

C2 ASSIGNMENT:

PG.P.10.4. Quantum Mechanics-1

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Part 1: Short answer questions

2. Show that linear momentum operator is Hermitian.

Solution: An operator \hat{A} is said to be Hermitian if

$$\langle \phi | \hat{A} \psi \rangle = \langle \hat{A} \phi | \psi \rangle \quad (1)$$

The momentum operator \hat{p} , in the position basis, is defined as:

$$\hat{\vec{p}} = -i\hbar \vec{\nabla} \quad (2)$$

In one dimension, this reduces to:

$$\vec{p} = p_x = -i\hbar \frac{\partial}{\partial x} \quad (3)$$

Consider two vectors $|\psi\rangle$ and $|\phi\rangle$.

$$\begin{aligned} \langle \phi | \hat{p} \psi \rangle &= \int_{-\infty}^{\infty} \phi^*(x) \hat{p} \psi(x) dx \\ &= \int_{-\infty}^{\infty} \phi^*(x) \left(-i\hbar \frac{d}{dx} \right) \psi(x) dx \\ &= \int_{-\infty}^{\infty} \phi^*(x) \left(-i\hbar \frac{d\psi(x)}{dx} \right) dx \\ &= -i\hbar \int_{-\infty}^{\infty} \phi^*(x) \left(\frac{d\psi(x)}{dx} \right) dx \end{aligned}$$

The integral is now of the form uv' . Hence this can be integrated by parts:

$$\langle \phi | \hat{p} \psi \rangle = -i\hbar \left(\phi^*(x) \psi(x) \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{d\phi^*(x)}{dx} \psi(x) dx \right)$$

Now, the wave functions vanish as $x \rightarrow \pm\infty$. Hence the first term becomes zero.
Hence,

$$\begin{aligned}
 \langle \phi | \hat{p} \psi \rangle &= i\hbar \int_{-\infty}^{\infty} \frac{d\phi^*(x)}{dx} \psi(x) dx \\
 &= \int_{-\infty}^{\infty} \left(i\hbar \frac{d\phi^*(x)}{dx} \right) \psi(x) dx \\
 &= \int_{-\infty}^{\infty} \left(-i\hbar \frac{d\phi(x)}{dx} \right)^* \psi(x) dx \\
 &= \int_{-\infty}^{\infty} [\hat{p} \phi(x)]^* \psi(x) dx \\
 &= \langle \hat{p} \phi | \psi \rangle \\
 \therefore \quad &\boxed{\langle \phi | \hat{p} \psi \rangle = \langle \hat{p} \phi | \psi \rangle}
 \end{aligned}$$

Hence, by equation (1), the linear momentum operator \hat{p} is a Hermitian operator.

4. **Show that Hermitian operators have real eigenvalues.**

Solution: Consider a Hermitian operator \hat{A} which has the eigen-value equation:

$$\hat{A} |\psi\rangle = a |\psi\rangle \quad (4)$$

Since these vectors are members of a Hilbert's space, they have finite inner products. Hence, we can take the inner product with $|\psi\rangle$ in the above equation:

$$\langle \psi | \hat{A} \psi \rangle = a \langle \psi | \psi \rangle \quad (5)$$

Since \hat{A} is Hermitian, by equation (1),

$$\langle \psi | \hat{A} \psi \rangle = \langle \hat{A} \psi | \psi \rangle = a^* \langle \psi | \psi \rangle \quad (6)$$

Therefore, from equations (5) and (6),

$$a = a^*$$

This will be true only if a is a real number, *i.e.*, $a \in \mathbb{R}$.

\therefore Hermitian operators have real eigenvalues.

