Linear operators

An operator $\hat{\alpha}$ is a linear operator if for arbitrary operands $\psi_1(x)$ and $\psi_2(x)$ we get

$$\hat{\alpha}(\psi_1 + \psi_2) = \hat{\alpha}\psi_1 + \hat{\alpha}\psi_2 \quad ; \text{——} (1)$$

and for an operator $\hat{c}$ we get

$$\hat{c}(\psi_1 + \psi_2) = \hat{c}\psi_1 + \hat{c}\psi_2 \quad ; \text{——} (2)$$

and for an arbitrary Constant c

$$\hat{\alpha} c = c \hat{\alpha} \quad \text{——} (3)$$

Hermitian operators → [An operator $\hat{A}$ or A associated with a dynamical variable is said to be Hermitian if its average value in any state is real.

For any two well-behaved functions $f(x)$ and $g(x)$ vanishing at infinity, an operator $\hat{O}$ satisfying the equation,

$$= \left[\int_{-\infty}^{+\infty} f^*(x) (\hat{O} g(x)) \, dx\right]^*$$

$$\int_{-\infty}^{+\infty} g^*(x) [\hat{O} f(x)] \, dx = \int_{-\infty}^{+\infty} [\hat{O} g(x)]^* f(x) \, dx \quad \text{——} (4)$$

is said to be Hermitian.

Any operator $\hat{A}$, representing some observable, must for state ψ, yield an expectation value

$$\langle \hat{A} \rangle = \int \psi^* \hat{A} \psi \, d\tau = (\psi, \hat{A}\psi)$$

which is a real number. Now $\hat{A}$ must satisfy the condition.

$$\left(\int \psi^* \hat{A} \psi \, d\tau\right)^* = \int \psi^* \hat{A} \psi \, d\tau$$

or $$\int (\hat{A}\psi)^* \psi \, d\tau = \int \psi^* \hat{A} \psi \, d\tau$$

or $$(\hat{A}\psi, \psi) = (\psi, \hat{A}\psi)$$

A linear operator which obey the above rule is called a Hermitian operator.

Thus the Hermitian operator can be applied to either factor in the scalar product.

More generally, a Hermitian operator satisfies the relation

$$(\psi, A\phi) = (A\psi, \phi)$$

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for any two functions ψ and ϕ. To prove the above equation, for Hermitian operator A and state function $(\psi+\phi)$, we have

$$\int(\psi+\phi)^* A(\psi+\phi)\, d^3r = \int[A(\psi+\phi)]^*(\psi+\phi)\, d^3r$$

or $$\int \psi^* A\psi\, d^3r + \int \psi^* A\phi\, d^3r + \int \phi^* A\psi\, d^3r + \int \phi^* A\phi\, d^3r$$

$$= \int (A\psi)^*\psi\, d^3r + \int (A\phi)^*\psi\, d^3r + \int (A\psi)^*\phi\, d^3r + \int (A\phi)^*\phi\, d^3r$$

As A is Hermitian, hence

$$\int \psi^* A\psi\, d^3r = \int (A\psi)^*\psi\, d^3r$$

and $$\int \phi^* A\phi\, d^3r = \int (A\phi)^*\phi\, d^3r$$

$$\cancel{\int \psi^* A\psi\, d^3r + \int \phi^* A\phi\, d^3r} =$$

$$\therefore \cancel{\int \psi^* A\psi\, d^3r} + \cancel{\int \phi^* A\phi\, d^3r} = \cancel{\int (A\psi)^*\psi\, d^3r} + \cancel{\int (A\phi)^*\phi\, d^3r}$$

Again for the state function $(\psi + i\phi)$ we have

$$\int(\psi+i\phi)^* A(\psi+i\phi)\, d^3r = \int[A(\psi+i\phi)]^*(\psi+i\phi)\, d^3r$$

or $$\int \psi^* A\psi\, d^3r + \int \phi^* A\phi\, d^3r + i\int \psi^* A\phi\, d^3r - i\int \phi^* A\psi\, d^3r$$

$$= \int (A\psi)^*\psi\, d^3r + \int (A\phi)^*\phi\, d^3r + i\int (A\psi)^*\phi\, d^3r - i\int (A\phi)^*\psi\, d^3r$$

or $\cancel{\int \psi^* A}$

Now $$\cancel{\int (A\psi)^*\psi\, d^3r} + \int \psi^* A\phi\, d^3r + \int \phi^* A\psi\, d^3r + \cancel{\int (A\phi)^*\phi\, d^3r}$$

$$= \cancel{\int (A\psi)^*\psi\, d^3r} + \int (A\phi)^*\psi\, d^3r + \int (A\psi)^*\phi\, d^3r + \cancel{\int (A\phi)^*\phi\, d^3r}$$

$$\therefore \int \psi^* A\phi\, d^3r + \int \phi^* A\psi\, d^3r = \int (A\phi)^*\psi\, d^3r + \int (A\psi)^*\phi\, d^3r \qquad (9)$$

