Chapter 6

The General Structure of Wave Mechanics

We had, $$H\, u_E(x) = E\, u_E(x) \qquad (1)$$

with $$H = \frac{P_{op}^2}{2m} + V(x) = \frac{1}{2m}\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 + V(x) \qquad (2)$$

H also determines the time development of a system;

Also we had the requirement;

$$\int dx\, \psi^*(x)\, \psi(x) < \infty \qquad (3)$$

$\psi(x)$; initial state of a system

$$\psi(x) \longrightarrow c\,\psi(x) \xrightarrow{\text{rename}} \psi(x)$$

such that $$\int dx\, \psi^*(x)\, \psi(x) = 1 \qquad (4)$$

The time-dep. Schrödinger eqn;

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = H\,\psi(x,t) \qquad (5)$$

Theorem: An arbitrary func. $\psi(x)$ can be expanded in a complete set of eigen funcs of H, that is,

$$\psi(x) = \sum_E C_E\, u_E(x) \qquad (6)$$

By the orthonormality cond.; that is;

$$\int u^*_{E'}(x)\, u_{E''}(x)\, dx = \delta_{E'E''} \qquad (7)$$

$$\rightarrow \int dx\, u^*_{E'}(x)\, \psi(x) = \sum_E C_E \int u^*_{E'}(x)\, u_E(x)\, dx$$

$$= \sum_E C_E\, \delta_{EE'} = C_{E'} \qquad (8)$$

Now, $u_E(x,t) = u_E(x)\, e^{-iEt/\hbar}$ (9)

As can be seen by;

$$(9) \xrightarrow{in} (5) \qquad i\hbar\left(-i\frac{E}{\hbar}\right) u_E(x) e^{-iEt/\hbar} = E\, u_E(x)\, e^{-iEt/\hbar}$$

$$\rightarrow \quad E\, u_E(x) = E\, u_E(x) \qquad (10)$$

Hence $\psi(x,t) = \sum_E C_E\, e^{-iEt/\hbar}\, u_E(x)$ (11)

In general;

$$\psi(x,t) = e^{-i\frac{H(t-t_0)}{\hbar}}\, \psi(x,t_0) \qquad (12)$$

Also in general;

$$\psi(x) = \sum_n C_n\, u_{E_n}(x) + \int dE\, C(E)\, u_E(x) \qquad (13)$$

where $\int u^*_{E_m}(x)\, u_{E_n}(x) = \delta_{mn}$

$$\int u^*_E(x)\, u_{E'}(x)\, dx = \delta(E-E') \qquad (14)$$

Postulate: $|C_E|^2$ is the probability that an energy measurement of the state described by $\psi(x)$ yields the particular eigenvalue E.

$$\text{Any measurement} \xrightarrow[\text{yields}]{\text{of observable } A} a' \text{ with the probability } |C_{a'}|^2$$

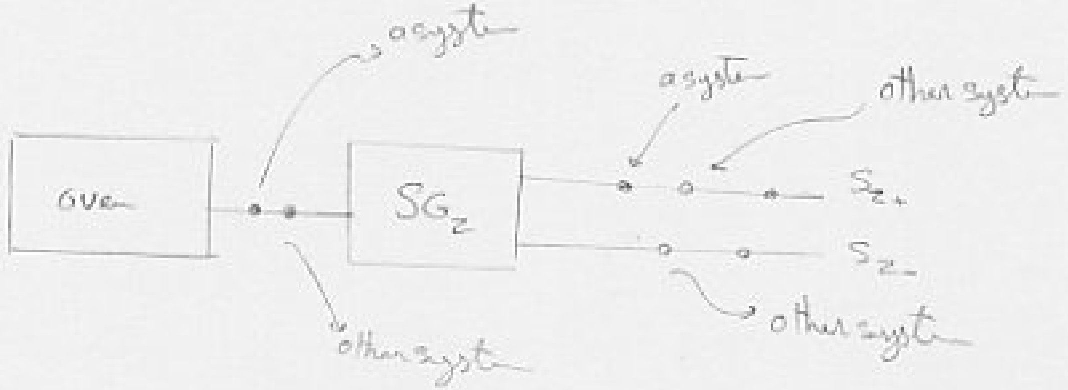
we cannot predict which a' will occur

In Q.M. as in classical theory, a measurement must be reproducible to have any meaning.

