Chapter 7

Operator Methods in Quantum Mechanics

For Harmonic Osc.; $H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$ (1)

Where we have the relation $[P, x] = \frac{\hbar}{i}$ between P and x ops. (2)

Classically,

$$H = \omega \left(\sqrt{\frac{m\omega}{2}}\, x - i \frac{p}{\sqrt{2m\omega}} \right)\left(\sqrt{\frac{m\omega}{2}}\, x - i \frac{p}{\sqrt{2m\omega}} \right) \quad (3)$$

But in Q.M. since, $[P, x] \neq 0$

$$\rightarrow \omega \left(\sqrt{\frac{m\omega}{2}}\, x - i \frac{p}{\sqrt{2m\omega}} \right)\left(\sqrt{\frac{m\omega}{2}}\, x - i \frac{p}{\sqrt{2m\omega}} \right) = \frac{p^2}{2m} + \frac{m\omega^2}{2} x^2 - \frac{i\omega}{2}(Px - xP)$$

$$= H - \frac{1}{2}\hbar\omega \quad (4)$$

We introduce the notation;
$$\begin{cases} A = \sqrt{\frac{m\omega}{2}}\, x + i \frac{p}{\sqrt{2m\omega}} \\ A^+ = \sqrt{\frac{m\omega}{2}}\, x - i \frac{p}{\sqrt{2m\omega}} \end{cases} \quad (5)$$

Remember, $P = P^+$, $x = x^+$

$$[A, A^+] = \left[\sqrt{\frac{m\omega}{2}}\, x, \, i \frac{p}{\sqrt{2m\omega}} \right] + \left[i \frac{p}{\sqrt{2m\omega}}, \sqrt{\frac{m\omega}{2}}\, x \right] = \hbar \quad (6)$$

$$\rightarrow H = \frac{1}{2}\hbar\omega + \omega A^+ A \quad (7)$$

$$[H, A] = [\omega A^{+}A\ , A] + 0 = \omega [A^{+}, A] A + 0 = -\hbar\omega A \qquad (8)$$

and,

$$[H, A^{+}] = [\omega A^{+}A\ , A^{+}] + 0 = \omega A^{+}[A, A^{+}] + 0 = \hbar\omega A^{+} \qquad (9)$$

Remark:
$$[A+B, C] = [A, C] + [B, C]$$
$$[AB, C] = A[B, C] + [A, C]B$$

Note also that $[A,B]^{+} = (AB - BA)^{+} = B^{+}A^{+} - A^{+}B^{+} = [B^{+}, A^{+}]$ (11)

$$\rightarrow [H, A]^{+} = [A^{+}, H^{+}] = [A^{+}, H] = -[H, A^{+}] = (-\hbar\omega A)^{+}$$
$$= -\hbar\omega A^{+}$$

$$\rightarrow [H, A^{+}] = \hbar\omega A^{+} \quad \text{(the same as (9))}$$

Now consider the eigenvalue equ.:

$$H u_E = E u_E \qquad (12)$$

In the past we discussed:

An observable like H. $\qquad H = H(\frac{d}{dx}, x, \ldots)$

and $\qquad u_E = u_E(x)_{p}\ , \quad \Psi = \Psi(x)_{p} \qquad (13)$

(square integrable)

But here, we are not being very specific about what our ops operate on (i.e. the details of ψ or $u_E \cdots$)

We shall assume that they are defined in some abstract vector space, and relate that abstract vector space to the space of funcs. of x later.

eigenfunctions $\xrightarrow{\text{now}}$ eigenstates

wave functions $\xrightarrow{\text{now}}$ state vectors

$$u_{a,b,\ldots m}(x) \longrightarrow u_{a,b,\ldots m}$$

where $a \longleftrightarrow A$, $b \longleftrightarrow B, \ldots \; m \longleftrightarrow M$

Now

$$(8) \rightarrow \quad HA\,u_E - AA\,u_E = -\hbar\omega A u_E \qquad (14)$$

$$(12) \text{ in } (14) \rightarrow \quad H\underbrace{Au_E} = (E-\hbar\omega)\underbrace{Au_E} \qquad (15)$$

take $\quad \epsilon = \hbar\omega$

$$(15) \rightarrow \quad A\,u_E = C(E)\,u_{E-\epsilon} \qquad (16)$$

The const. $C(E)$ is necessary, because even if u_E is normalized to 1, $A u_E$ need not be.

