Observables:

If $\mathcal{E}$ were a finite dimensional vector space then obviously eigenfunctions of any Hermitian operator will form a complete basis. However, when $\mathcal{E}$ is infinite dimensional, that is no longer the case.

Therefore, we define an observable as a Hermitian operator whose eigenvectors form a complete basis in the state space $\mathcal{E}$, irrespective of the dimension of $\mathcal{E}$.

Let $A = A^{+}$ whose eigenvalues form a discrete spectrum $\{a_n, n=1,2,\ldots\}$ and that each eigenvalue is g_n fold degenerate with eigenvectors $|\psi_n^i\rangle$, $i=1,2,\ldots g_n$, i.e.,

$$A|\psi_n^i\rangle = a_n|\psi_n^i\rangle$$

with

$$\langle\psi_n^i|\psi_{n'}^i\rangle = 0 \quad \text{when } n \neq n'.$$

and vectors $|\psi_n^i\rangle$ can be chosen to be orthogonal

$$\langle\psi_n^i|\psi_n^{i'}\rangle = 0 \quad i \neq i'$$

Thus, for an orthonormal set we have

$$\boxed{\langle \psi_n^{i} | \psi_{n'}^{i'} \rangle = \delta_{nn'} \delta_{ii'}} \quad (66)$$

The completeness of the set $|\psi_n^i\rangle$ implies that

$$\boxed{\sum_{i,n} |\psi_n^i\rangle\langle\psi_n^i| = \mathbb{1}} \quad (67)$$

Thus only those infinite dimensional Hermitian operators will be called observables whose eigenvectors satisfy the closure property (67).

Set of Commuting Observables:

We will find that sets of commuting observables play an important role in quantum mechanics, particularly ~~~~ when one of those observables is the Hamiltonian of the system. Next we will prove ~~~~ the very important result that a set of commuting observables are simultaneously diagonalizable, i.e. share a common set of eigenvectors. The proof, however, will be ~~~~ completed in three steps.

(a) Theorem I:

If two operators A and B commute, and if $|\psi\rangle$ is an eigenvector of A, then $B|\psi\rangle$ is also an eigenvector of A with the same eigenvalue.

Proof: We are given that

$$[A, B] = AB - BA = 0$$

and let $|\psi\rangle$ be an eigenvector of A with eigenvalue a

$$A|\psi\rangle = a|\psi\rangle$$

Now

$$[A,B]|\psi\rangle = AB|\psi\rangle - BA|\psi\rangle = 0$$

$$\Rightarrow \quad A(B|\psi\rangle) = a(B|\psi\rangle)$$

$\Rightarrow$ $B|\psi\rangle$ is an eigenket of A with eigenvalue a. QED.

Here two possibilities arise:

(i) If a is a non-degenerate eigenvalue then clearly $B|\psi\rangle$ must be proportional to $|\psi\rangle$, i.e., ~~$B|\psi\rangle = b|\psi\rangle$~~

$$B|\psi\rangle = b|\psi\rangle$$

$\Rightarrow$ $|\psi\rangle$ is an eigenvector of B as well.

(ii) Let a be a degenerate eigenvalue with degeneracy g_a. Then eigenvectors $\{|\psi_a^i\rangle, i = 1, \ldots g_a\}$ span the subspace $\mathcal{E}_a$ and $|\psi\rangle \in \mathcal{E}_a$

Then all we can say

$$B|\psi\rangle \in \mathcal{E}_a.$$

$\Rightarrow$ $\mathcal{E}_a$ is globally invariant under the action of B.

(b) Theorem II :

If two observables A and B commute, and if $|\psi_1\rangle$ and $|\psi_2\rangle$ eigenvectors of A with distinct eigenvalues, then $\langle\psi_1|B|\psi_2\rangle = 0$.