5. **Find $[x, p^2]$ or $[x^2, p]$ or $[x, p^n]$ or $[x^n, p]$.**

Solution:

$$[x, p] = i\hbar \quad (7)$$

By the properties of commutators:

$$[A, BC] = B[A, C] + [A, B]C \quad (8)$$

$$\begin{aligned}
[x, p^2] &= p[x, p] + [x, p]p \\
&= i\hbar p + i\hbar p \\
&= 2i\hbar p
\end{aligned}$$

$$\begin{aligned}
[x^2, p] &= x[x, p] + [x, p]x \\
&= i\hbar x + i\hbar x \\
&= 2i\hbar x
\end{aligned}$$

$$\begin{aligned}
[x^3, p] &= [x x^2, p] \\
&= x[x^2, p] + [x, p]x^2 \\
&= x(2i\hbar x) + i\hbar x^2 \\
&= 3i\hbar x^2
\end{aligned}$$

$$\begin{aligned}
[x, p^3] &= [x, p p^2] \\
&= p[x, p^2] + [x, p]p^2 \\
&= p(2i\hbar p) + i\hbar p^2 \\
&= 3i\hbar p^2
\end{aligned}$$

So, in general,

$$\boxed{[x^n, p] = ni\hbar x^{n-1}} \tag{9}$$

$$\boxed{[x, p^n] = ni\hbar p^{n-1}} \tag{10}$$

Long Answer Questions

8. Derive the expression for general uncertainty relation for non-commuting operators \hat{A} , \hat{B} satisfying

$$[\hat{A}, \hat{B}] = i\hat{C}$$

Solution:

If $|\psi\rangle$ is an eigenstate of \hat{A} , then

$$\hat{A}|\psi\rangle = \lambda|\psi\rangle \quad (11)$$

where λ is real. The uncertainty in the measurement of \hat{A} is

$$\Delta A = \sqrt{\langle (\hat{A} - \langle \hat{A} \rangle)^2 \rangle} = \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}$$

Consider the uncertainty in the measurement of \hat{A} in the eigenstate $|\psi\rangle$:

$$\begin{aligned} (\Delta A)^2 &= \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2 \\ &= \langle \psi | \hat{A}^2 | \psi \rangle - \langle \psi | \hat{A} | \psi \rangle^2 \\ &= \lambda^2 - \lambda^2 \\ &= 0 \end{aligned} \quad (12)$$

Suppose \hat{A} , \hat{B} are non-commuting Hermitian operators satisfying

$$[\hat{A}, \hat{B}] = i\hat{C}$$

\hat{C} is Hermitian:

$$\begin{aligned} \hat{C} &= -i[\hat{A}, \hat{B}] \\ &= -i(\hat{A}\hat{B} - \hat{B}\hat{A}) \end{aligned}$$

$$\begin{aligned} \hat{C}^\dagger &= [-i(\hat{A}\hat{B} - \hat{B}\hat{A})]^\dagger \\ &= (\hat{A}\hat{B} - \hat{B}\hat{A})^\dagger (-i)^\dagger \\ &= i(\hat{A}\hat{B} - \hat{B}\hat{A})^\dagger \\ &= i[(\hat{A}\hat{B})^\dagger - (\hat{B}\hat{A})^\dagger] \\ &= i[\hat{B}\hat{A} - \hat{A}\hat{B}] \\ &= -i[\hat{A}, \hat{B}] \\ &= \hat{C} \end{aligned}$$

Suppose the system is in some state $|\phi\rangle$. Define :

$$|\chi\rangle \equiv (\hat{A} - \langle\hat{A}\rangle \hat{I}) |\phi\rangle \quad (13)$$

$$|\zeta\rangle \equiv (\hat{B} - \langle\hat{B}\rangle \hat{I}) |\phi\rangle \quad (14)$$

By Schwarz inequality,

$$\langle\chi|\chi\rangle \langle\zeta|\zeta\rangle \geq \|\langle\chi|\zeta\rangle\|^2 \quad (15)$$