Thus if the observer, upon making a single measurement on a system finds that the eigenvalue is, say, a_1, then a subsequent measurement for the system must again yield a_1 (the eigenvalue of the observable A).

Hence after the first measurement, the state of the system is described by a new wave func. namely $u_{a_1}(x)$, only then will a repeated measurement (with the same observable A) yield a_1 with probability 1.

In other words, a measurement projects a state into an eigenstate of the observable.



Remark: The expansion theorem may be viewed as a generalization of the expansion of a vector $\bar{A}$ in terms of orthonormal unit vectors in N-dimensional vector space,

$$A = a_1\hat{i}_1 + a_2\hat{i}_2 + \cdots a_N \hat{i}_N \quad (15)$$

where $\hat{i}_k \cdot \hat{i}_\ell = \delta_{k\ell}$

and $\quad a_k = \hat{i}_k \cdot A \quad (16)$

(8) and analogy to (16) $\longrightarrow C_F = \int u_F^*(x)\, \Psi(x)\, dx \quad (17)$

(scalar product)

A convenient notation (following Dirac):

$$\int \varphi^*(x)\, \Psi(x) = \langle \varphi | \Psi \rangle \quad (18)$$

Remark: Similitary

$\bar{A} + \bar{B} = \bar{C} \quad \longleftrightarrow \quad \varphi(x) + \chi(x) = \Psi(x) \quad (19)$

vectors $\qquad\qquad$ square integrable funcs.

$$c\bar{A} = \bar{B} \quad \longleftrightarrow \quad c\varphi(x) = \psi(x) \qquad (20)$$

In both cases we have linear vector space.

We define the notation:

$$\langle A|B\rangle = A\cdot B \qquad (21)$$

$$\langle \varphi|\psi\rangle = \int dx\, \varphi^*(x)\, \psi(x) \qquad (22)$$

In Q.M. the vector space is infinite dimensional.

In fact, since in (22) it is the continuous label $\underline{x}$ that play the role that the index $\underline{i}$ plays in

$$A\cdot B = \sum_{i=1}^{N} a_i b_i \qquad (23)$$

we see that the space is continuously infinite.

In mathematical parlance, the square integrable fncs. form a Hilbert space and the energy eigenfncs form a complete set of basis vectors.

In Q.M. we are interested in linear ops. with the property:

$$A(\alpha\psi_1 + \beta\psi_2) = \alpha A\psi_1 + \beta A\psi_2 \qquad (24)$$

α, β: complex numbers

Def.: $$\langle A \rangle_\psi = \int \psi^*(x)\, A\, \psi(x)\, dx \qquad (25)$$

In chap. 4 in a simple example (P59) we showed that

$$\langle H \rangle_\psi = \int \psi^*(x)\, H\, \psi(x)\, dx \qquad (26)$$

is <u>real</u>, (expected for a physical measurable quantity).
Such operators are called <u>Hermitian</u>.

Also
$$\langle A \rangle_\psi^* = \int [A\psi(x)]^* \psi(x)\, dx \qquad (27)$$

Def.: A^+ (A-dagger) (Hermitian conjugate op.)

$$\int [A\psi(x)]^* \psi(x)\, dx = \int \psi^*(x)\, A^+ \psi(x)\, dx \qquad (28)$$