Again for the state function $(\psi + i\phi)$, we have

$$\int (\psi + i\phi)^* A (\psi + i\phi) d^3r = \int [A(\psi + i\phi)]^* (\psi + i\phi) d^3r$$

or $$\cancel{\int \psi^* A \psi d^3r} + \cancel{\int \phi^* A \phi d^3r} + i\int \psi^* A \phi d^3r - i\int \phi^* A \psi d^3r$$

$$= \cancel{\int (A\psi)^* \psi d^3r} + \cancel{\int (A\phi)^* \phi d^3r} + i\int (A\psi)^* \phi d^3r - i\int (A\phi)^* \psi d^3r$$

or $$\int \psi^* A \phi d^3r - \int \phi^* A \psi d^3r = \int (A\psi)^* \phi d^3r - \int (A\phi)^* \psi d^3r \quad \text{(b)}$$

Now both equations (a) and (b) holds good simultaneously if

$$\left.\begin{aligned} \int \psi^* A \phi d^3r &= \int (A\psi)^* \phi d^3r \\ \text{i.e } (\psi, A\phi) &= (A\psi, \phi) \\ \text{and } \int \phi^* A \psi d^3r &= \int (A\phi)^* \psi d^3r \\ \text{i.e } (\phi, A\psi) &= (A\phi, \psi) \end{aligned}\right\} \quad \text{— (c)}$$

i.e the operator can be applied to either factor in the scalar product.

If an operator satisfies equations (c) whenever ψ and ϕ are normalisable, we call it Hermitian, self adjoint or real.

Thus ψ and ϕ are two acceptable normalised wave functions defined over a certain range of configuration space d^3r or $d\tau$ then the operator A associated with a dynamical variable is Hermitian if the equations (c) are satisfied.

We conclude that every Schrodinger operator associated with a real dynamical variable is Hermitian

Properties of Hermitian operators

(i) Every eigen value of Hermitian operator is real.

Proof → ~~the~~ Let ψ be an eigen function of Hermitian operator A belonging to the eigen value λ.

According to the condition of Hermitian oper

$$\int_{-\infty}^{\infty} \psi^* A \phi \, dx = \int_{-\infty}^{\infty} A^* \psi^* \cdot \phi \, dx$$

Putting $\phi = \psi$ in above relation, we get

$$\int \psi^* A \psi \, dx = \int A^* \psi^* \cdot \psi \, dx$$

But according to eigen value equation

$A\psi = \lambda\psi$ where λ is the eigen value of the operator A and ψ is eigen function

Hence $\int \psi^* \lambda \psi \, dx = \int \lambda^* \psi^* \cdot \psi \, dx$

and λ is a number, therefore

$$\lambda \int \psi^* \psi \, dx = \lambda^* \int \psi^* \psi \, dx$$

and hence $\lambda = \lambda^*$

This is only possible if λ is a real number.

This proves that every Hermitian operator gives real eigen values.

(ii) Prove that the eigenfunctions of a Hermitian operator corresponding to different eigenvalues will be orthogonal functions.

Proof → Let P be any Hermitian operator and ψ_1 and ψ_2 be two eigen functions of operator P. If λ_1 and λ_2 are eigen values corresponding to two

The operator (AB − BA) is called the commutator of A and B and is represented by eigen functions of the same operator, then

$$P\psi_1 = \lambda_1\psi_1$$
$$P\psi_2 = \lambda_2\psi_2$$

Scalar product of $P\psi_1$ and ψ_2 is

$$(\psi_2, P\psi_1) = (\psi_2, \lambda_1\psi_1) = \lambda_1(\psi_2, \psi_1) \quad \text{—— (1)}$$

Since λ_1 is real number

Similarly the scalar product of $P\psi_2$ and ψ_1

is $$(P\psi_2, \psi_1) = (\lambda_2\psi_2, \psi_1)$$
$$= \lambda_2(\psi_2, \psi_1)$$

as λ_2 is also real number

But $(P\psi_2, \psi_1) = (\psi_2, P\psi_1)$ Since P is Hermitian operator.

~~Hence~~ $= \cancel{(\psi_2, \lambda_1\psi_1)}$

Hence $\cancel{(P\psi_2, \psi_1) = \psi_2}$

$$(\psi_2, P\psi_1) = \lambda_2(\psi_2, \psi_1) \quad \text{—— (2)}$$

Subtracting (1) from (2)

$$(\lambda_2 - \lambda_1)(\psi_2, \psi_1) = 0$$

But $(\lambda_2 - \lambda_1)$ is not zero.