Note that: $$\int u_E^*(x)\, u_E(x)\, dx = 1 \longrightarrow \langle u_E | u_E \rangle = 1 \quad (17)$$

without explicit x-dep.

Also $$\langle u_E | u_{E'} \rangle = \delta_{EE'}$$

$$(18)$$

$$\langle u_E | u_{E'} \rangle = \delta(E-E')$$

Now if we apply (8) on $u_{E-\epsilon}$:

$\longrightarrow$ $A u_{E-\epsilon} \sim A^2 u_E$ has the energy $E-2\epsilon$

$\longrightarrow$ A: lowering op

$A^n u_E$ has the energy $E-n\epsilon$

But there is a limitation for this process:

From (1) $\longrightarrow$ $\langle H \rangle \geq 0$

Because,

$$\langle \psi | p^2 | \psi \rangle = \int \psi^*(x)\, p^2 \psi(x)\, dx = \int [p^\dagger \psi(x)]^* (p\psi)\, dx$$

$$= \int [p\psi(x)]^* [p\psi(x)]\, dx = \hbar^2 \int \left| \frac{d\psi(x)}{dx} \right|^2 dx \geq 0$$

(19)

which we rewrite in our coordinate-deemphasizing way as:

$$\langle \psi | p^2 | \psi \rangle = \langle p^{+} \psi | p \psi \rangle = \langle p\psi | p\psi \rangle \geq 0 \qquad (20)$$

Similarly: $\langle \psi | x^2 | \psi \rangle = \langle x^{+} \psi | x \psi \rangle = \langle x\psi | x\psi \rangle \geq 0 \qquad (21)$

The limit: $\underset{\substack{\uparrow \\ \text{ground state}}}{A u_0} = 0 \qquad (22)$

The energy of the ground state:

$$(7) \rightarrow H u_0 = (\omega A^{+} A + \tfrac{1}{2}\hbar\omega) u_0 = 0 + \tfrac{1}{2}\hbar\omega u_0 \qquad (23)$$

$$E_0 = \tfrac{1}{2}\hbar\omega \qquad (24)$$

Apply (9) on u_0:

$$H A^{+} u_0 - A^{+} H u_0 = \hbar\omega A^{+} u_0$$

$$\rightarrow H A^{+} u_0 = (\hbar\omega + \tfrac{1}{2}\hbar\omega) A^{+} u_0 \qquad (24)$$

$\rightarrow A^{+}$: raising op.

$$\rightarrow \begin{cases} A^{+} u_0 = C u_1 \\ A u_1 = C' u_0 \end{cases} \qquad (25)$$

$\rightarrow \quad E_n = (n+\frac{1}{2})\hbar\omega \qquad n=0,1,2,\dots$ the energy of the system

(26)

We have succeeded in obtaining the energy spectrum without solving any differential equ.

Remark: We write $N = A^+A$

$$[N,A] = [A^+A, A] = A^+[A,A] + [A^+,A]A = -\hbar A$$

Similarly $[N,A^+] = \hbar A^+$ (27)

As a result;

(7) $\rightarrow \quad H = \frac{1}{2}\hbar\omega + \omega N$ (28)

Note that $[H,N] = 0$ (29)

(26) $\rightarrow \quad H\,u_{E_n} = (n+\frac{1}{2})\hbar\omega\, u_{E_n}$ (30)

(28) (30) $\rightarrow \quad (\frac{1}{2}\hbar\omega + \omega N)\,u_{E_n} = (n+\frac{1}{2})\hbar\omega\, u_{E_n}$ (31)

$\rightarrow \quad N\,u_{E_n} = n\hbar\, u_{E_n} \quad \rightarrow N$: number op.