Remark:
$\langle Ax, y \rangle = \langle x, A^+ y \rangle$

Ex. — $OP = \frac{d}{dx}$

$$\int dx \left(\frac{d\psi}{dx}\right)^* \psi = \int dx \frac{d}{dx}(\psi^* \psi) - \int dx\, \psi^* \frac{d\psi}{dx}$$

$$= (\psi^*\psi)\Big|_{-\infty}^{\infty} - \int dx\, \psi^* \frac{d}{dx}\psi = 0 - \int dx\, \psi^* \frac{d\psi}{dx}$$

$$\rightarrow \left(\frac{d}{dx}\right)^+ = -\frac{d}{dx}$$

Ex – It can be shown,

$$\left(\frac{d^2}{dx^2} - a e^{ix}\right)^{\dagger} = \left(\frac{d^2}{dx^2} - a^* e^{-ix}\right)$$

For Hermitian op. :

$$\langle A\rangle_{\psi}^{*} = \overbrace{\int [A\psi(x)]^{*}\psi(x)\,dx = \int \psi^{*}(x)\, A^{\dagger}\, \psi(x)\,dx}^{\text{H.C. Def.}}$$

$$\underbrace{\qquad = \langle A\rangle}_{\text{H. Def.}} = \int \psi^{*}(x)\, A\,\psi(x)\,dx \qquad (29)$$

$$\forall \psi(x)$$

$$\rightarrow \quad A^{\dagger} = A$$

In Dirac notation;

$$\int \varphi^{*}(x)\, A\,\psi(x)\,dx = \langle\varphi|A|\psi\rangle$$

$$\rightarrow \quad \langle\varphi|A|\psi\rangle^{*} = \int (A\psi(x))^{*}\,\varphi(x)\,dx \qquad (30)$$

$$\left\{\begin{array}{l}\text{Remark;}\\ \langle x,y\rangle^{*} = \langle y,x\rangle\end{array}\right.$$

Now take $\psi = \psi_1 + \lambda\psi_2$

$$(28) \rightarrow \int (A\psi_1 + \lambda A\psi_2)^{*}(\psi_1 + \lambda\psi_2)\,dx = \int (\psi_1 + \lambda\psi_2)^{*} A^{\dagger}(\psi_1 + \lambda\psi_2)\,dx$$

$$\rightarrow \cancel{\int (A\psi_1)^{*}\psi_1\,dx} + \lambda\int (A\psi_1)^{*}\psi_2\,dx + \lambda^{*}\int (A\psi_2)^{*}\psi_1\,dx + |\lambda|^2 \cancel{\int (A\psi_2)^{*}\psi_1\,dx}$$

$$= \cancel{\int \psi_1^{*} A^{\dagger}\psi_1\,dx} + \lambda\int \psi_1^{*}A^{\dagger}\psi_2\,dx + \lambda^{*}\int \psi_2^{*}A^{\dagger}\psi_1\,dx + |\lambda|^2 \cancel{\int \psi_2^{*}A^{\dagger}\psi_2\,dx}$$

(31)

Equating the coeffs. of λ and λ^* from both sides;

$$\rightarrow \int (A\psi_1)^* \psi_2 \, dx = \int \psi_1^* A^\dagger \psi_2 \, dx \quad (32)$$

$$\begin{matrix}(30)\\(32)\end{matrix} \rightarrow \quad \langle \varphi | A | \psi \rangle^* = \int (A\psi(x))^* \varphi(x) \, dx =$$

$$= \int \psi^*(x) A^\dagger \varphi(x) \, dx = \langle \psi | A^\dagger | \varphi \rangle \quad (33)$$

All Hermitian ops. have eigen funcs. with the property;

$$A\, u_{a'}(x) = a'\, u_{a'}(x) \quad (34)$$

$\{u_a(x)\}$: discrete and/or continuous

Ex. $\{u_p(x)\}$: continuous (momentum)

$\{u_n(x)$: discrete (eigenvalues $= \pm 1$) (parity)

We have; $$\int u_a^*(x)\, u_{a'}(x) = \delta(a, a') \quad (35)$$

where $\delta(a, a') = \begin{cases} \delta_{aa'} & \text{Kroenecker } \delta\text{-func} \\ \text{or} & \\ \delta(a-a') & \text{Dirac } \delta\text{-func.} \end{cases}$