Proof:

$$[A, B] = 0 = AB - BA$$

and let

$$A|\psi_1\rangle = a_1|\psi_1\rangle$$

$$A|\psi_2\rangle = a_2|\psi_2\rangle$$

with $a_1 \neq a_2$.

$$\cancel{AB|\psi_1\rangle = BA|\psi_1\rangle = a_1 B|\psi_1\rangle}$$

$$\cancel{AB|\psi_2\rangle}$$

$$(AB - BA)|\psi_1\rangle = 0$$

$$\Rightarrow \langle\psi_2|(AB - BA)|\psi_1\rangle = 0$$

$$\cancel{\Rightarrow \langle\psi_2| a_1 B}$$

$$\Rightarrow a_2\langle\psi_2|B|\psi_1\rangle - a_1\langle\psi_2|B|\psi_1\rangle = 0$$

$$\Rightarrow (a_2 - a_1)\langle\psi_2|B|\psi_1\rangle = 0$$

since $a_2 - a_1 \neq 0$

$$\Rightarrow \boxed{\langle\psi_2|B|\psi_1\rangle = 0}$$

(c) Theorem III:

If two observables A and B commute, one can construct an orthonormal basis of the state space with eigenvectors common to A and B

Proof: Since A and B are both observables so they ~~are~~ are both diagonalizable with a orthonormal set of eigenvectors which span $\mathcal{E}$. Let us consider the eigenset of A

$$A|u_n^i\rangle = a_n|u_n^i\rangle \; ; \quad n = 1, 2, \ldots \quad i = 1, 2, \ldots g_n$$

such that

$$\langle u_n^i | u_{n'}^{i'}\rangle = \delta_{nn'}\delta_{ii'}$$

Let us construct operator B w.r.t. ~~rep~~ basis spanned by $|u_n^i\rangle$. Defining

$$B_{nn'}^{ii'} = \langle u_n^{i'} | B | u_{n'}^{i}\rangle$$

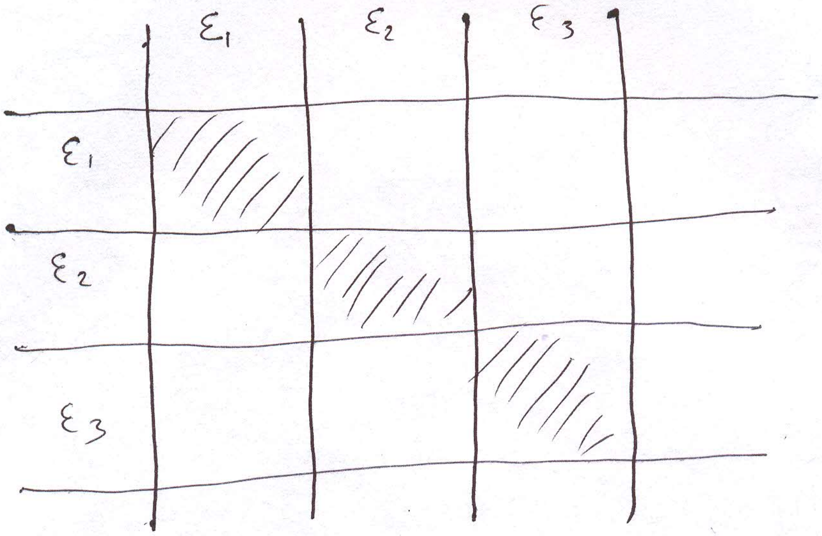
using the result of theorem II, we obtain

$$B_{n'n}^{i'i} = b_n^{i'i}\,\delta_{nn'}$$

Thus, if we arrange our basis in the order

$$|u_1^1\rangle\, |u_1^2\rangle \ldots |u_1^{g_1}\rangle, \; |u_2^1\rangle \ldots |u_2^{g_2}\rangle$$

we will obtain a block diagonal form for B



where $\mathcal{E}_n$ is the g_n dimensional subspace spanned by $\{|u_n^1\rangle, |u_n^2\rangle \dots |u_n^{g_n}\rangle\}$. Two possibilities exist:

(i) ~~Thus~~ For those eigenvalues a_n ~~of~~ which are nondegenerate ($g_n=1$), $\mathcal{E}_n$ will be one dimensional and hence $|u_n^i\rangle$ will also be an eigenvector of B.