(32)

The general representation:

$$u_n = \frac{1}{\sqrt{n!}} \left(\frac{A^+}{\sqrt{\hbar}} \right)^n u_0 \qquad (33)$$

Proof:
$$A | u_n \rangle = c_{n-1} | u_{n-1} \rangle \qquad (34)$$

$$\rightarrow \quad \langle u_n | A^+ A | u_n \rangle = |c_{n-1}|^2 \langle u_{n-1} | u_{n-1} \rangle$$

$$n\hbar \langle u_n | u_n \rangle = |c_{n-1}|^2 \quad \rightarrow n\hbar = |c_n|^2 \qquad (35)$$

C: Positive, real (by conversion)

$$\rightarrow \quad A | u_n \rangle = \sqrt{n\hbar} \, | u_{n-1} \rangle$$

(36)

Similarly, $A^+ | u_n \rangle = \sqrt{(n+1)\hbar} \, | u_{n+1} \rangle$ (use $[A, A^+] = \hbar$)

$$A^2 | u_n \rangle = \sqrt{n(n-1)\hbar^2} \, | u_{n-2} \rangle$$
$$A^3 | u_n \rangle = \sqrt{n(n-1)(n-2)\hbar^3} \, | u_{n-3} \rangle$$

$\vdots$

Then (33) is proved.

Orthogonality:

$$\langle u_m | u_n \rangle = ?$$

$$\langle u_m | u_n \rangle \sim \langle u_0 | A^m (A^+)^n | u_0 \rangle = ?$$

$$A^m (A^+)^n = ?$$

For example; $A^2 (A^+)^3 = A A A^+ (A^+)^2 = A(A^+A + \hbar)(A^+)^2$

$$= AA^+AA^+A^+ + \hbar A(A^+)^2 = AA^+(A^+A+\hbar)A^+ + \hbar A(A^+)^2$$

$$= AA^+A^+(A^+A+\hbar) + 2\hbar A(A^+)^2 = A(A^+)^3 A + 3\hbar A(A^+)^2$$

$$= A(A^+)^3 A + 3\hbar (A^+A+\hbar) A^+$$

Now $\langle u_0 | A (A^+)^3 A | u_0 \rangle = 0$ (since $A|u_0\rangle = 0$)

$\langle u_0 | A^+ A | u_0 \rangle = 0$ (")

$$\langle u_0 | A^+ | u_0 \rangle = \langle u_0 | A^+ u_0 \rangle = \langle \underbrace{A u_0}_{0} | u_0 \rangle = 0$$

$$\rightarrow \langle u_2 | u_3 \rangle = 0$$

$\rightarrow \langle u_m | u_n \rangle = 0$ for $m \neq n$

$\langle u_m | u_n \rangle = \delta_{mn}$ for normalized eigenstates

(37)

The expansion principle in the coordinate-indep. way;

$$\Psi = \sum_{n=0}^{\infty} C_n u_n \qquad (38)$$

$$(37)(38) \rightarrow C_m = \langle u_m | \Psi \rangle \qquad (39)$$

Now, $(22) \rightarrow \left(\sqrt{\frac{m\omega}{2}}\, x + i \frac{p}{\sqrt{2m\omega}} \right) u_0(x) = 0 \qquad (40)$

$$\rightarrow \left(m\omega x + \hbar \frac{d}{dx} \right) u_0(x) = 0 \qquad (41)$$

$$\rightarrow u_0(x) = C e^{-m\omega x^2/2\hbar} \qquad (42)$$

$$\int u_0^*(x)\, u_0(x)\, dx = 1 \rightarrow C^2 \int_{-\infty}^{\infty} dx\, e^{-m\omega x^2/\hbar} = 1 \qquad (43)$$

$$C^2 \left(\frac{\hbar \pi}{m\omega} \right)^{1/2} = 1 \qquad \rightarrow C = \left(\frac{m\omega}{\hbar \pi} \right)^{1/4} \qquad (44)$$

$$u_n(x) = \frac{\hbar^{-n/2}}{\sqrt{n!}} (A^+)^n u_0(x) = \frac{1}{\sqrt{n!}} \left(\frac{m\omega}{\hbar \pi} \right)^{1/4} \left(\sqrt{\frac{m\omega}{2\hbar}}\, x - \sqrt{\frac{\hbar}{2m\omega}} \frac{d}{dx} \right)^n e^{-m\omega x^2/2\hbar} \qquad (45)$$

As we remarked $a, b, \ldots m$ are the quantum numbers needed to specify the eigenstates (P139), here the only quantum number is n;

i.e. $\underbrace{a, b, \ldots m} = n$

and thus the complete set of commuting observables consists of H alone,

i.e. $[\underset{A}{\Pi}, \underset{B}{H}] = [\underset{C}{N}, H] = \cdots = 0$

$$\underset{A}{\Pi} \longleftrightarrow \underset{a}{n}\ , \quad \underset{B}{H} \longleftrightarrow \underset{b}{n}\ , \quad \underset{C}{N} \longleftrightarrow \underset{c}{n} \quad \cdots$$

$$\rightarrow \ u_{a,b,c\ldots} \longrightarrow u_n$$

Thus the label n on the eigenstate u_n describes its whole content.