Therefore, $(\psi_2, \psi_1) = \int \psi_2^* \psi_1 \, dx = 0$

Hence two eigenfunctions are ~~oth~~ orthogonal.

(iii) The product of the Hermitian operators is Hermitian if and only if they commute.

or

~~If β and γ are Commuting Hermitian operators~~, then ~~operator $\beta\gamma$ is also Hermitian.~~

~~Ans~~ Proof $\rightarrow$ To prove this, we write

$$\int \psi^* \beta\gamma\phi \, dx = \int \psi^* \beta(\gamma\phi) \, dx$$

If β is Hermitian, then

$$\int \psi^* \beta(\gamma\phi) \, dx = \int \beta^* \psi^* \gamma\phi \, dx \quad \text{—— (1)}$$

and of $\hat{\gamma}$ is also Hermitian. Hence

$$\int \hat{\beta}^* \hat{\gamma}^* \psi^* \phi \, dx = \int \hat{\gamma}^* \hat{\beta}^* \psi^* \phi \, dx \qquad (2)$$

Now if $\hat{\beta}$ and $\hat{\gamma}$ are both Hermitian, then

$$\int \psi^* \hat{\beta} \hat{\gamma} \phi \, dx = \int \hat{\beta}^* \psi^* \hat{\gamma} \phi \, dx$$

$$= \int \hat{\gamma}^* \hat{\beta}^* \psi^* \phi \, dx \qquad (3)$$

Now since $\hat{\beta}$ and $\hat{\gamma}$ commute i.e.

$$[\hat{\beta}, \hat{\gamma}] = 0$$

$$\hat{\beta}\hat{\gamma} - \hat{\gamma}\hat{\beta} = 0$$

$$\hat{\beta}\hat{\gamma} = \hat{\gamma}\hat{\beta}$$

So equation (3) can be expressed as

$$\int \psi^* \hat{\beta} \hat{\gamma} \phi \, dx = \int (\hat{\beta}\hat{\gamma})^* \psi^* \phi \, dx \qquad (4)$$

If A is a Hermitian operator then we have

$$\int \psi^* A \phi \, dx = \int A^* \psi^* \phi \, dx \qquad (5)$$

Comparing (4) and (5), we see that $\hat{\beta}\hat{\gamma}$ is Hermitian operator if $\hat{\beta}$ and $\hat{\gamma}$ commute.

~~Proof — it we shall prove that if $\hat{\beta}$ and $\hat{\gamma}$ are commuting.~~

Proof → Let $\hat{\beta}$ and $\hat{\gamma}$ are two commuting Hermitian operators.

We have to prove that

~~We shall prove that~~

We have to prove that if $\hat{\beta}$ and $\hat{\gamma}$ are commuting Hermitian operators, then the operator $\hat{\beta}\hat{\gamma}$ is also Hermitian.

Let ψ and ϕ be two functions. Consider the value of the integral $\int \psi^* \hat{\beta} \hat{\gamma} \phi \, dx$

If β is Hermitian, then we have

$$\int \psi^* \beta \gamma \phi \, dx = \int \beta^* \psi^* \gamma \phi \, dx \quad \text{——— (1)}$$

Again if γ is also Hermitian, we have

$$\int \beta^* \psi^* \gamma \phi \, dx = \int \gamma^* \beta^* \psi^* \phi \, dx \quad \text{——— (2)}$$

Now considering $\beta\gamma$ as the Hermitian operator

$$\int \psi^* \beta \gamma \phi \, dx = \int \beta^* \gamma^* \psi^* \phi \, dx \quad \text{——— (3)}$$

As ~~do~~ β and γ are commuting operators

$$\cancel{\beta\gamma - \gamma\beta} \ [\beta, \gamma] = 0$$

$$\text{or} \quad \beta\gamma - \gamma\beta = 0$$

$$\beta\gamma = \gamma\beta \quad \text{——— (4)}$$

Now equation (3) becomes

$$\int \psi^* \beta \gamma \phi \, dx = \int \gamma^* \beta^* \psi^* \phi \, dx \quad \text{——— (5)}$$

Now right hand sides of (2) & (5) will be equal.

Thus $\beta\gamma$ will be Hermitian if β and γ commute.

(iv) show that the momentum operator $\frac{\hbar}{i} \frac{\delta}{\delta x}$ is Hermitian.