(ii) If a_n is nondegenerate ($g_n>1$) the corresponding block of B will not be diagonal and hence $|u_n^i\rangle$, $i=1,\dots g_n$ will not be its eigenvectors. However, since the submatrix of B $b^n_{i'i}$ is also Hermitian, it can be diagonalized to obtain ~~a new~~ ~~set of~~ eigenvectors

$$B|u_n^{i}\rangle = b_n^i |u_n^{i}\rangle$$

since these new vectors $|u_n^{'i}\rangle$ are ~~eigen~~ linear combinations of the old set $|u_n^i\rangle$ so they will still be eigenvectors of A

$$A|u_n^{'i}\rangle = a_n|u_n^{'i}\rangle$$

This procedure can be applied to ~~each~~ each block of B leading to a new set of eigenvectors $|u_n^{'i}\rangle$, $n = 1, 2, -$ ~~g_n~~ $i = 1, 2, - g_n$ which are eigenvectors of both A and B

$$A|u_n^{'i}\rangle = a_n|u_n^{'i}\rangle \quad i = 1, -- g_n$$

$$B|u_n^{'i}\rangle = b_n^i|u_n^{'i}\rangle$$

which are orthonormal

$$\langle u_{n'}^{'i'}|u_n^{'i}\rangle = \delta_{nn'}\delta_{ii'}$$

QED

Complete Set of Commuting Observables:

Suppose ~~for~~ all the eigenvalues of a given observable are non degenerate. Then each eigenvector of A can be labeled by the corresponding eigenvalue in a unique manner. However, if the eigenvalues are degenerate, the eigenvectors cannot be determined in a unique manner because within a degenerate subspace, ~~eigenvectors~~ ~~are to~~ any ~~lin~~ orthogonal linear combination of a given eigenvectors is another set of possible eigenvectors. Suppose B is another observable which commutes with ~~to~~ A. As we saw earlier, the common set of eigenvectors within a given E_n, may not be degenerate with respect to the eigenvalues of B. In that case we can uniquely label the common eigenvectors of E_n by the eigenvalues of B. If there are still some degeneracies even with respect to the eigenvalues of B, one can look for a third observable C which commutes both with A and B. This process can be continued until all the ~~eigenvalues of A~~ common eigenvectors can be ~~completely~~ uniquely labeled. Such a set of commuting observables, which allows unique labeling of all its eigenvectors is called a complete set of commuting observables.

The $|\vec{r}\rangle$ and $|\vec{p}\rangle$ Representations:

Here we define two basis called the position and momentum basis

$$\xi_{r_0}(\vec{r}) = \delta(\vec{r}-\vec{r}_0) \quad \text{—— (68)}$$

$$v_{p_0}(\vec{r}) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{p}_0\cdot\vec{r}/\hbar} \quad \text{—— (69)}$$

note that $\xi_{r_0}(\vec{r})$ defines a well defined position $(\vec{r}_0)$ while $v_{p_0}(\vec{r})$ defines a well-defined momentum $\vec{p}_0$. ξ_{r_0} and $v_{p_0}(\vec{r})$ are the basis in $\mathcal{F}$ while their counterparts in the state space $\mathcal{E}$ are defined by

$$\xi_{r_0}(\vec{r}) \Longleftrightarrow |\vec{r}_0\rangle \quad \text{—— (70a)}$$

$$v_{p_0}(\vec{r}) \Longleftrightarrow |\vec{p}_0\rangle \quad \text{—— (70b)}$$

(a) Orthonormalization & Closure Relation

$$\langle r_0|\vec{r}_0'\rangle = \int \xi^*_{r_0}(\vec{r})\, \xi_{r_0'}(\vec{r})\, d^3\vec{r} = \delta(\vec{r}_0-\vec{r}_0') \quad \text{(71a)}$$

~~[illegible]~~ fo

$$\langle p_0 | p_0' \rangle = \int U_{p_0}^{*}(\bar{r})\, U_{p_0'}(\bar{r})\, d^3\bar{r}$$

$$= \frac{1}{(2\pi\hbar)} \int e^{i(\bar{p}_0' - p_0)\cdot\bar{r}}\, d^3\bar{r}$$

$$\boxed{\langle p_0 | p_0' \rangle = \delta(\bar{p}_0 - \bar{p}_0')} \quad \text{—— } 71b$$

thus $|\bar{r}\rangle$ and $|\bar{p}\rangle$ basis set ~~spans~~ forms an orthonormal basis in $\mathcal{E}$ and hence it will satisfy closure properties

$$\boxed{\begin{aligned} \int d^3\bar{r}_0\, |r_0\rangle\langle \bar{r}_0| &= 1 \quad \text{—— } 72a \\ \int d^3\bar{p}_0\, |\bar{p}_0\rangle\langle \bar{p}_0| &= 1 \quad \text{—— } 72b \end{aligned}}$$