(34) $\Rightarrow$ $a = \int u_a^*(x)\, A\, u_a(x)\, dx$ (36)

or, $a = \langle u_a | A | u_a \rangle$ (37)

For Hermitian op.,

(33) $\rightarrow$ $\langle u_a | A | u_a \rangle^* = \langle u_a | A | u_a \rangle = a$ real (38)

in general $\langle \psi | A | \psi \rangle^* = \langle \psi | A | \psi \rangle$ real

Just as for the Hamiltonian, the eigenfuncs. of any Hermitian op. like A also form a complete set; $\{u_a\}$,

so that the expansion theorem

$$\psi(x) = \sum_a c_a u_a(x) \quad (39)$$

where $c_a = \int u_a^*(x)\, \psi(x)\, dx = \langle u_a | \psi \rangle$ (40)

holds. c_a: probability amplitude

$|c_a|^2$: the probability of finding the eigenvalue $\underline{a}$ in making a measurement of A on a system described by $\psi(x)$

Before the measurement of A : $\psi(x)$ system description

After " " " " : $u_a(x)$ " "

Now,

$$A\, u_a(x) = a\, u_a(x)$$
$$B\, u_a(x) = b\, u_a(x) \qquad (41)$$

$u_a(x)$: Simultaneous eigenfunc. of A and B.

$$(41) \rightarrow A(B u_a(x)) = A(b u_a(x)) = b(A u_a(x)) = ab\, u_a(x)$$
$$B(A u_a(x)) = B(a u_a(x)) = a(B u_a(x)) = ab\, u_a(x) \qquad (42)$$

$$\rightarrow (AB-BA)u_a(x) = 0 \qquad \forall\, u_a(x) \in \{u_a(x)\} \qquad (43)$$

$\rightarrow$ For all $\psi(x) = \sum_a C_a u_a(x)$ (square integrable func.)

$$\sum_a C_a (AB-BA) u_a(x) = (AB-BA) \sum C_a u_a(x)$$
$$= (AB-BA)\psi(x) = 0 \qquad (44)$$

$$\rightarrow [A,B] = 0 \qquad (45)$$

Now; if $[A,B]=0$

$$\rightarrow AB\, u_a(x) = BA\, u_a(x) = aB\, u_a(x) \qquad (46)$$

$$\rightarrow A[B u_a(x)] = a[B u_a(x)] \qquad (47)$$

$\rightarrow B u_a(x)$ is an eigenfunc. of A, with eigenvalue $\underline{a}$.

i) Nondegenerate case,

In this case, there is only one eigenfunc of A $\xleftrightarrow[\text{to}]{\text{corresponding}}$ a

$$\longrightarrow B u_a(x) \sim u_a(x) \quad \longrightarrow B u_a(x) = b\, u_a(x) \quad (48)$$

$\longrightarrow u_a(x)$: Simultaneous eigenfunc. of A and B

Ex. - A particle in the box,

$$A = H \,, \quad B = \Pi \qquad [H, \Pi] = 0$$

ii) Degenerate case;

$$\begin{aligned} A\, u_a^{(1)}(x) &= a\, u_a^{(1)}(x) \\ A\, u_a^{(2)}(x) &= a\, u_a^{(2)}(x) \end{aligned} \qquad (49)$$

Ex. - A free particle,

$$A = H \,, \quad B = P \qquad , \quad [H, P] = 0$$

$u_a^{(1)} = e^{iP/\hbar\, x}$ and $u_a^{(2)} = e^{-iP/\hbar\, x}$ have the same energy.