Now consider,

$$\begin{aligned} \langle\chi|\chi\rangle &= \langle\chi|(\hat{A} - \langle\hat{A}\rangle \hat{I})|\phi\rangle \\ &= \langle\phi|(\hat{A} - \langle\hat{A}\rangle \hat{I})(\hat{A} - \langle\hat{A}\rangle \hat{I})|\phi\rangle \\ &= \langle\phi|(\hat{A}^2 - 2\langle\hat{A}\rangle \hat{A} + \langle\hat{A}\rangle^2)|\phi\rangle \\ &= \langle\phi|\hat{A}^2|\phi\rangle - 2\langle\hat{A}\rangle^2 + \langle\hat{A}\rangle^2 \\ &= \langle\phi|\hat{A}^2|\phi\rangle - \langle\hat{A}\rangle^2 \\ &= (\Delta A)^2 \end{aligned} \quad (16)$$

Similarly,

$$\langle\zeta|\zeta\rangle = (\Delta B)^2 \quad (17)$$

Now consider the third term required in equation (15)

$$\begin{aligned} \langle\chi|\zeta\rangle &= \langle\phi|(\hat{A} - \langle\hat{A}\rangle \hat{I})(\hat{B} - \langle\hat{B}\rangle \hat{I})|\phi\rangle \\ &= \langle\phi|(\hat{A}\hat{B} - \langle\hat{B}\rangle \hat{A} - \langle\hat{A}\rangle \hat{B} + \langle\hat{A}\rangle \langle\hat{B}\rangle)|\phi\rangle \\ &= \langle\phi|\hat{A}\hat{B}|\phi\rangle - \langle\hat{A}\rangle \langle\hat{B}\rangle \end{aligned} \quad (18)$$

$$\begin{aligned} \langle\phi|\hat{A}\hat{B}|\phi\rangle &= \left\langle\phi\left|\left\{\left(\frac{\hat{A}\hat{B} - \hat{B}\hat{A}}{2}\right) + \left(\frac{\hat{A}\hat{B} + \hat{B}\hat{A}}{2}\right)\right\}\right|\phi\right\rangle \\ &= \left\langle\phi\left|\frac{i\hat{C}}{2}\right|\phi\right\rangle + \frac{1}{2}\langle\phi|\hat{A}\hat{B} + \hat{B}\hat{A}|\phi\rangle \\ &= \frac{i}{2}\langle\hat{C}\rangle + \frac{1}{2}\langle\phi|\hat{A}\hat{B} + \hat{B}\hat{A}|\phi\rangle \end{aligned} \quad (19)$$

Substituting equation (19) in equation (18),

$$\begin{aligned} \langle\chi|\zeta\rangle &= \frac{i}{2}\langle\hat{C}\rangle + \frac{1}{2}\langle\phi|\hat{A}\hat{B} + \hat{B}\hat{A}|\phi\rangle - \langle\hat{A}\rangle \langle\hat{B}\rangle \\ &= \frac{i}{2}\langle\hat{C}\rangle + \frac{1}{2}\langle\phi|\hat{A}\hat{B} + \hat{B}\hat{A}|\phi\rangle - \langle\hat{A}\rangle \langle\hat{B}\rangle \langle\phi|\phi\rangle \\ &= \frac{i}{2}\langle\hat{C}\rangle + \frac{1}{2}\langle\phi|\hat{A}\hat{B} + \hat{B}\hat{A}|\phi\rangle - \langle\phi|\langle\hat{A}\rangle \langle\hat{B}\rangle|\phi\rangle \\ &= \frac{i}{2}\langle\hat{C}\rangle + \frac{1}{2}\left\langle\phi\left|\left\{(\hat{A}\hat{B} + \hat{B}\hat{A}) - 2\langle\hat{A}\rangle \langle\hat{B}\rangle\right\}\right|\phi\right\rangle \end{aligned}$$

Let $\hat{D} \equiv [(\hat{A}\hat{B} + \hat{B}\hat{A}) - 2\langle A \rangle \langle B \rangle]$. Note that this is also an operator.