(b) Components of a ket :

For the ~~more~~ sake of a more general notation instead of calling these kets $|r_0\rangle$ and $|p_0\rangle$, we call them $|\bar{r}\rangle$ and $|\bar{p}\rangle$. Let us ~~some~~ represent a general ket $|\psi\rangle$ in these two representations using the resolution of identity

$$\int |\bar{r}\rangle\langle\bar{r}|\, d^3\bar{r} = \mathbb{1}$$

$$\int |\vec{p}\rangle\langle\vec{p}|\, d^3\vec{p} = 1$$

we can write

$$|\psi\rangle = \mathbb{1}|\psi\rangle = \int d^3\bar{r}\; |\vec{r}\rangle\langle\bar{r}|\psi\rangle \quad \text{— (73a)}$$

$$|\psi\rangle = \int d^3\vec{p}\; |\vec{p}\rangle\langle\vec{p}|\psi\rangle \quad \text{— (73b)}$$

using the definition of inner product

$$\langle\bar{r}|\psi\rangle = \int d^3\bar{r}'\, \xi_{\bar{r}}(\bar{r}')\, \psi(\bar{r}') = \psi(\bar{r}) \quad \text{— (74a)}$$

$$\langle\bar{p}|\psi\rangle = \int d^3\bar{p}'\, v_{p}(\bar{r}')\, \psi(\bar{r}') = \bar{\psi}(\bar{p}) \quad \text{— (74b)}$$

where $\bar{\psi}(\bar{p})$ is the F. T. of $\psi(\bar{r})$

This is a very important result which shows that the value of a wave function at a given point in space is nothing but the component of ket $|\psi\rangle$ on basis vector $|\bar{r}\rangle$ and similarly for $\bar{\psi}_p(\bar{r})$.

Inner Product in Momentum Space

$$\langle \phi | \psi \rangle = \int d^3\bar{p} \, \langle \phi | p \rangle \langle p | \psi \rangle$$

$$\langle \phi | \psi \rangle = \int d^3\bar{p} \; \bar{\phi}^*(p) \, \bar{\psi}(p)$$

Change of basis from $\bar{r}$ to $\bar{p}$ space and vice-versa:

It is obvious

$$\langle \bar{r} | \bar{p} \rangle = \int d^3\bar{r}' \, \xi_r^*(\bar{r}') \, U_p(\bar{r}') = U_p(\bar{r}) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\bar{p}\cdot\bar{r}/\hbar}$$

so

$$\boxed{\begin{aligned} \langle \bar{r} | \bar{p} \rangle &= \frac{1}{(2\pi\hbar)^{3/2}} e^{i\bar{p}\cdot\bar{r}/\hbar} \quad \text{— (75a)} \\ \langle p | \bar{r} \rangle &= \langle \bar{r} | \bar{p} \rangle^* = \frac{1}{(2\pi\hbar)^{3/2}} e^{-i\bar{p}\cdot\bar{r}/\hbar} \quad \text{— (75b)} \end{aligned}}$$

Now.

$$\psi(\bar{r}) = \langle \bar{r} | \psi \rangle = \int d^3p \, \langle \bar{r} | p \rangle \langle p | \psi \rangle$$

$$\boxed{\psi(r) = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3\bar{p} \, e^{i\bar{p}\cdot\bar{r}/\hbar} \, \bar{\psi}(p) \quad \text{— (76a)}}$$

and

$$\tilde{\psi}(p) = \langle \bar{p} \langle p|\psi\rangle = \int d^3\bar{r}\, \langle p|\bar{r}\rangle\langle\bar{r}|\psi\rangle$$

$$\boxed{\tilde{\psi}(p) = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3\bar{r}\, e^{-i\bar{p}\cdot\bar{r}/\hbar}\, \psi(\bar{r}) \quad (76b)}$$

