negative eigenvalues. So if $\hat{a}^{p-1}|\lambda\rangle$ is an eigenstate with the smallest non-negative eigenvalue $(\lambda-p+1)$, then the action of $\hat{a}$ on $\hat{a}^{p-1}|\lambda\rangle$ should not give a new eigenstate with eigenvalue $(\lambda-p)$. We enforce this condition by requiring that,

$$\hat{a}\left(\hat{a}^{p-1}|\lambda\rangle\right) = \hat{a}^p|\lambda\rangle = 0 .$$

But this implies that,

$$\hat{a}^+\hat{a}\left(\hat{a}^{p-1}|\lambda\rangle\right) = \hat{n}\,\hat{a}^{p-1}|\lambda\rangle = 0$$

But from the previous analysis we had reached the conclusion that $\hat{a}^{p-1}|\lambda\rangle$ is an eigenstate of $\hat{n}$ with a non-negative eigenvalue $(\lambda-p+1)$. The only way both these conclusions can be true is if $\lambda-p+1=0 \Rightarrow \lambda=p-1$. This means that λ is an integer and the smallest eigenvalue is zero. Therefore, all eigenvalues of the operator $\hat{n}$ are integers. This eigenstate of $\hat{n}$ with zero eigenvalue is denoted by $|0\rangle$.

It follows from the analysis above that $\hat{a}^+|0\rangle$ is an eigenstate of $\hat{n}$ with eigenvalue 1. And $(\hat{a}^+)^n|0\rangle$ is an eigenstate of $\hat{n}$ with eigenvalue n. Thus, starting from $|0\rangle$ and applying $\hat{a}^+$ operator we can generate all the eigenstates of $\hat{n}$ which will have integral eigenvalues. We label the eigenstate with eigenvalue n as $|n\rangle$. So,

$$\hat{n}|n\rangle = n|n\rangle .$$

Normalization of the Eigenstates: From previous analysis,

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

So $\hat{a}|n\rangle \propto |n-1\rangle$. We require that $|n\rangle$ be properly normalized, i.e. $\langle n\,|\,m\rangle = \delta_{n\,m}$. Suppose,

$$\hat{a}|n\rangle = c_n\,|n-1\rangle$$

then taking the inner product on both sides of the states with themselves we get,

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

$$\Rightarrow n = |c_n|^2$$

$$\Rightarrow |c_n| = \sqrt{n}$$

The phase of c_n is chosen by convention so that,

$$\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle$$

Similarly, since,

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

This implies, $\hat{a}^{+}|n\rangle \propto |n+1\rangle$. Let, $\hat{a}^{+}|n\rangle = b_n\,|n+1\rangle$. Then,

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

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

$$\Rightarrow n+1 = |b_n|^2$$

$$\Rightarrow |b_n| = \sqrt{n+1}$$

Again the phase of b_n is chosen by conversion so that,

$$\hat{a}^{+}|n+1\rangle = \sqrt{n+1}\,|n+1\rangle .$$

We can write all the eigenstates as follows,

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

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

$$\Rightarrow |3\rangle = \frac{\hat{a}^{+}}{\sqrt{3}}||2\rangle\rangle = \frac{(\hat{a}^{+})^2}{\sqrt{3.2.}}|2\rangle = \frac{(\hat{a}^{+})^3}{\sqrt{3!}}|0\rangle$$

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

Since the Hamiltonian is proportional to $\hat{n}$,

$$\hat{H} = \hbar\omega_o\left(\hat{n}+\frac{1}{2}\right)$$

the eigenstates of $\hat{n}$ are also the eigenstates of $\hat{H}$,

$$\hat{H}|n\rangle = \hbar\omega_o\left(\hat{n}+\frac{1}{2}\right)|n\rangle = \hbar\omega_o\left(n+\frac{1}{2}\right)$$

where, $n = 0, 1, 2......$ The eigenenergies are,

$$\frac{1}{2}\hbar\omega_o,\ \hbar\omega_o + \frac{1}{2}\hbar\omega_o,\ 2\hbar\omega_o + \frac{1}{2}\hbar\omega_o,\ ......$$

The lowest energy eigenstate $|0\rangle$ has energy equal to $\hbar\omega_o/2$.

Completeness Relation for the Eigenstates:

$$\sum_{n=0}^{\infty} |n\rangle\langle n| = \hat{1}$$

Orthogonalily Relation for the Eigenstates:

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

4.1.5 Creation and Destruction Operators

The operators $\hat{a}^{+}$ and $\hat{a}$ are called creation and destruction operators since they increase and decrease the energy of an eigenstate by $\hbar\omega_o$, respectively. The name "creation" and "destruction" comes from quantum electrodynamics where these operators create and destroy photons. The operator $\hat{n} = \hat{a}^{+}\hat{a}$ is called the number operator since it gives the number of energy quanta (of magnitude $\hbar\omega_o$) in an energy eigenstate above the lowest energy $\hbar\omega_o/2$. In quantum electrodynamics, the number operator gives the number of photons in a state.

