21st Feb 2024

⊛ Dirac notation →

Dot or inner product between two wave functions ψ and ϕ :

$$(\phi, \psi) \equiv \langle \phi , \psi \rangle = \int^{L_2} \psi^* \psi \, dx$$

$\langle \phi | \cdot | \psi \rangle$

$\langle$ bra |(c)| ket $\rangle$

$\psi \rightarrow |\psi\rangle$ is called a ket state

Dual (conjugate) wave function

$\psi^* \rightarrow \langle \psi | \rightarrow$ bra state.

⊛ Eigenvalue eqn →

$$\boxed{\hat{O}\psi = \lambda\psi} \quad , \psi \rightarrow |\psi\rangle$$

↳ In dirac notation

↳ $\hat{O}|\psi\rangle = \lambda|\psi\rangle$

⊛ It is convenient to use the eigenvalue to denote the state.

$$\hat{O}|\lambda\rangle = \lambda|\lambda\rangle \quad \Big|\; |\psi\rangle \longrightarrow |\lambda\rangle$$

For e.g. : Two different states with different eigenvalues of the operator $\hat{O}$.

$$\hat{O}\,|\lambda_1\rangle = \lambda_1 |\lambda_1\rangle$$

$$\hat{O}\,|\lambda_2\rangle = \lambda_2 |\lambda_2\rangle$$

∘ Normalization →

Squared norm of $\psi = ||\psi||^2 = (\psi, \psi) = \int_{L_1}^{L_2} \psi^* \psi \, dx$

$= \langle \psi | \psi \rangle$

If ψ is normalized, then,

$$\langle \psi | \psi \rangle = 1 = ||\psi||^2$$

∘ Recasting quantum SHO in Dirac notation →

(*) The action of the operator $\hat{N}$, $\hat{a}$, $\hat{a}^\dagger$

$\hat{N} \psi = n \psi$

$\phi = \hat{a} \psi$

$\Rightarrow \hat{N} \phi = (n-1) \psi$

$\psi \to |n\rangle$

$\phi \to |n-1\rangle$

Complex no.

$\therefore \boxed{\hat{N} |n\rangle = n |n\rangle}$

operator   Element of vec space

(*) If $|n\rangle$ is normalized, ~~then,~~ i.e $\langle n|n\rangle = 1$,
then is the ket $|n-1\rangle = \hat{a} |n\rangle$

~~$\langle n-1 | an$~~, ~~$\langle n-1 | n-1 \rangle = \langle a n | a^\dagger a | n \rangle$~~

Sq norm of $|n-1\rangle$ →

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

$= (\langle n | \hat{a}^\dagger) (\hat{a} |n\rangle)$

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

$\Rightarrow \langle n-1|n-1\rangle = \langle n|\hat{N}|n\rangle = n\langle n|n\rangle = n$

$\rightarrow |n-1\rangle$ is not normalized.

$|n\rangle, |n-1\rangle$ should be normalized.

In general,

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

$$\therefore |c|^2\langle n-1|n-1\rangle = n$$

$$\Rightarrow \boxed{c=\sqrt{n}}$$

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

Now both are normalized.

⊛ Raising operator:

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

Now,

$$|c|^2\langle n+1|n+1\rangle$$

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

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

$$= \langle n|\{[\hat{a},\hat{a}^{+}]+\hat{N}\}|n\rangle$$

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

$$= (n+1)$$

$$\therefore \boxed{c=\sqrt{n+1}}$$

$$\Rightarrow \boxed{\hat{a}^{+} |n\rangle = \sqrt{n+1}\; |n+1\rangle}$$

So now, $\langle n+1 | n+1 \rangle = 1$

Hamiltonian of $\hat{H}$ →

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

$$\Rightarrow \hat{H}|n\rangle = \left(\hat{N} + \tfrac{1}{2}\mathbb{I}\right)\hbar\omega |n\rangle$$

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

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

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

$|n\rangle$ kets are also eigenstates of the Hamiltonian operator with eigenvalues,

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

What is the domain of n?

Inner product : $(\psi, \psi) \geq 0$

$$\langle \psi | \psi \rangle \geq 0 \quad \forall |\psi\rangle$$

$$\therefore |\psi\rangle = \hat{a}\,|n\rangle \Rightarrow \langle \psi | \psi \rangle = \langle n | \hat{a}^{+}\hat{a} | n \rangle$$

$$= n$$

Atleast $n \geq 0$ → a +ve real number.