Therefore

$$\langle \chi | \zeta \rangle = \frac{i}{2} \langle \hat{C} \rangle + \frac{1}{2} \langle \phi | \hat{D} | \phi \rangle \quad (20)$$

Now,

$$\| \langle \chi | \zeta \rangle \|^2 = \frac{1}{4} \langle \hat{C} \rangle^2 + \frac{1}{4} \langle \phi | \hat{D} | \phi \rangle^2 \quad (21)$$

$$(\because |(a + ib)|^2 = (a + ib)(a - ib) = a^2 + b^2)$$

Since all the terms in the above equation are real,

$$\| \langle \chi | \zeta \rangle \|^2 \geq \frac{1}{4} \langle \hat{C} \rangle^2 \quad (22)$$

Combining equation(15) with the above equation,

$$\langle \chi | \chi \rangle \langle \zeta | \zeta \rangle \geq \| \langle \chi | \zeta \rangle \|^2 \geq \frac{1}{4} \langle \hat{C} \rangle^2$$

Now, using the results from (16) and (17),

$$(\Delta A)^2 (\Delta B)^2 \geq \frac{1}{4} \langle \hat{C} \rangle^2 \quad (23)$$

$$\boxed{(\Delta A) (\Delta B) \geq \frac{1}{2} |\langle \hat{C} \rangle|} \quad (24)$$

The above gives the general uncertainty principle for any two non-commuting Hermitian operators:

If \hat{A} and \hat{B} are two non-commuting Hermitian operators, then the product of the uncertainties in \hat{A} and \hat{B} is always greater than $\frac{|\langle \hat{C} \rangle|}{2}$.

12. Solve the Schrödinger equation for the oscillator using the operator method and obtain the energy eigenvalues.

Solution: The time-independent Schrödinger equation is given by:

$$\hat{H}\psi = E\psi \quad (25)$$

By using the fact that any potential $V(x)$ is approximately parabolic in the neighbourhood of a local minimum,

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

where $\omega = \sqrt{k/m}$.

Substituting the equation for the Hamiltonian operator as

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$$

Equation 25 becomes

$$\frac{1}{2m} [\hat{p}^2 + (m\omega\hat{x})^2] \psi(x) = E\psi(x) \quad (26)$$

(Note that p and x are operators.)

We define two operators:

$$\hat{a} = \frac{1}{\sqrt{2\hbar m\omega}} (i\hat{p} + m\omega\hat{x}) \quad (27)$$

$$\hat{a}^\dagger = \frac{1}{\sqrt{2\hbar m\omega}} (-i\hat{p} + m\omega\hat{x}) \quad (28)$$

Now, consider

$$\begin{aligned} \hat{a}\hat{a}^\dagger &= \frac{1}{2\hbar m\omega} (i\hat{p} + m\omega\hat{x}) (-i\hat{p} + m\omega\hat{x}) \\ &= \frac{1}{2\hbar m\omega} \{\hat{p}^2 + (m\omega\hat{x})^2 - im\omega(\hat{x}\hat{p} - \hat{p}\hat{x})\} \\ &= \frac{1}{2\hbar m\omega} \{\hat{p}^2 + (m\omega\hat{x})^2 - im\omega[\hat{x}, \hat{p}]\} \end{aligned}$$

Now,

$$[x, p] = i\hbar$$

$$\therefore \hat{a}\hat{a}^\dagger = \frac{1}{2\hbar m\omega} \{\hat{p}^2 + (m\omega\hat{x})^2 + m\omega\hbar\}$$

Using the equation for Hamiltonian as in equation (26),

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

$$\therefore \hat{a}\hat{a}^\dagger = \left(\frac{\hat{H}}{\hbar\omega} + \frac{1}{2} \right) \quad (29)$$

Now, consider the following commutator relations:

$$\begin{aligned} [\hat{a}, \hat{a}^\dagger] &= \frac{1}{2m\hbar\omega} (i\hat{p} + m\omega\hat{x}, -i\hat{p} + m\omega\hat{x}) \\ &= \frac{1}{2m\hbar\omega} (im\omega[\hat{p}, \hat{x}] - im\omega[\hat{x}, \hat{p}]) \\ &= \frac{1}{2m\hbar\omega} (2m\hbar\omega) \\ &= 1 \end{aligned} \quad (30)$$