Solution → Momentum operator $P_{op} = \frac{\hbar}{i} \frac{\delta}{\delta x}$

Complex conjugate of P_{op} is $P_{op}^* = -\frac{\hbar}{i} \frac{\delta}{\delta x}$

If p is hermitian operator then its expectation value $\langle P \rangle$ in any state ψ must be real i.e

$$\langle P \rangle = \int_{-\infty}^{+\infty} \psi^* \frac{\hbar}{i} \frac{\delta \psi}{\delta x} \, dx \; ; \quad \text{——— (1)}$$

must be real.

Integrating (1) by parts we ~~have~~ get

$$\langle P \rangle = \frac{\hbar}{i} \left[\psi^* \psi \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{\hbar}{i} \frac{\delta \psi^*}{\delta x} \psi \, dx$$

$$= \int_{-\infty}^{+\infty} \psi \left(-\frac{\hbar}{i} \frac{\delta \psi^*}{\delta x} \right) dx \quad \text{—— (2)}$$

It is obvious from (1) and (2) that $\langle P \rangle$ is equal to its complex conjugate. In other words $\langle P \rangle$ is real. Hence we may say that momentum operator $P_{op} = \frac{\hbar}{i} \frac{\delta}{\delta x}$ is Hermitian.

Schwartz Inequality

Schwartz Inequality states that

$$\sum_i \sum_j |A_i|^2 |B_j|^2 \geq \left| \sum_{ij} A_i^* B_j \right|^2 \quad \text{—— (1)}$$

To prove this we write

$$\sum_{ij} |A_i^* B_j|^2 = \sum_{ij} A_i^* B_i A_j B_j^* \quad \text{—— (2)}$$

Then we consider the following quantity

$$Q = \sum_{ij} |A_i|^2 |B_j|^2 - \left| \sum A_i^* B_j \right|^2$$

$$= \sum_{ij} \left(|A_i|^2 |B_j|^2 - A_i^* B_i A_j B_j^* \right) \quad \text{—— (3)}$$

We note that if $i = j$, the contribution to Q in the sum vanishes. But if i and j are each given values, not equal to each other, then the corresponding terms are

$$|A_i|^2 |B_j|^2 + |A_j|^2 |B_i|^2 - A_i^* B_j^* A_j B_i - A_j^* B_i^* A_i B_j$$

$$= |A_i B_j - A_j B_i|^2 \quad \text{—— (4)}$$

This quantity, however is always either positive or zero. Hence Q is made up of terms which are

The operator $(AB - BA)$ is called the commutator of A and B and is represented by $[A, B] = AB - BA$. The operators satisfying the equation $[A, B] = 0$ are said to commute.

never negative and we may conclude that

$$Q \geq 0$$

This proves Schwartz inequality. It is clear that $Q = 0$ only if each term in the series is zero or if $A_i B_j - A_j B_i = 0$. This means that

$$\frac{A_i}{A_j} = \frac{B_i}{B_j}$$

or that $A_i = c B_{ij}$

where c is a constant.

Therefore,

$$\sum_{ij} |A_i|^2 |B_j|^2 \geq \left| \sum_i A_i^* B_i \right|^2$$

Altier → We can prove Schwartz inequality in other way also.

Let f and g be any two functions of x such that

$$A = \int f^* f \, dx, \quad B = \int f^* g \, dx, \quad C = \int g^* g \, dx \quad \text{exist} \quad (1)$$

The integration extends over any definite range of the variable x. Certainly the integral

$$\int [\lambda f^*(x) + g^*(x)] [\lambda f(x) + g(x)] \, dx = A\lambda^2 + (B^* + B)\lambda + C, \quad (2)$$

in which λ is to be consider as a real variable, independent of x and is always positive or zero (zero only when g is directly proportional to f) and hence has no real roots in λ. But the roots of $A\lambda^2 + (B^*+B)\lambda + C$ are given by

$$\lambda = -\frac{B^* + B}{2A} \pm \frac{1}{2A}\sqrt{(B+B^*)^2 - 4AC} \quad (3)$$

Then are real unless

$$4AC \geq (B^* + B)^2 \quad \text{or} \quad AC \geq B^2 \quad (4)$$

The equality sign here holds only when $g = \text{constant} \times f$.

The R.H.S of (4) is twice the real part of B. Hence if f and g are real functions, the inequality becomes

$$\int f^2 dx \int g^2 dx \geq \left[\int f g \, dx\right]^2 ; \quad (5)$$

which is one form of Schwartz inequality.