Then we can only assert that (acc. to the Dirac explanation about the measurement of $[A,B]=0$ observables).

$$\begin{aligned} B\, u_a^{(1)}(x) &= b_{11}\, u_a^{(1)}(x) + b_{12}\, u_a^{(2)}(x) \\ B\, u_a^{(2)}(x) &= b_{21}\, u_a^{(1)}(x) + b_{22}\, u_a^{(2)}(x) \end{aligned} \qquad (50)$$

However, we can take linear combinations of these equs. to obtain equs. of the type,

$$B\, V_a^{(1)}(x) = b_1 V_a^{(1)}(x)$$
$$B\, V_a^{(2)}(x) = b_2 V_a^{(2)}(x) \qquad (51)$$

For example; $\quad B(u_a^{(1)} + \lambda u_a^{(2)}) = (b_{11} + \lambda b_{21}) u_a^{(1)} + (b_{21} + \lambda b_{22}) u_a^{(2)}$

$$= b_{1,2}(u_a^{(1)} + \lambda u_a^{(2)}) \qquad (52)$$

Provided we choose λ such that;

$$(52) \rightarrow \quad \frac{b_{12} + \lambda b_{22}}{b_{11} + \lambda b_{21}} = \frac{\lambda}{1} \qquad (53)$$

(equating the coeffs. of the independent vectors)

$$\xrightarrow{\text{Sol.}} \lambda_1, \lambda_2 \xleftrightarrow[\text{to}]{\text{corresponding}} b_1, b_2$$

It is more appropriate to denote the simultaneous eigenfncs of A and B in (51) by,

$$u_{ab}^{(1)}(x) \longrightarrow b_1 \quad , \quad u_{ab}^{(2)}(x) \longrightarrow b_2$$

$$\int u_{ab}^{(1)*}(x)\, u_{ab}^{(2)}(x)\, dx = 0 \qquad \text{(orthogonal)} \qquad (54)$$

In practice, for <u>2-fold</u> degeneracy, the degenerate eigenfncs. of A, if they are taken to be or<u>thogonal</u> to each other, will automatically be eigenfncs. of B.

Ex. – For free particles,

$$u^{(1)}_{ab}(x) = u^{(1)}_{Ep}(x) = e^{ikx} \quad , \quad u^{(2)}_{ab}(x) = u^{(2)}_{Ep}(x) = e^{-ikx}$$

$$\int_{-\infty}^{\infty} [e^{ikx}]^* e^{-ikx}\, dx = \int_{-\infty}^{\infty} e^{ix(k+k)}\, dx = \delta(k-(-k)) = 0$$

$$A = H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \qquad B = P_{op} = \frac{\hbar}{i}\frac{d}{dx} \quad \rightarrow [A, B] = 0$$

$$u^{(1)}_a = u^{(1)}_E = \frac{1}{\sqrt{2\pi}} e^{ikx} \qquad u^{(2)}_a = u^{(2)}_E = \frac{1}{\sqrt{2\pi}} e^{-ikx}$$

$$H\, u^{(1)}_E = \frac{\hbar^2 k^2}{2m} u^{(1)}_E = \frac{p^2}{2m} u^{(1)}_E = E\, u^{(1)}_E$$

(2-fold degeneracy)

$$H\, u^{(2)}_E = \frac{\hbar^2 k^2}{2m} u^{(2)}_E = \frac{p^2}{2m} u^{(2)}_E = E\, u^{(2)}_E$$

$$P\, u^{(1)}_E(x) = P_{11}\, u^{(1)}_E(x) + P_{12}\, u^{(2)}_E(x)$$

$$P\, u^{(2)}_E(x) = P_{21}\, u^{(1)}_E(x) + P_{22}\, u^{(2)}_E(x)$$

$$P_{ji} = \int u^{(i)*}_E(x)\, P\, u^{(j)}_E(x)\, dx$$

$$P_{11} = \frac{1}{2\pi}\int (e^{ikx})^* \left(\frac{\hbar}{i}\frac{d}{dx}\right) e^{ikx}\, dx = \hbar k = p$$

$$P_{22} = \frac{1}{2\pi}\int (e^{-ikx})^* \left(\frac{\hbar}{i}\frac{d}{dx}\right) e^{-ikx}\, dx = -\hbar k = -p$$