→ We would therefore be quite willing to give up the privileged role of the eigenfunc. in x-space $u_n(x)$ – <u>except</u> for one point: $u_n(x)$ does provide us with more information in that it gives us the probability density (via $|u_n(x)|^2$) of finding the particle <u>at</u> x.

Now, from;

$$\psi(x) = \int_{-\infty}^{\infty} dp\ \varphi(p)\ \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}$$

$$\varphi(p) = \int_{-\infty}^{\infty} dx\ \psi(x)\ \frac{e^{-ipx/\hbar}}{\sqrt{2\pi\hbar}} \qquad (46)$$

we see that:

$\varphi(p)$ is merely an expansion coeff. of an arbitrary $\psi(x)$ in eigenstates of momentum op.

$\longrightarrow |\varphi(p)|^2$: the probability of finding a mom. p for that state

Similarly:

The fact that $|\psi(x)|^2$: " " " " position x for the system

$\longrightarrow$ Could be interpreted by the statement that $\psi(x)$ is the expansion coeff. of an arbitrary abstract state in eigenstates of the position operator X_{op}.

$$X_{op}\varphi_x = x\,\varphi_x \qquad (X|x'\rangle = x'|x'\rangle) \qquad (47)$$

continuous

$$\psi = \sum_{n=0}^{\infty} c_n u_n \longrightarrow \psi = \int dx\, C(x)\,\varphi_x \qquad (48)$$

$$\langle \varphi_x | \varphi_{x'} \rangle = \delta(x-x') \qquad (49)$$

$$C(x) = \langle \varphi_x | \psi \rangle \equiv \psi(x) \qquad (50)$$

$$\overset{(48)}{\underset{(50)}{\rightarrow}} |\psi\rangle = \int dx\, |\varphi_x\rangle\langle\varphi_x|\psi\rangle = \int dx\, \psi(x)\,|\varphi_x\rangle \qquad (51)$$

Remark: Note that $\psi(x)$ is not eigenfunc of X_{op}

Note that,

$$|\alpha\rangle = \int |p\rangle\langle p|\alpha\rangle\, dp \longrightarrow \langle x|\alpha\rangle = \int \langle x|p\rangle\langle p|\alpha\rangle\, dp$$

$$\rightarrow \quad \psi(x) = \int u_p(x)\, \varphi(p)\, dp \qquad (52)$$

$$|\alpha\rangle = \int |x\rangle\langle x|\alpha\rangle\, dx \longrightarrow \langle p|\alpha\rangle = \int \langle p|x\rangle\langle x|\alpha\rangle\, dp$$

$$\rightarrow \quad \varphi(p) = \int u_p^*(x)\, \psi(x) \qquad (53)$$

(See 46)

Ex. - $|\alpha\rangle = \sum_{n=0}^{\infty} |u_n\rangle\langle u_n|\alpha\rangle = \sum_{n=0}^{\infty} C_n |u_n\rangle$

where $|u_n\rangle$: energy eig. state

Also $|\alpha\rangle = \int |\varphi_x\rangle\langle\varphi_x|\alpha\rangle\, dx = \int \psi(x)\, |\varphi_x\rangle$

Suppose $|\alpha\rangle = a_0|u_0\rangle + a_2|u_2\rangle$

$$\longrightarrow \quad a_0 = \langle u_0|\alpha\rangle \quad , \quad a_2 = \langle u_2|\alpha\rangle$$

$$|\alpha\rangle = \int |\varphi_x\rangle \underbrace{\langle\varphi_x|\left[a_0|u_0\rangle + a_2|u_2\rangle\right]}_{\psi(x)}\, dx$$

$$\psi(x) = a_0\langle\varphi_x|u_0\rangle + a_2\langle\varphi_x|u_2\rangle$$

Time Evolution of a System
in Representation-Indep. Way:

$$i\hbar \frac{\partial \Psi(t)}{\partial t} = H\Psi(t) \qquad (54)$$

$\Psi(t)$: a vector in abstract vector space (not necessarily x-space)