For complex functions f and g equation inequality (4) may be modified. Taking f and g in polar form:

$$f(x) = \rho_1(x)\, e^{i\theta_1(x)} \; ; \; g(x) = \rho_2(x)\, e^{i\theta_2(x)}$$

$$B^* = \int f g^* dx$$

then $$B^* = \int \rho_1 \rho_2\, e^{i(\theta_1 - \theta_2)} dx$$

Since (4) holds for every pair of functions f and g then it must also be true when g is replaced by

$$g' = g\, e^{i(\theta_1 - \theta_2)}$$

But the substitution of g' for g leaves the values of A and c unchanged while it converts both B^* and B into

$$\int \rho_1 \rho_2 \, dx = |B|$$

which is modulus of B. Hence

$$\int f^* f\, dx \int g^* g\, dx \geq \left| \int f^* g\, dx \right|^2 \quad \text{——} \quad (6)$$

This is more general form of Schwartz inequality. Further generalisation to functions of more than one real variables is obvious.

The relation (6) is also valid for sums:

$$\left(\sum_1^n f_i^* f_i\right)\left(\sum_1^n g_i^* g_i\right) \geq \left|\sum_1^n f_i^* g_i\right|^2 \quad (7)$$

For ordinary vectors U and V this is equivalent to

$$U^2 V^2 \geq (U, V)^2$$

The operator (AB − BA) is called the commutator of A and B and is represented by $[A, B] = AB - BA$.

Heisenberg's Uncertainty Relation derived from operators.

Let u and v be two acceptable functions in the sense specified in Connection with the definition of Hermitian operator, then

$$\int u^* u \, d\tau \int v^* v \, d\tau \geq \frac{1}{4}\left[\int (u^* v + v^* u) \, d\tau\right]^2 \quad \text{--- (1)}$$

This relation is due to Schwartz inequality. We assume a system to be in a state ϕ which need not be an eigen state of any particular operator and we are interested in the results of measurements on the observables belonging to two operators P and Q at present unspecified. So let us introduce the function.

$$u = (P - \bar{p})\phi \quad \text{and} \quad v = i(Q - \bar{q})\phi \quad \text{--- (2)}$$

where $\bar{p}$ and $\bar{q}$ are mean values associated with P and Q as

$$\bar{p} = \underset{\tau \to \infty}{\text{Let}} \frac{\int_\tau \phi^* P \phi \, d\tau}{\int_\tau \phi^* \phi \, d\tau}$$

and

$$\bar{q} = \underset{\tau \to \infty}{\text{Let}} \frac{\int_\tau \phi^* Q \phi \, d\tau}{\int \phi^* \phi \, d\tau}$$

Now substituting the value of u and v from equation (2) in equation (1), we get

$$\int (P - \bar{p})^* \phi^* (P - \bar{p})\phi \, d\tau \int (Q - \bar{q})^* \phi^* (Q - \bar{q})\phi \, d\tau$$

$$\geq \frac{1}{4}\left[i\int (P - \bar{p})^* \phi^* (Q - \bar{q})\phi \, d\tau - i\int (Q - \bar{q})^* \phi^* (P - \bar{p})\phi \, d\tau\right]^2$$

$$\geq \frac{1}{4}\left[i\int \phi^* (P - \bar{p})(Q - \bar{q})\phi \, d\tau - i\int \phi^* (Q - \bar{q})(P - \bar{p})\phi \, d\tau\right]^2$$

--- (3)

As P and Q are Hermitian operators satisfy the following relation:

$$\int_\tau u^* P v \, d\tau = \int_\tau P^* u^* v \, d\tau \quad \text{——— (4)}$$

$\bar{p}$ and $\bar{q}$ are constants, therefore inequality (3) reduces to

$$\int \phi^* (P-\bar{p})^2 \phi \, d\tau \int \phi^* (Q-\bar{q})^2 \phi \, d\tau \geq -\frac{1}{4}\left[\int \phi^* (PQ-QP)\phi \, d\tau\right]^2$$

——— (5)

Let us consider the meaning of the quantity

$$\int \phi^* (P-\bar{p})^2 \phi \, d\tau$$

$$\int \phi^* (P-\bar{p})^2 \phi \, d\tau = \langle (P-\bar{p})^2 \rangle = \langle P^2 \rangle - \langle 2P\bar{p} \rangle + \langle \bar{p}^2 \rangle$$

$$= \langle P^2 \rangle - 2\bar{p}\langle P \rangle + \langle \bar{p}^2 \rangle$$

$$= \langle P^2 \rangle - \bar{p}^2$$

$$= \langle P^2 \rangle - \langle P \rangle^2$$

$$= (\Delta P)^2$$

[By standard deviation]

Similarly, $\int \phi^* (Q-\bar{q})^2 \phi \, d\tau = (\Delta q)^2$,

Hence $(\Delta P)^2 (\Delta q)^2 \geq -\frac{1}{4}\left[\int \phi^* (PQ-QP)\phi \, d\tau\right]^2$ ——— (6)

If operators P and Q commute, the right hand side is zero since $PQ = QP$ or $PQ - QP = 0$ and it is possible for $(\Delta P)^2$ or $(\Delta q)^2$ to be zero or even both to vanish.