An operator A in $\bar{r}$ representation will be

$$A(\bar{r}', \bar{r}) = \langle\bar{r}'|A|\bar{r}\rangle = \iint d^3\bar{p}\, d^3\bar{p}' \langle\bar{r}'|\bar{p}'\rangle \langle\bar{p}'|A|\bar{p}\rangle\langle p|\bar{r}\rangle$$

$$\boxed{A(\bar{r}, \bar{r}') = \frac{1}{(2\pi\hbar)} \iint d^3p\, d^3\bar{p}'\, A(\bar{p}', \bar{p})\, e^{\frac{i}{\hbar}(\bar{p}'\cdot\bar{r}' - \bar{p}\cdot\bar{r})} \quad (77a)}$$

Similarly

$$A(\bar{p}', \bar{p}) = \langle\bar{p}'|A|\bar{p}\rangle = \iint d^3r\, d^3\bar{r}' \langle\bar{p}'|\bar{r}'\rangle\langle\bar{r}'|A|\bar{r}\rangle \langle\bar{r}|\bar{p}\rangle$$

$$\boxed{A(\bar{p}', \bar{p}) = \iint d^3\bar{r}\, d^3\bar{r}'\, e^{\frac{i}{\hbar}(\bar{p}\cdot\bar{r} - \bar{p}'\bar{r}')}\, A(\bar{r}', \bar{r}) \quad (77b)}$$

The $\vec{R}$ and $\vec{P}$ operators:

Let $|\psi\rangle \in \mathcal{E}_r$ with $\langle \bar{r}|\psi\rangle = \psi(\bar{r})$ the corresponding wave function $\psi(\bar{r})$. If X is the operator corresponding to the x coordinate then ~~we want to obtain~~ the representation of the ket

$$|\psi'\rangle = X|\psi\rangle$$

in $|\bar{r}\rangle$ basis is given by

$$\psi'(\bar{r}) = \langle \bar{r}|\psi'\rangle = x\,\psi(\bar{r})$$

Therefore we define the X, Y, and Z operators by the formulas

$$\boxed{\begin{aligned} \langle \bar{r}|X|\psi\rangle &= x\,\langle \bar{r}|\psi\rangle && \text{— (78a)} \\ \langle \bar{r}|Y|\psi\rangle &= y\,\langle \bar{r}|\psi\rangle && \text{— (78b)} \\ \langle \bar{r}|Z|\psi\rangle &= z\,\langle \bar{r}|\psi\rangle && \text{— (78c)} \end{aligned}}$$

Similarly, we define the three components of the momentum operator

$$\boxed{\begin{aligned} \langle p|P_x|\psi\rangle &= p_x\langle p|\psi\rangle \quad \text{— (79 a)} \\ \langle \bar{p}|P_y|\psi\rangle &= p_y\langle p|\psi\rangle \quad \text{— (79 b)} \\ \langle p|P_z|\psi\rangle &= p_z\langle p|\psi\rangle \quad \text{— (79 c)} \end{aligned}}$$

Let us investigate as to how $\bar{P}$ operator operates in the $|\bar{r}\rangle$ representation and $\bar{R}$ operator in the $|\bar{p}\rangle$ representation.

$$\langle \bar{r}|P_x|\psi\rangle = \int d^3p\,\langle \bar{r}|\bar{p}\rangle\langle p|P_x|\psi\rangle$$

$$= \frac{1}{(2\pi\hbar)^{3/2}}\int d^3p\, e^{i\bar{p}\cdot\bar{r}/\hbar}\, p_x\,\psi(p)$$

$$= \frac{\hbar}{i}\frac{\partial}{\partial x}\left\{\frac{1}{(2\pi\hbar)^{3/2}}\int d^3\bar{p}\, e^{i\bar{p}\cdot\bar{r}/\hbar}\,\psi(p)\right\}$$

$$\Rightarrow \quad \langle \bar{r}|P_x|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle \bar{r}|\psi\rangle$$

$$\Rightarrow \quad \boxed{\langle \bar{r}|\bar{P}|\psi\rangle = \frac{\hbar}{i}\bar{\nabla}\langle \bar{r}|\psi\rangle} \quad \text{— (80)}$$