Now, using the result in (30) and commutator property,

$$[\hat{a}^\dagger, \hat{a}] = -1 \quad (31)$$

Now, consider

$$\begin{aligned} [\hat{a}^\dagger\hat{a}, \hat{a}] &= \hat{a}^\dagger[\hat{a}, \hat{a}] + [\hat{a}^\dagger, \hat{a}]\hat{a} \\ &= -\hat{a} \end{aligned}$$

$$\begin{aligned} [\hat{a}^\dagger\hat{a}, \hat{a}^\dagger] &= \hat{a}^\dagger[\hat{a}, \hat{a}^\dagger] + [\hat{a}^\dagger, \hat{a}^\dagger]\hat{a} \\ &= \hat{a}^\dagger \end{aligned}$$

Now, define

$$\hat{N} \equiv \hat{a}^\dagger\hat{a} \quad (32)$$

Note that \hat{N} is Hermitian.

Let us rewrite the commutator relations we have obtained so far, using the definition (32) for $\hat{a}^\dagger\hat{a}$,

- $[\hat{a}, \hat{a}^\dagger] = 1$
- $[\hat{N}, \hat{a}] = -\hat{a}$
- $[\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger$

Now, from equation (29), using equations (31) and (32), we can write

$$\hat{H} = \hbar\omega \left(\hat{N} + \frac{1}{2} \right) \quad (33)$$

\hat{N} possesses eigen states with real eigenvalues. Let $|n\rangle$ be an eigenstate of \hat{N} , with eigenvalue n .

$$\hat{N} |n\rangle = n |n\rangle \quad (34)$$

Let $|\chi\rangle \equiv \hat{a}|n\rangle$. Operating \hat{N} on $|\chi\rangle$, we see that:

$$\begin{aligned}
\hat{N}|\chi\rangle &= \hat{N}\hat{a}|n\rangle \\
&= (\hat{a}\hat{N} - \hat{a})|n\rangle \quad (\text{from commutator relation } [\hat{N}, \hat{a}]) \\
&= \hat{a}\hat{N}|n\rangle - \hat{a}|n\rangle \\
&= n\hat{a}|n\rangle - \hat{a}|n\rangle \quad (\text{from the eigenvalue equation (34)}) \\
&= (n-1)\hat{a}|n\rangle \\
&= (n-1)|\chi\rangle
\end{aligned} \tag{35}$$

which means, $|\chi\rangle$ is also an eigen state of \hat{N} with eigenvalue $(n-1)$. Similarly, $(\hat{a})^2|n\rangle$ is also an eigenstate of \hat{N} with eigenvalue $(n-2)$.

Now, let $|\xi\rangle \equiv \hat{a}^\dagger|n\rangle$. Similar to equation (35),

$$\begin{aligned}
\hat{N}|\xi\rangle &= \hat{N}\hat{a}^\dagger|n\rangle \\
&= (\hat{a}^\dagger + \hat{a}^\dagger\hat{N})|n\rangle \quad (\text{from commutator relation } [\hat{N}, \hat{a}^\dagger]) \\
&= \hat{a}^\dagger|n\rangle + \hat{a}^\dagger\hat{N}|n\rangle \\
&= \hat{a}^\dagger|n\rangle + n\hat{a}^\dagger|n\rangle \quad (\text{from the eigenvalue equation (34)}) \\
&= (n+1)\hat{a}^\dagger|n\rangle \\
&= (n+1)|\xi\rangle
\end{aligned} \tag{36}$$

which means, $|\xi\rangle$ is also an eigen state of \hat{N} with eigenvalue $(n+1)$.

Similarly, $(\hat{a}^\dagger)^2|n\rangle$ is also an eigenstate of \hat{N} with eigenvalue $(n+2)$.

Due to these properties, the operators \hat{a} and \hat{a}^\dagger are known as *annihilation* and *creation* operators respectively. This is because, given a particular state, one can apply \hat{a}^\dagger and \hat{a} on that state to get new states with higher and lower eigenvalues respectively.

$$\langle\chi|\chi\rangle = \langle n|\hat{a}^\dagger\hat{a}|n\rangle = \langle n|\hat{N}|n\rangle = n\langle n|n\rangle \geq 0$$

So n is non-negative and real.