The operator $(AB-BA)$ is called the commutator of A and B and is represented by

When P and Q do not commute, the relation (6) sets a lower limit for the product of the dispersion, often called - uncertainties.

Uncertainty relation for position and momentum

Suppose for instance that P is the operator $-i\hbar\frac{\delta}{\delta q}$ or $\frac{\hbar}{i}\frac{\delta}{\delta q}$ associated with the linear momentum p and Q stands for the Co-ordinate q. Then

$$(PQ-QP)\psi = \left(\frac{\hbar}{i}\frac{\partial}{\partial q}\cdot q - q\frac{\hbar}{i}\frac{\partial}{\partial q}\right)\psi$$

$$= \frac{\hbar}{i}\left[\left\{q\cdot\frac{\partial\psi}{\partial q} + \psi\right\} - q\frac{\partial\psi}{\partial q}\right]$$

$$(PQ-QP)\psi = \frac{\hbar}{i}\psi$$

$$\therefore PQ - QP = \frac{\hbar}{i} \quad \text{——— (7)}$$

Putting (7) in (6), we get

$$(\Delta p)^2(\Delta q)^2 \geq -\frac{1}{4}\frac{\hbar^2}{i^2}$$

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

$$\text{or } \boxed{\Delta p\,\Delta q \geq \frac{\hbar}{2}} \quad \text{——— (8)}$$

This is Heisenberg's uncertainty relation for position and momentum.

Uncertainty relation for Energy and time

Let operator P represents energy operator and the operator Q as time operator i.e

$$P = E_{op} = i\hbar\frac{\partial}{\partial t}$$

$$Q = t$$

$$\therefore (PQ-QP)\psi = \left(i\hbar\frac{\partial}{\partial t}t - t\,i\hbar\frac{\partial}{\partial t}\right)\psi$$

$$= i\hbar\frac{\partial}{\partial t}(t\psi) - t\,i\hbar\frac{\partial\psi}{\partial t}$$

$$= i\hbar\psi + \cancel{i\hbar t\frac{\partial\psi}{\partial t}} - \cancel{i\hbar t\frac{\partial\psi}{\partial t}}$$

$$= i\hbar\psi \quad \text{——— (9)}$$

Putting this value in (1)

$$(\Delta E)^2 (\Delta t)^2 \geq -\frac{(i\hbar)^2}{4}$$

$$\geq \frac{\hbar^2}{4}$$

$$\therefore \boxed{\Delta E \Delta t \geq \frac{\hbar}{2}} \quad \text{——— (1}$$

This is Heisenberg's uncertainty for energy and time.

Commutation rules for the Components orbital angular momentum.

The Orbital angular momentum is defined

$$L = r \times p$$

where r is the position vector of the from the axis of rotation and p be the momentum the body. If x, y, z are the Cartesian Coordin and L_x, L_y, L_z the components of orbital angu momentum along x, y and Z axes, then

$$L_x = yP_z - zP_y = y\left(\frac{\hbar}{i}\frac{\partial}{\partial z}\right) - z\left(\frac{\hbar}{i}\frac{\partial}{\partial y}\right)$$

$$L_y = zP_x - xP_z = z\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) - x\left(\frac{\hbar}{i}\frac{\partial}{\partial z}\right)$$

$$L_z = xP_y - yP_x = x\left(\frac{\hbar}{i}\frac{\partial}{\partial y}\right) - y\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)$$

Commutation rules for the Components of orbital angul momentum with position:

Commutation rule for L_x and x

$[L_x, x] = 0$	$[L_y, x] = -i\hbar z$	$(L_z, x) = i$
$[L_x, y] = i\hbar z$	$[L_y, y] = 0$	$(L_z, y) = -i$
$[L_x, z] = -i\hbar y$	$[L_y, z] = i\hbar x$	$(L_z, z) = 0$