23rd Feb 2024

1st Class → (Copied from Adrika)

$\hat{a}^{+}$ is a dual operator corresponding to $\hat{a}$.

n is such that $n \geq 0$, $n \in \mathbb{R}$

$$\Rightarrow \quad n \begin{cases} \to n \in \mathbb{Z} \\ \to n \notin \mathbb{Z} \end{cases}$$

Let us assume that n is not an integer.

Let there be a state $|\alpha\rangle$ where $0 < \alpha < 1$

⊛ Action of lowering operator on α →

$\hat{a}\,|\alpha\rangle \longrightarrow |x\rangle$ → should be a vector with norm-squared positive.

By construction →

$$|x\rangle = \sqrt{\alpha}\,|\alpha - 1\rangle$$

$$\hat{N}\,|\alpha-1\rangle = (\alpha-1)\,|\alpha-1\rangle$$

$$\hat{N}\,|x\rangle = \alpha\,\hat{N}\,|\alpha-1\rangle = (\alpha-1)\left(\sqrt{\alpha}\,|\alpha-1\rangle\right)$$

$$= (\alpha-1)\,|x\rangle$$

Say, we have $|m\rangle$

$$\hat{N}\,|m\rangle = m\,|m\rangle$$

Here, $m = (\alpha - 1)$, which is less than 0.

But we have established $m \geq 0$

Hence our assumption must be wrong.

$\therefore$ n must be ~~ans~~ an integer (By contradiction)

(*) In summary, we have established

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

where $\boxed{E_n = (n+\frac{1}{2})\hbar\omega}$

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

We have thus solved the SHO solutions without solving Schroedinger's equation..

We are also going to do this using SE, by using Hermite polynomials.

What happens if we chose 2?

$$\hat{a}|2\rangle = \sqrt{2}|1\rangle$$

$$\hat{a}|1\rangle = \sqrt{1}|0\rangle$$

What is $|0\rangle$? It is $|n=0\rangle$

$\Rightarrow$ It is not a null state.

$$\hat{H}|0\rangle = \frac{1}{2}\hbar\omega|0\rangle$$

$$E_0 = \frac{1}{2}\hbar\omega$$

$\Rightarrow$ Energy of QHO must be be $\geq \frac{1}{2}\hbar\omega$

Classically,

- Hamiltonian $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2$

Minimum energy $= 0$

But, $\hat{x}, \hat{p} \rightarrow$ cannot both be zero, otherwise we would have violated the uncertainty principle.

Zero-point energy $= \frac{1}{2}\hbar\omega$

Qualitatively, you cannot ever bring something to complete rest.

What happen to the state $|0\rangle$ if we act on it by $\hat{a}$?

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

for $n = 0$

$\hat{a}|0\rangle = \sqrt{0}\ |0-1\rangle = \phi \rightarrow$ null state.

Since $\sqrt{0}$ is $\mathbb{C}$.

Thus, we hit null state, we cannot go further down.

Lowering operator $\hat{a}$ annihilated the ground state

$\Rightarrow$ annihilation operator.

Raising operator $\rightarrow$

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

$n = 0$

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

Thus, we create a higher energy eigenstate starting from the null state (ground state, really).

2nd Class →

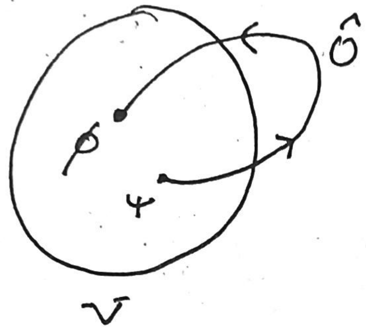
Recall: $\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right)$

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

$\lambda \xrightarrow{\text{Conjugate}} \lambda^{*}$ (for c-number)

$(x+iy) \xrightarrow{\text{Conjugate}} (x-iy)$

(*) Operator $\hat{O}$ is a map from a vector space V to itself.,
i.e $\forall$ ~~$\forall$~~ $\psi \in V$, $\psi \xrightarrow{\hat{O}} \phi = \hat{O}\psi$
and $\phi \in V$



$\{\psi\} \to$ domain of the operator.