and similarly

$\cancel{\langle \bar{p} | \bar{R} | \psi \rangle}$

$$\langle \bar{p} | X | \psi \rangle = \int d^3\bar{r} \langle p | \bar{r} \rangle \langle \bar{r} | X | \psi \rangle$$

$$= \frac{1}{(2\pi\hbar)^{3/2}} \int d^3\bar{r}\, e^{-i\bar{p}\cdot\bar{r}/\hbar}\, x\, \psi(\bar{r})$$

$$= -\frac{\hbar}{i} \frac{\partial}{\partial p_x} \left\{ \frac{1}{(2\pi\hbar)^{3/2}} \int d^3\bar{r}\, e^{-i\bar{p}\cdot\bar{r}/\hbar}\, \psi(\bar{r}) \right\}$$

$$\langle \bar{p} | X | \psi \rangle = -\frac{\hbar}{i} \frac{\partial}{\partial p_x} \langle \bar{p} | \psi \rangle$$

$\Rightarrow$ ~~$\langle \bar{p} | X | \psi \rangle = -\hbar$~~

$$\boxed{\langle \bar{p} | \bar{R} | \psi \rangle = -\frac{\hbar}{i} \bar{\nabla}_p \langle \bar{p} | \psi \rangle} \quad (81)$$

Thus it is easy to show that

$$\boxed{\langle \bar{r} | [X, P_x] | \psi \rangle = i\hbar \langle \bar{r} | \psi \rangle}$$

~~and, in general~~

$$\Rightarrow \boxed{[X, P_x] = i\hbar}$$

or, in general,

$$\boxed{\begin{aligned} [R_i, R_j] &= 0 \\ [P_i, P_j] &= 0 \\ [R_i, P_j] &= i\hbar\delta_{ij} \end{aligned}} \quad \text{—— (82)}$$

it is easy to show that the operators $\vec{R}$ and $\vec{P}$ are Hermitian.

$$\boxed{\begin{aligned} \langle\phi|X|\psi\rangle &= \langle\psi|X|\phi\rangle^* \\ \langle\phi|P_x|\psi\rangle &= \langle\psi|P_x|\phi\rangle^* \end{aligned}}$$

$\vec{R}$ and $\vec{P}$ are observables:

$$\langle\vec{r}|X|\vec{r}_0\rangle = x\langle\vec{r}|\vec{r}_0\rangle = x\,\delta(\vec{r}-\vec{r}_0) = x_0\delta(\vec{r}-\vec{r}_0)$$

$$\boxed{\langle\vec{r}|X|\vec{r}_0\rangle = x_0\langle\vec{r}|\vec{r}_0\rangle} \quad \text{—— (83)}$$

$$\Rightarrow \quad X|\vec{r}_0\rangle = x_0|\vec{r}_0\rangle$$

$$X|\bar{r}\rangle = x|\bar{r}\rangle$$

$$Y|\bar{r}\rangle = y|\bar{r}\rangle$$

$$Z|\bar{r}\rangle = z|\bar{r}\rangle$$

$\Rightarrow$ kets $|\bar{r}\rangle$ are eigenkets of $\bar{R}$ operator. Similarly one can show that

$$\boxed{\begin{aligned} P_x|\bar{p}\rangle &= p_x|\bar{p}\rangle \\ P_y|\bar{p}\rangle &= p_y|\bar{p}\rangle \\ P_z|\bar{p}\rangle &= p_z|\bar{p}\rangle \end{aligned}} \quad \text{—— (84)}$$

but we already know that $|\bar{r}\rangle$ and $|\bar{p}\rangle$ from a basis for the state space $\mathcal{E}_r$, so $\bar{R}$ and $\bar{P}$ are observables.

Now we note that the operator involved in the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2 + V(r) \equiv \frac{p^2}{2m} + V(r) \equiv \mathcal{H}\text{amiltonian}$$

Thus the operator of the Schrödinger equation is nothing but the nonrelativistic Hamiltonian of the system leading to $\mathcal{H}\psi = i\hbar\frac{\partial\psi}{\partial t}$