For example

$$[L_x, x] = L_x x - x L_x$$

$$= \left\{ y\left(\frac{\hbar}{i}\frac{\partial}{\partial z}\right) - z\left(\frac{\hbar}{i}\frac{\partial}{\partial y}\right) \right\} x - x\left\{ y\left(\frac{\hbar}{i}\frac{\partial}{\partial z}\right) - z\left(\frac{\hbar}{i}\frac{\partial}{\partial y}\right) \right\}$$

$$= \cancel{y \frac{\hbar}{i} \frac{\partial x}{\partial}}$$

$$(L_x x - x L_x)\psi = \left\{ y\left(\frac{\hbar}{i}\frac{\partial}{\partial z}(x\psi)\right) - z\left(\frac{\hbar}{i}\frac{\partial}{\partial y}(x\psi)\right)\right\} - x\left\{ y\frac{\hbar}{i}\frac{\partial \psi}{\partial z} - z\frac{\hbar}{i}\frac{\partial \psi}{\partial y}\right\}$$

$$= 0$$

Similar relation can be obtained between L and p

$$[L_x, p_x] = 0, \quad [L_x, p_y] = i\hbar p_z$$

$$[L_x, p_z] = -i\hbar p_y$$

The orbital angular momentum $\vec{L}$ of a particle having momentum $\vec{p}$ and position vector $\vec{r}$ relative to an arbitrary origin is defined as

Knowledge Plus → $\quad L = r \times p$ ——— (1)

This defines the components of L about x, y and z axes respectively. By vector analysis

$$\vec{L} = \hat{i}L_x + \hat{j}L_y + \hat{k}L_z$$
$$\vec{r} = \hat{i}x + \hat{j}y + \hat{k}z$$
$$\vec{p} = \hat{i}p_x + \hat{j}p_y + \hat{k}p_z$$

$$\hat{i}L_x + \hat{j}L_y + \hat{k}L_z = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} = \hat{i}(yp_z - zp_y) + \hat{j}(zp_x - xp_z) + \hat{k}(xp_y - yp_x)$$

Substituting these values, we get

$$\hat{i}L_x + \hat{j}L_y + \hat{k}L_z = (\hat{i}x + \hat{j}y + \hat{k}z) \times (\hat{i}p_x + \hat{j}p_y + \hat{k}p_z)$$

$$= \hat{i}(yp_z - zp_y) + \hat{j}(zp_x - xp_z) + \hat{k}(xp_y - yp_x)$$

Comparing the coefficients of $\hat{i}$, $\hat{j}$ and $\hat{k}$ on either sides

$$\left.\begin{aligned} L_x &= yp_z - zp_y \\ L_y &= zp_x - xp_z \\ L_z &= xp_y - yp_x \end{aligned}\right\} \text{——— (2)}$$

Substituting operators for P_x, P_y and P_z i.e

$$P_x = \frac{\hbar}{i}\frac{\partial}{\partial x}, \quad P_y = \frac{\hbar}{i}\frac{\partial}{\partial y}, \quad P_z = \frac{\hbar}{i}\frac{\partial}{\partial z}$$

∴ The components of orbital angular momentum are defined as

$$\left.\begin{aligned} L_x &= \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \\ L_y &= \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \\ L_z &= \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \end{aligned}\right\}$$

<u>Commutation rules for the various components of orbital angular momentum.</u>

Consider the commutation relation between L_x and L_y

$$[L_x, L_y] = L_x L_y - L_y L_x \quad \text{———} (1)$$

Let us first consider $L_x L_y$

$$L_x L_y = \left\{y\left(\frac{\hbar}{i}\frac{\partial}{\partial z}\right) - z\left(\frac{\hbar}{i}\frac{\partial}{\partial y}\right)\right\} \times \left\{z\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) - x\left(\frac{\hbar}{i}\frac{\partial}{\partial z}\right)\right\}$$

$$= -\hbar^2\left\{\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\right\}$$

$$= -\hbar^2\left\{y\frac{\partial}{\partial z}\left(z\frac{\partial}{\partial x}\right) - y\frac{\partial}{\partial z}\left(x\frac{\partial}{\partial z}\right) - z\frac{\partial}{\partial y}\left(z\frac{\partial}{\partial x}\right) + z\frac{\partial}{\partial y}\left(x\frac{\partial}{\partial z}\right)\right\}$$

$$= -\hbar^2\left(y\frac{\partial}{\partial x} + yz\frac{\partial^2}{\partial z\,\partial x} - yx\frac{\partial^2}{\partial z^2} - z^2\frac{\partial^2}{\partial y\,\partial x} + zx\frac{\partial^2}{\partial y\,\partial z}\right) \quad \text{———} (2)$$