$$\rightarrow \frac{\partial \Psi(t)}{\partial t} = -\frac{i}{\hbar} H\Psi(t) \rightarrow \Psi(t) = e^{-iHt/\hbar}\Psi(t=0) \qquad (55)$$

$$e^{-iHt/\hbar} = \sum_{n=0}^{\infty} \frac{(-iHt/\hbar)^n}{n!} \qquad (56)$$

$$\langle B\rangle_t = \langle \Psi(t)|B|\Psi(t)\rangle = ? \qquad \text{where } B \neq B(t)$$

$$\langle e^{-iHt/\hbar}\Psi(0)|B e^{-iHt/\hbar}\Psi(0)\rangle = \langle \Psi(0)|e^{iHt/\hbar} B e^{-iHt/\hbar}\Psi(0)\rangle$$

$$= \langle \Psi(0)|B(t)\Psi(0)\rangle = \langle \Psi(0)|B(t)|\Psi(0)\rangle = \langle B(t)\rangle_0$$

$$(57)$$

where we have used $(e^{-iHt/\hbar})^+ = e^{iH^+t/\hbar} = e^{iHt/\hbar}$

and where $B(t) = e^{iHt/\hbar} B e^{-iHt/\hbar} \qquad (58)$

$$\begin{cases} |\Psi(t)\rangle = e^{iHt/\hbar}|\Psi(0)\rangle \\ B: t\text{-indep} \end{cases} \text{Schrödinger Pict.} \qquad \begin{cases} |\Psi(0)\rangle : t\text{-indep} \\ B(t) = e^{\pm iHt/\hbar} B e^{\mp iHt/\hbar} \end{cases} \text{Heisenberg Pict}$$

$$(59)$$

$$\frac{d}{dt}B(t) = \left(\frac{iH}{\hbar}e^{iHt/\hbar}\right)B\,e^{-iHt/\hbar} + e^{iHt/\hbar}B\left(-\frac{iH}{\hbar}e^{-iHt/\hbar}\right) + 0$$

$$= \frac{i}{\hbar}\left(HB(t) - B(t)H\right) = \frac{i}{\hbar}\left[H, B(t)\right] \qquad (60)$$

Ex. – For Harmonic OSC.;

$$H = \omega A^{+}A + \tfrac{1}{2}\hbar\omega$$

$$\rightarrow \quad H(t) = \omega A^{+}(t)A(t) + \tfrac{1}{2}\hbar\omega \quad \rightarrow \quad H = \omega A^{+}(t)A(t) + \tfrac{1}{2}\hbar\omega \qquad (61)$$

(Since H is const. of motion)

Now;

$$\left[A(t), A^{+}(t)\right] = \left[e^{iHt/\hbar}A\,e^{-iHt/\hbar},\; e^{+iHt/\hbar}A^{+}e^{-iHt/\hbar}\right]$$

$$= \left[A(0), A^{+}(0)\right] = \hbar \qquad (62)$$

Note that; $e^{iHt/\hbar}He^{-iHt/\hbar} = H \qquad (63)$

and $\left[H, A(t)\right] = \left[\omega A^{+}(t)A(t), A(t)\right] = \omega\left[A^{+}(t), A(t)\right]A(t)$

$$= -\hbar\omega A(t)$$

$$\left[H, A^{+}(t)\right] = \left[\omega A^{+}(t)A(t), A^{+}(t)\right] = \omega A^{+}(t)\left[A(t), A^{+}(t)\right]$$

$$= \hbar\omega A^{+}(t) \qquad (64)$$

$$\begin{matrix}(60)\\(64)\end{matrix} \rightarrow \begin{cases} \dfrac{d}{dt}A(t) = -i\omega A(t) \\[2ex] \dfrac{d}{dt}A^{+}(t) = i\omega A^{+}(t) \end{cases} \qquad (65)$$

$$\rightarrow \begin{cases} A(t) = e^{-i\omega t} A(0) \\ A^+(t) = e^{i\omega t} A^+(0) \end{cases} \qquad (66)$$

$$(5)(66) \rightarrow \begin{cases} P(t) = P(0)\cos\omega t + m\omega X(0)\sin\omega t \\ X(t) = X(0)\cos\omega t + \frac{P(0)}{m\omega}\sin\omega t \end{cases}$$