\hat{a} cannot be applied indefinitely on a given state. At some point, on repeated application of \hat{a} , a *lowest energy state* is obtained. To satisfy this condition, n must be an integer. Therefore, n is a non-negative integer.

The lowest energy state, $|0\rangle$ has eigenvalue zero:

$$\begin{aligned}
\hat{N}|0\rangle &= 0 \\
\implies \hat{a}|0\rangle &= 0
\end{aligned} \tag{37}$$

Call $|0\rangle$ as $\psi_0(x)$

$$\begin{aligned}
&\Rightarrow \frac{1}{\sqrt{2\hbar m\omega}} (i\hat{p} + m\omega\hat{x}) \psi_0(x) = 0 \\
&\frac{1}{\sqrt{2\hbar m\omega}} \left(i \left(-i\hbar \frac{d}{dx} \right) + m\omega\hat{x} \right) \psi_0(x) = 0 \\
&\Rightarrow \frac{d\psi_0(x)}{dx} + \frac{m\omega}{\hbar} x \psi_0(x) = 0 \\
&\text{Solving, } \psi_0(x) = A e^{-\left(\frac{m\omega x^2}{2\hbar}\right)}
\end{aligned}$$

To get the constant of integration A , apply the normalization condition:

$$\begin{aligned}
\int_{-\infty}^{\infty} \psi_0^*(x) \psi_0(x) dx &= 1 \\
\Rightarrow A^2 &= \sqrt{\frac{m\omega}{\pi\hbar}} \\
\Rightarrow A &= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}
\end{aligned}$$

Therefore, the time-independent wave function of the lowest energy state is:

$$\boxed{\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\left(\frac{m\omega x^2}{2\hbar}\right)}} \quad (38)$$

The time dependent wave function is therefore

$$\Psi_0(x, t) = \psi_0(x) e^{\frac{-iE_0 t}{\hbar}} \quad (39)$$

Now, from equation (33) it is clear that,

$$[\hat{H}, \hat{N}] = 0$$

In other words, the operators \hat{H} and \hat{N} , commute. Since, they commute, the eigenstates of \hat{H} are also eigenstates of \hat{N} (since they are Hermitian).

This means that, since $|n\rangle$, $|\chi\rangle$ and $|\xi\rangle$ are eigenstates of \hat{N} , they must be eigenstates of \hat{H} also.

$$\begin{aligned}
\hat{H} |n\rangle &= \hbar\omega \left(\hat{N} + \frac{1}{2} \right) |n\rangle \\
&= \hbar\omega \left(\hat{N} |n\rangle + \frac{1}{2} |n\rangle \right) \\
&= \hbar\omega \left(n |n\rangle + \frac{1}{2} |n\rangle \right) \\
&= \left(n + \frac{1}{2} \right) \hbar\omega |n\rangle
\end{aligned} \quad (40)$$

Using $\hat{H} |n\rangle = E_n |n\rangle$, we see that

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega \quad (41)$$

Hence, even when $n = 0$, the energy is non-zero. In other words, there is no zero energy state. From (38) and (41),

$$\begin{aligned} \Psi_0(x, t) &= \psi_0(x) e^{-\frac{iE_0 t}{\hbar}} \\ &= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\left(\frac{m\omega x^2}{2\hbar}\right)} e^{-\frac{i\left(\frac{1}{2}\hbar\omega\right)t}{\hbar}} \\ &= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}} e^{-\frac{i\omega t}{2}} \end{aligned} \quad (42)$$

Any higher state can be obtained by applying the creation operator on the ground state $\psi_0(x)$ and continuing the same procedure discussed above.

The general wave function of the harmonic oscillator can be written in terms of the Hermite polynomials as:

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2} \quad (43)$$

where $H_n(x)$ are the Hermite polynomials and $\xi = \sqrt{\frac{m\omega}{\hbar}}x$