(*) ~~Ag~~ <u>Adjoint of an operator</u> →
If given two operators say $\hat{A}$ and $\hat{B}$ satisfy

$$(\phi, \hat{A}\psi) = (\hat{B}\phi, \psi) \quad \forall\ \phi, \psi \in V,$$

then the operator $\hat{B}$ is called the Hermitian ~~co~~ conjugate or the adjoint of the operator $\hat{A}$.
$\hat{B}$ is often denoted as $\hat{A}^{+}$

Ex 1: By using the definition, find the ~~adjoint operator~~ action of the adjoint operator $\hat{O}$ on ψ if $\hat{O}\psi = \lambda\psi$, i.e., $\hat{O}^{+}\psi = ?$

Defn: $(\hat{O}^{+}\phi, \psi) = (\phi, \hat{O}\psi)$

Say, $\phi = \psi$ (arbitrary ϕ and ψ)

$\therefore$ ~~$(\hat{O}^{+}$~~

$\therefore (\hat{O}^{+}\psi = \psi) = (\psi, \hat{O}\psi)$

$$\Rightarrow \int_{-\infty}^{\infty} (\hat{O}^{+}\psi)^{*}\psi\, dx = \int_{-\infty}^{\infty} \psi^{*}(\hat{O}\psi)\, dx$$

$$\Rightarrow \int_{-\infty}^{\infty} (\hat{O}^{+}\psi)^{*}\psi\, dx = \int_{-\infty}^{\infty} \psi^{*}(\lambda^{*})^{*}\psi\, dx$$

$$= \int_{-\infty}^{\infty} (\hat{O}^{+}\psi)^{*}\psi\, dx = \int_{-\infty}^{\infty} (\lambda\psi)^{*}\psi\, dx$$

$$= (\lambda^{*}\psi, \psi)$$

$$\Rightarrow \boxed{\hat{O}^{+}\psi = \lambda^{*}\psi}$$

$$\hat{p} = \frac{\hbar}{i}\frac{d}{dx} \longrightarrow \hat{p}^{+} = -\frac{\hbar}{i}\frac{d}{dx} \text{ ? No.}$$

Ex 2. Find the adjoint operator $\hat{O}^{+}$ for the operator $\hat{O} = \frac{d}{dx}$

Defn: $(\hat{O}^{+}\phi, \psi) = (\phi, \hat{O}\psi)$

$$\Rightarrow \int_{-\infty}^{\infty} (\hat{O}^{+} \phi)^{*} \, \psi \, dx = \int_{-\infty}^{\infty} \psi^{*} \, (\hat{O} \psi) \, dx$$

$$\Rightarrow \int_{-\infty}^{\infty} (\hat{O}^{+} \phi)^{*} \, \psi \, dx = \int_{-\infty}^{\infty} \psi^{*} \left(\frac{d}{dx} \psi \right) dx$$

Doing integration by parts on RHS,

$$\int_{-\infty}^{\infty} (\hat{O}^{+} \phi)^{*} \, \psi \, dx = \int_{-\infty}^{\infty} dx \left[\frac{d}{dx} (\phi^{*} \psi) - \frac{d\phi^{*}}{dx} \psi \right]$$

$$\Rightarrow \int_{-\infty}^{\infty} dx \, (\hat{O}^{+} \phi)^{*} \, \psi = \phi^{*} \psi \Big|_{L_1}^{L_2} + \int_{-\infty}^{\infty} dx \left(- \frac{d\phi}{dx} \right)^{*} \psi$$

Term has to go to zero

1. Vanishes at boundary
2. Periodic boundary conditions.

$$\therefore \hat{O}^{+} = - \frac{d}{dx}$$

$\Rightarrow$ momentum is a self-adjoint operator.

(*) A7/Q2 Find the adjoint operator $\hat{p}^{+}$ if

$$\hat{p} = \frac{\hbar}{i} \frac{d}{dx}$$

(*) An operator is called (self-adjoint) or Hermitian

if $\hat{O}^{+} = \hat{O}$

(and domain of $\hat{O}$ = domain of $\hat{O}^{+}$)

(*) In Dirac's bra-ket notation →

$$\hat{O}|\alpha\rangle \quad \| \quad \langle\alpha|\hat{O}^{+}$$

Claim: Eigenvalues of Hermitian operator $\hat{O}$, i.e. $\hat{O}^{+} = \hat{O}$ are real.

Say, $\hat{O}|n\rangle = n|n\rangle$ — (I)

$\langle m|\hat{O}^{+} = \langle m|m^{*}$ — (II)

$\langle m|\cdot$ (I) $\Rightarrow \langle m|\hat{O}|n\rangle = n\langle m|n\rangle$ — (III)

II $\cdot|n\rangle \Rightarrow \langle m|\hat{O}^{+}|n\rangle = \cancel{\langle} m^{*}\langle m|n\rangle$ — (IV)

Subtract (III) from (IV)

$$(m^{*} - n)\langle m|n\rangle = \langle m|\hat{O}^{+}|n\rangle - \langle m|\hat{O}|n\rangle$$
$$= 0$$

$\Rightarrow (n - m^{*})\langle m|n\rangle = 0$

(i) if $m = n$, $\langle n|n\rangle = 1$ (or any other +ve no.)