4.1.6 Wavefunctions for the Eigenstates

The wavefunctions corresponding to the eigenstates can be obtained as follows. Consider the first the lowest energy state $|0\rangle$. The wavefunction is, $\psi_0(x) = \langle x|0\rangle$. We know that,

$$\hat{a}|0\rangle = 0$$

$$\Rightarrow \langle x|\hat{a}|0\rangle = 0$$

$$\Rightarrow \langle x|\frac{\omega_o\hat{x} + i\hat{p}}{\sqrt{2\hbar\omega_o}}|0\rangle = 0$$

$$\Rightarrow \left(\omega_o x + \hbar\frac{\partial}{\partial x}\right)\psi_0(x) = 0$$

The properly normalized solution to the above differential equation is,

$$\psi_0(x) = \left(\frac{\omega_o}{\pi\,\hbar}\right)^{\frac{1}{4}} e^{-\frac{x^2\omega_o}{2\,\hbar}}$$

The wavefunction for the state $|n\rangle$ can be obtained from $\psi_0(x)$ as follows,

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

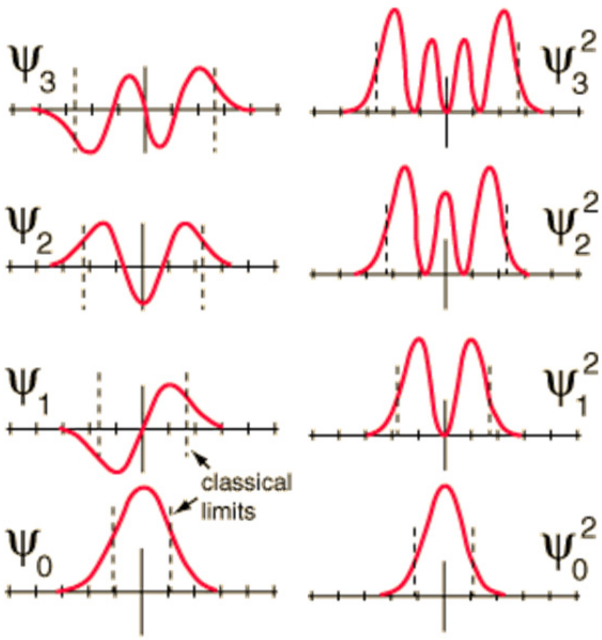
$$\Rightarrow \psi_n(x) = \langle x|n\rangle = \langle x|\frac{(\hat{a}^{+})^n}{\sqrt{n!}}|0\rangle$$

$$= \frac{1}{\sqrt{n!}}\left(\frac{\omega_o x - \hbar\frac{\partial}{\partial x}}{\sqrt{2\hbar\omega_o}}\right)^n \psi_0(x)$$

All the wavefunctions $\psi_n(x)$ belong to a set of functions called the Hermite Gaussians and can be written as,

$$\psi_n(x) = \left(\frac{\omega_o}{\pi \hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{\omega_o}{\hbar}}\, x\right) e^{-\frac{x^2 \omega_o}{2\hbar}}$$

where, H_n are Hermite polynomials. The first four Hermite Gaussians, along with their squared magnitudes, are sketched in the Figure below.



4.1.7 Two Independent Harmonic Oscillators

The Hamiltonian of two independent harmonic oscillators is

$$\hat{H} = \hat{H}_1 + \hat{H}_2 = \left\{\frac{\hat{p}_1^2}{2} + \frac{1}{2}\omega_1^2\,\hat{x}_1^2\right\} + \left\{\frac{\hat{p}_2^2}{2} + \frac{1}{2}\omega_2^2\,\hat{x}_2^2\right\}$$

which can also be written as,

$$\hat{H} = \hbar\omega_1\left[\hat{a}_1^+\hat{a}_1 + \frac{1}{2}\right] + \hbar\omega_2\left[\hat{a}_2^+\hat{a}_2 + \frac{1}{2}\right]$$

The eigenstates are of the form, $|\,n\rangle_1 \otimes |\,m\rangle_2$, and,

$$\hat{H}|\,n\rangle_1 \otimes |\,m\rangle_2 = \left[\hbar\omega_1\left(n + \frac{1}{2}\right) + \hbar\omega_2\left(m + \frac{1}{2}\right)\right]|\,n\rangle_1 \otimes |\,m\rangle_2$$

Note that a more formal expression would be,

$$\hat{H} = \hat{H}_1 + \hat{H}_2 = \hat{H}_1 \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{H}_2$$