$$P_{12} = P_{21} = 0$$

$$P\,u_E^{(1)}(x) = P\,u_E^{(1)}(x) + 0$$

$$P\,u_E^{(2)}(x) = 0 - P\,u_E^{(2)}(x)$$

$$(52) \rightarrow \quad P\left(u_E^{(1)} + \lambda u_E^{(2)}\right) = (P_{11} + \lambda P_{21})\,u_E^{(1)} + (P_{21} + \lambda P_{22})\,u_E^{(2)}$$

$$P\left(u_E^{(1)} + \lambda u_E^{(2)}\right) = P_{1,2}\left(u_E^{(1)} + \lambda u_E^{(2)}\right)$$

$$(53) \rightarrow \quad \lambda = \frac{P_{12} + \lambda P_{22}}{P_{11} + \lambda P_{21}} = \frac{0 - \lambda P}{P + 0}$$

$$\lambda = \frac{-\lambda P}{P} \qquad \lambda P = -\lambda P \quad \rightarrow \lambda = 0$$

$$\rightarrow \quad P\left(u_E^{(1)} + 0\right) = P_1\left(u_E^{(1)} + 0\right)$$

$$\rightarrow \quad \frac{\hbar}{i}\frac{d}{dx}\left(\frac{1}{\sqrt{2}} e^{ikx}\right) = \underbrace{\hbar k}_{P}\left(\frac{1}{\sqrt{2}} e^{ikx}\right)$$

Instead if we take;

$$P\left(\lambda u_E^{(1)} + u_E^{(2)}\right) = \cdots = P_{1,2}\left(\lambda u_E^{(1)} + u_E^{(2)}\right)$$

$$\longrightarrow \quad \lambda = 0$$

$$\longrightarrow \quad P\left(0 + u_E^{(2)}\right) = P_{1,2}\left(0 + u_E^{(2)}\right)$$

$$\longrightarrow \quad \frac{\hbar}{i}\frac{d}{dx}\left(\frac{1}{\sqrt{2}} e^{-ikx}\right) = \underbrace{-\hbar k}_{-P}\left(\frac{1}{\sqrt{2}} e^{-ikx}\right)$$

$$\rightarrow \quad u_{E,P}^{(1)} = u_{E,P}^{+P} = \frac{1}{\sqrt{2\pi}} e^{ikx} \qquad\qquad u_{E,P}^{(2)} = u_{E,P}^{-P} = \frac{1}{\sqrt{2\pi}} e^{-ikx}$$

Even after finding eigenfuncs. of A and then making linear combinations that are eigenfuncs. of a commuting op. B, there may still be some degeneracy, that is there are several eigenfuncs. of A and B simultaneously, with the same a and b.

This means that → there must be a third operator C that commutes with A and B and the funcs. can be recombined to be simultaneous eigenfuncs. of A, B and C whose eigenvalues distinguish the degenerate eigenfuncs of A and B.

This will go on until there is no more degeneracy.

The set of mutually commuting ops. $\{A, B, C, \ldots M\}$ of which our set of funcs. is a set of common eigenfuncs. is called a complete set of commuting observables.

$$[A,B] = [A,C] = \cdots = [A,M] = 0$$
$$[B,C] = [B,D] = \cdots = [B,M] = 0 \qquad (55)$$
$$\vdots$$

$$A\,u_{ab\ldots m}(x) = a\,u_{ab\ldots m}(x)$$
$$B\,u_{ab\ldots m}(x) = b\,u_{ab\ldots m}(x) \qquad (56)$$
$$\vdots$$
$$M\,u_{ab\ldots m}(x) = m\,u_{ab\ldots m}(x)$$

This is the <u>largest</u> possible amount of information that we can have about the system <u>all at once</u>.