$\Rightarrow n - n^{*} = 0 \Rightarrow n^{*} = n$

$\Rightarrow$ n must be real.

(ii) If $m \neq n$

$\Rightarrow \boxed{\langle m|n\rangle = 0}$

→ Vectors are orthogonal to each other

⇒ ① The eigenvalues are real
② The eigenstates are orthogonal to each other.

(*) The eigenstates of ~~an~~ a Hermitian operator forms an orthonormal basis set ~~$\{|n\rangle\}$~~.

$\{|n\rangle\}$

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

(*) An arbitrary quantum state $|\psi\rangle$ can be expressed as,

$$|\psi\rangle = \sum_n a_n |n\rangle$$

$$\therefore a_n = \langle n|\psi\rangle$$

So,
$$|\psi\rangle = \sum_n a_n |n\rangle$$
$$= \sum_n \langle n|\psi\rangle |n\rangle$$
$$= \sum_n |n\rangle\langle n|\psi\rangle$$

$$\sum_n |n\rangle\langle n| = \mathbb{I}$$

Completeness relation of the basis $\{|n\rangle\}$.

(*) Copied from Sabarno's notes.

26th Feb 2024

(*) If $\hat{B}\,(=\hat{A}^{+}) = \hat{A}$, then it is called a Hermitian operator.

→ Its eigenvalues are real.

→ Eigenvectors form an orthonormal basis.

(*) Expectation value of an operator $\hat{O}$ w.r.t to a state ~~θ~~ $|\Psi\rangle$ is defined as,

$$\langle \Psi | \hat{O} | \Psi \rangle$$

Ex: ~~H~~ Find the expectation value of the Hamiltonian operator $\hat{H}$ w.r.t the state $|n\rangle$

$$\langle n | \hat{H} | n \rangle = \langle n | (\hat{N} + \tfrac{1}{2}) \hbar\omega | n \rangle$$

$$= \hbar\omega \langle n | (n + \tfrac{1}{2}) | n \rangle$$

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

$$= E_n$$

(*) In QM, expectation values are physically measurable quantities.

Ex2: Compute the expectation value of the position operator $\hat{x}$ in the eigenstate $|n\rangle$

$$\langle \hat{x} \rangle_{|n\rangle} = \langle n | \hat{x} | n \rangle$$

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

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

$$\Rightarrow \left(\hat{a} + \hat{a}^\dagger\right)\sqrt{\frac{\hbar}{2m\omega}} = \hat{x}$$

$$\Rightarrow \langle \hat{x} \rangle_{|n\rangle} = \langle n | \hat{x} | n \rangle$$

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

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

$$= 0$$

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

<u>Ex 6</u>: Compute the expectation $\langle n | \hat{x}^2 | n \rangle$

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

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

$$= m \langle n | \hat{a}^2 + 2\hat{N} - i\hbar + (\hat{a}^\dagger)^2 | n \rangle$$

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

$$= m(2n+1) + \langle n | \hat{a} (\sqrt{n} | n-1 \rangle) + \langle n | \hat{a}^+ (\sqrt{n+1} | n+1 \rangle)$$

Ex: Compute the expectation value of $\hat{p}$ w.r.t $|n\rangle$

$$\langle n|\hat{p}|n\rangle = \left(\sqrt{\frac{\hbar}{2m\omega}}\right)\left(\frac{i}{m\omega}\right) \langle n|(\hat{a}^{+} - \hat{a})|n\rangle = 0$$

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

$$\therefore \langle n|\hat{p}^2|n\rangle = \lambda^2 \langle n|(\hat{a}^{+})^2 - \hat{a}^{+}\hat{a} - \hat{a}\hat{a}^{+} + \hat{a}^2|n\rangle$$

$$= \lambda^2 \langle n|(\hat{a}^{+})^2 - 2\hat{N} - [a, a^{+}] + \hat{a}^2|n\rangle$$

$$= -\lambda^2 (2n+1)$$

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

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

(*) Variance of the operator:

$$\Delta x^2 = \sigma_x^2 \equiv \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2$$

$$\sigma_p^2 \equiv \langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2$$

Product of σ_x^2 and σ_p^2,

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

$$= \frac{\hbar^2}{4}(2n+1)^2$$

$$\Rightarrow \cancel{\sigma_x^2 \sigma} \quad \boxed{\sigma_x \sigma_p \geq \frac{\hbar}{2}}$$ as min value of $(2n+1)$ is 1

(*) This is the Heisenberg Uncertainty principle.