Similarly,

$$L_y L_x = (zP_x - xP_z)(yP_z - zP_y)$$

$$= \left\{z\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) - x\left(\frac{\hbar}{i}\frac{\partial}{\partial z}\right)\right\} \times \left\{y\left(\frac{\hbar}{i}\frac{\partial}{\partial z}\right) - z\left(\frac{\hbar}{i}\frac{\partial}{\partial y}\right)\right\}$$

$$= -\hbar^2\left\{\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\right\}$$

$$= -\hbar^2\left\{z\frac{\partial}{\partial x}\left(y\frac{\partial}{\partial z}\right) - z\frac{\partial}{\partial x}\left(z\frac{\partial}{\partial y}\right) - x\frac{\partial}{\partial z}\left(y\frac{\partial}{\partial z}\right) + x\frac{\partial}{\partial z}\left(z\frac{\partial}{\partial y}\right)\right\}$$

$$= -\hbar^2 \left(zy \frac{\partial^2}{\partial x \partial z} - z^2 \frac{\partial^2}{\partial x \partial y} - xy \frac{\partial^2}{\partial z^2} + xz \frac{\partial^2}{\partial z \partial y} + x \frac{\partial}{\partial y} \right) \quad \text{--- } (3)$$

Putting the values of (2) and (3) in (1)

$$[L_x, L_y] = -\hbar^2 \left(y \frac{\partial}{\partial x} - x \frac{\partial}{\partial y} \right)$$

Provided x, y and z are perfect differentials

i.e $\frac{\partial^2}{\partial x \partial z} = \frac{\partial^2}{\partial z \partial x}$ and $\frac{\partial^2}{\partial y \partial z} = \frac{\partial^2}{\partial z \partial y}$ and so on.

Then $[L_x, L_y] = \hbar^2 \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$

$$= i\hbar \left\{ \frac{\hbar}{i} \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \right\}$$

$$[L_x, L_y] = i\hbar L_z$$

Similarly, we get

$$\left.\begin{aligned} [L_y, L_z] &= i\hbar L_x \\ [L_z, L_x] &= i\hbar L_y \end{aligned}\right\}$$

Commutation relation of L^2 with components L_x, L_y and L_z:

The total angular momentum is defined by the relation $L^2 = L_x^2 + L_y^2 + L_z^2$.

$$[L^2, L_x] = [L_x^2 + L_y^2 + L_z^2, L_x]$$

$$= (L_x^2 + L_y^2 + L_z^2) L_x - L_x (L_x^2 + L_y^2 + L_z^2)$$

$$= (L_x^2 L_x + L_y^2 L_x + L_z^2 L_x) - (L_x L_x^2 + L_x L_y^2 + L_x L_z^2)$$

$$= (L_y^2 L_x - L_x L_y^2) + (L_z^2 L_x - L_x L_z^2)$$

$$= [L_y^2, L_x] + [L_z^2, L_x]$$

We know that,

$[ab, c] = a[b, c] + [a, c] b$.

So, $[L^2, L_x] = [L_y L_y, L_x] + [L_z L_z ; L_x]$

$= L_y [L_y, L_x] + [L_y, L_x] L_y + L_z [L_z, L_x] + [L_z, L_x] L_z$

Since $[L_x, L_y] = i\hbar L_z$

and $[L_y, L_x] = -i\hbar L_z$

Also $[L_z, L_x] = i\hbar L_y$

Then

~~$[L^2, L_x] = L_y(-i\hbar L_z) + (-i\hbar L_z) L_y +$~~

$$[L^2, L_x] = L_y(-i\hbar L_z) + (-i\hbar L_z) L_y + L_z(i\hbar L_y) + (i\hbar L_y) L_z$$

$$= i\hbar(-\cancel{L_y L_z} - \cancel{L_z L_y} + \cancel{L_z L_y} + \cancel{L_y L_z})$$

$$= 0$$

Similarly,

$[L^2, L_y] = 0$ and $[L^2, L_z] = 0$

Hence L^2 commutes with any of the three components of the angular momentum operator. Thus L^2, L_x and L_x have simultaneous eigenfunctions.

<u>Eigenvalues of L_z →</u> Eigenvalue equation of L_z may be written as —

$$L_z \psi = c\psi \quad \text{———} (1)$$

i.e. $$\frac{\hbar}{i} \frac{\partial \psi}{\partial \phi} = c\psi \quad \text{———} (2)$$

The solution of equation (2) is

$$\psi = f(r, \theta)\, e^{ic\phi/\hbar} \quad \text{———} (3)$$

where $f(r,\theta)$ is an arbitrary function of r and θ. Now ψ must be a single valued function of x, y, z. In this case increase in the angle ϕ by 2π should not change the wave function so that

$$f(r,\theta)\, e^{ic\phi/\hbar} = f(r,\theta)\, e^{\frac{ic(\phi + 2\pi)}{\hbar}}$$

or $e^{ic\cdot\frac{2\pi}{\hbar}} = 1$

$\frac{2\pi c}{\hbar} = 2m\pi$

$c = m\hbar$ where m is an integer

Thus eigenvalues of L_z are $L_z = m\hbar$

The operator (AB-BA) is called the commutator of A and ...