Because if we consider another op. F, that

$$F \notin \{A, B, \dots M\} \quad \text{(or any func. of them)}$$

$$U_{ab\dots m}(x) \xrightarrow[\text{measurement}]{F} \neq f\, U_{ab\dots m}(x)$$

What happens when $[A,B] \neq 0$ (57)

Def.: $(\Delta A)^2 = \langle A^2 \rangle - \langle A \rangle^2$ dispersion (58)

Note that $(\Delta A)^2 = \langle (A - \langle A \rangle)^2 \rangle$

Since, $\langle A^2 - 2A\langle A \rangle + \langle A \rangle^2 \rangle = \langle A^2 \rangle - \langle A \rangle \langle A \rangle$
$= \langle A^2 \rangle - \langle A \rangle^2$

$\rightarrow$ $(\Delta A)^2$ deals with the magnitude of fluctuations about the mean.

The uncertainty relation:

$$(\Delta A)^2 (\Delta B)^2 \geqslant \frac{1}{4} \left(\langle i[A,B] \rangle \right)^2 \quad (59)$$

A, B: Hermitian ops.

Proof: Let $U = A - \langle A \rangle$

$$V = B - \langle B \rangle \qquad (60)$$

and consider $\varphi = U\psi + i\lambda V\psi \qquad (61)$

The $I(\lambda) = \int dx\, \varphi^* \varphi \geq 0 \qquad (62)$

λ: real

$$I(\lambda) = \int dx\, (U\psi + i\lambda V\psi)^* (U\psi + i\lambda V\psi)$$

$$= \int dx\, (U\psi)^* (U\psi) + \lambda^2 \int dx\, (V\psi)^* (V\psi)$$

$$+ i\lambda \int dx\, \left[(U\psi)^* (V\psi) - (V\psi)^* (U\psi) \right] \qquad (63)$$

A, B: Hermitian $\longrightarrow$ U, V: Hermitian

$$\rightarrow I(\lambda) = \int dx\, \psi^* \left(U^2 + \lambda^2 V^2 + i\lambda [U, V] \right) \psi$$

$$= (\Delta A)^2 + \lambda^2 (\Delta B)^2 + i\lambda \int dx\, \psi^* [U, V] \psi$$

$$= (\Delta A)^2 + \lambda^2 (\Delta B)^2 + i\lambda \langle [A, B] \rangle \geq 0 \qquad (64)$$

$$\frac{\partial I(\lambda)}{\partial \lambda} = 0 \rightarrow 2\lambda (\Delta B)^2 + i \langle [A, B] \rangle = 0$$

$$\rightarrow \lambda = -i \frac{\langle [A, B] \rangle}{2(\Delta B)^2} \qquad \text{Min. of the expression}$$

(65)

$(65) \to (64)$ $$(\Delta A)^2 - \frac{\langle [A,B] \rangle^2}{4(\Delta B)^2} + \frac{\langle [A,B] \rangle^2}{2(\Delta B)^2} \geq 0$$

$$\to \quad (\Delta A)^2 (\Delta B)^2 \geq \frac{1}{4} \langle i[A,B] \rangle^2$$

Ex. – $A = x$, $B = P$, $[x,p] = i\hbar$

$$(\Delta x)^2 (\Delta p)^2 \geq \frac{\hbar^2}{4}$$

Notice that in the derivation no use was made of wave properties x-space or p-space wave funcs. or particle-wave duality. Our result depends entirely on the op. properties of the observables A and B.

Now, What is cl. limit of Q. theory?

To answer this first;

$$\frac{d}{dt} \langle A \rangle_t = ? \qquad A: \text{observable}$$

$$\langle A \rangle_t = \int \psi^*(x,t) A \psi(x,t) dx$$

$$\frac{d}{dt} \langle A \rangle_t = \int \psi^* \frac{\partial A}{\partial t} \psi dx + \int \frac{\partial \psi^*}{\partial t} A \psi dx + \int \psi^* A \frac{\partial \psi}{\partial t} \tag{66}$$

$$\frac{d}{dt}\langle A\rangle_t = \langle \frac{\partial A}{\partial t}\rangle_t + \int \left(\frac{1}{i\hbar} H\Psi\right)^* A\Psi\, dx + \int \Psi^* A \left(\frac{1}{i\hbar} H\Psi\right) dx$$

$$= \langle \frac{\partial A}{\partial t}\rangle_t + \frac{i}{\hbar}\int \Psi^* H A \Psi\, dx - \frac{i}{\hbar}\int \Psi^* A H \Psi\, dx$$

$$\frac{d}{dt}\langle A\rangle_t = \langle \frac{\partial A}{\partial t}\rangle_t + \frac{i}{\hbar}\langle [H,A]\rangle_t \qquad (67)$$

where we have used $H = H^+$ and the schrödinger op.

If $\frac{\partial A}{\partial t} = 0 \rightarrow \frac{d}{dt}\langle A\rangle_t = \frac{i}{\hbar}\langle [H,A]\rangle_t \qquad (68)$

If $[H,A] = 0 \rightarrow \frac{d}{dt}\langle A\rangle_t = 0 \rightarrow \langle A\rangle_t = \text{const.}$

(69)

$\rightarrow$ A: Const. of motion

Ex. – Let us consider successively $A = x$ and $A = P$,

$$\frac{d}{dt}\langle x\rangle = \frac{i}{\hbar}\langle [H,x]\rangle = \frac{i}{\hbar}\langle \left[\frac{P^2}{2m} + V(x), x\right]\rangle$$

since $[V(x), x] = 0$

and $[P^2, x] = P[P,x] + [P,x]P = 2\frac{\hbar}{i}P$

where we have used $[AB, C] = ABC - CAB =$

$$= ABC - ACB + ACB - CAB = A[B,C] + [A,C]B$$

(70)

$$\frac{d}{dt}\langle x\rangle = \langle \frac{p}{m} \rangle \qquad (71)$$

Now, $\frac{d}{dt}\langle p\rangle = \frac{i}{\hbar}\langle [\frac{p^2}{2m}+V(x), p] \rangle = -\frac{i}{\hbar}\langle [p, V(x)]\rangle$

Since $[p^2, p] = 0$

$[p, V(x)] = ?$ $\qquad [p, V(x)]\psi(x) = pV(x)\psi(x) - V(x)p\psi(x)$

$$= \frac{\hbar}{i}\frac{d}{dx}\left(V(x)\psi(x)\right) - \frac{\hbar}{i}V(x)\frac{d}{dx}\psi(x) = \frac{\hbar}{i}\frac{dV(x)}{dx}\psi(x)$$

$$\rightarrow [p, V(x)] = \frac{\hbar}{i}\frac{dV(x)}{dx} \qquad (72)$$

$$\frac{d}{dt}\langle p\rangle_t = -\langle \frac{dV(x)}{dx} \rangle_t \qquad (73)$$

$$(71)(72) \rightarrow \quad m\frac{d^2}{dx^2}\langle x\rangle_t = -\langle \frac{dV(x)}{dx}\rangle_t \qquad (74)$$

This looks very much like the equ. of motion of a classical point particle in a pot. $V(x)$;

$$m\frac{d^2 x_{cl}}{dt^2} = -\frac{dV(x_{cl})}{dx_{cl}}$$

The only thing that keeps us from making the identification

$$x_{cl} = \langle x\rangle$$

is that

$$\langle \frac{dV(x)}{dx}\rangle \neq \frac{dV(\langle x\rangle)}{d\langle x\rangle}$$

Under circumstances where the above inequality becomes an approximate equality, the motion is essentially classical, as was first noted by Ehrenfest.

This requires that the pot. be a slowly varying func. of its argument.

$$F(x) = -\frac{dV(x)}{dx}$$

$$F(x) = F(\langle x\rangle) + (x - \langle x\rangle)F'(\langle x\rangle) + \frac{(x-\langle x\rangle)^2}{2!}F''(\langle x\rangle) + \cdots$$

If uncertainty $(\Delta x)^2 = \langle (x-\langle x\rangle)^2\rangle \rightarrow$ small

$$\langle F(x)\rangle \simeq F(\langle x\rangle) + \langle x - \langle x\rangle\rangle F'(\langle x\rangle)$$

$$\simeq F(\langle x\rangle)$$