T.2) Operators, Eigenvalues and Observables

So far we have considered mappings of $\mathcal{H}$ (or $\hat{\mathcal{H}}$) into the complex numbers, the linear functionals. We next consider mappings of $\mathcal{H}\,(\hat{\mathcal{H}})$ into $\mathcal{H}\,(\hat{\mathcal{H}})$.

A linear operator, denoted A, is a mapping of vectors into vectors, $|\psi\rangle \xrightarrow{A} |\phi\rangle$, where we denote the vector $|\phi\rangle$ as $|\phi\rangle = |A\psi\rangle = A|\psi\rangle$ (old notation $\psi \xrightarrow{A} \phi = A\psi$), such that

$$A\left(|\psi\rangle + |\phi\rangle\right) = A|\psi\rangle + A|\phi\rangle$$

$$A\left(\lambda|\psi\rangle\right) = \lambda\left(A|\psi\rangle\right),$$ so that A is linear.

If $\{|\phi_k\rangle\}$ is an orthonormal basis, then $A|\phi_k\rangle$ is again a vector which can be expanded in this basis

$$A|\phi_k\rangle = \sum_l{}' A_{lk}|\phi_l\rangle$$

with A_{lk} called the <u>matrix elements</u> of A,

$$\langle\phi_l|A|\phi_k\rangle = \langle\phi_l|\sum_{l'}{}' A_{l'k}\,\phi_{l'}\rangle$$

$$= \sum_{l'}{}' A_{l'k}\underbrace{\langle\phi_l|\phi_{l'}\rangle}_{=\delta_{ll'}}$$

$$= A_{lk}\,.$$

Further if $|\psi\rangle = \sum_k{}' \psi_k|\phi_k\rangle$ then

$$A|\psi\rangle = \sum_k{}' \psi_k A|\phi_k\rangle = \sum_{k,l}{}' A_{lk}\psi_k|\phi_l\rangle.$$

So $\langle\phi_l|A|\psi\rangle = \sum_k{}' A_{lk}\psi_k$. Of course $A|\psi\rangle$ is a vector, call it $|\psi'\rangle$

$$|\psi'\rangle \equiv A|\psi\rangle = |A\psi\rangle,$$

which has its own expansion in terms of $\{|\phi_k\rangle\}$

$$|\psi'\rangle = \sum_k{}' \psi'_k|\phi_k\rangle.$$

So
$$\langle \phi_\ell | \psi' \rangle = \psi'_\ell$$
$$= \langle \phi_\ell | A | \psi \rangle = \sum_k{}' A_{\ell k} \psi_k$$

$$\Rightarrow \quad \boxed{\psi'_\ell = \sum_k{}' A_{\ell k} \psi_k}$$

Expansion of vectors and operators on vectors in terms of an orthonormal basis makes clear that we can represent our ket-vectors by column vectors $|\psi\rangle \longrightarrow \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \end{pmatrix}$ and

our bra-vectors by hermitean conjugate row vectors
$$\langle \psi | \longrightarrow (\psi_1^* \psi_2^* \cdots)$$

with $\langle \phi | \psi \rangle = (\phi_1^* \phi_2^* \cdots) \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \vdots \end{pmatrix} = \sum_k{}' \phi_k^* \psi_k$.

Further linear operators can be represented by matrices
$$A \longrightarrow \begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & \cdot & \\ \vdots & & \ddots \\ \vdots & & \end{pmatrix}$$

whose action on the ket vectors is represented by matrix multiplication of the matrix representative of A and the column vector representation of the ket

$$A|\psi\rangle \longrightarrow \begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & \ddots & \\ \vdots & & \ddots \end{pmatrix}\begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \end{pmatrix}.$$

In the $\{|\phi_k\rangle\}$ basis then the action of a linear operator is in 1-1 correspondence with matrix manipulations:

1) Addition:

$$(A+B)|\psi\rangle \equiv A|\psi\rangle + B|\psi\rangle$$

$$\Longleftrightarrow \quad (A+B)_{\ell k} = A_{\ell k} + B_{\ell k}$$

2) Multiplication:

$$(AB)|\psi\rangle \equiv A(B|\psi\rangle)$$

$$\Longleftrightarrow \quad (AB)_{\ell k} = \sum_m A_{\ell m} B_{mk}$$

(i.e. $(AB)|\phi_k\rangle = A(B|\phi_k\rangle) = A\left(\sum_m B_{mk}|\phi_m\rangle\right)$

$= \sum_m B_{mk} A|\phi_m\rangle = \sum_{m,\ell} B_{mk} A_{\ell m}|\phi_\ell\rangle$

$$= \sum_{m,l}{}' A_{lm} B_{mk} |\phi_l\rangle$$

$$\Rightarrow \langle \phi_l | (AB) | \phi_k \rangle \equiv (AB)_{lk}$$
$$= \sum_{m}{}' A_{lm} B_{mk} \;)$$

3) Scalar Multiplication:

$$(\lambda A)|\psi\rangle \equiv \lambda (A|\psi\rangle)$$

$$\Leftrightarrow (\lambda A)_{kl} = \lambda A_{kl} \; .$$

So we see that linear operators exhibit all the properties that matrices do, for example

<u>Associativity</u> : <u>$A(BC) = (AB)C$</u>

$$[A(BC)]|\psi\rangle \equiv A[(BC)|\psi\rangle] = AB[C|\psi\rangle]$$
$$= [(AB)C]|\psi\rangle.$$

<u>Distribution</u>: $A(B+C) = AB + AC$.

$$[A(B+C)]|\psi\rangle \equiv A\{(B+C)|\psi\rangle\} = A\{B|\psi\rangle + C|\psi\rangle\}$$
$$= A(B|\psi\rangle) + A(C|\psi\rangle) = (AB)|\psi\rangle + (AC)|\psi\rangle$$
$$= [AB + AC]|\psi\rangle.$$

We also uniquely define the identity operator $\mathbb{1}$ and the zero operator $\mathbb{O}$ by

$$\mathbb{1}|\psi\rangle \equiv |\psi\rangle \; ; \; \mathbb{O}|\psi\rangle \equiv 0 \leftarrow \text{number zero}$$

for arbitrary $|\psi\rangle$. Also in general linear operators, like matrices, do not commute, so that $AB \neq BA$. The difference being defined as the <u>commutator</u> of A and B

$$[A, B] \equiv AB - BA.$$

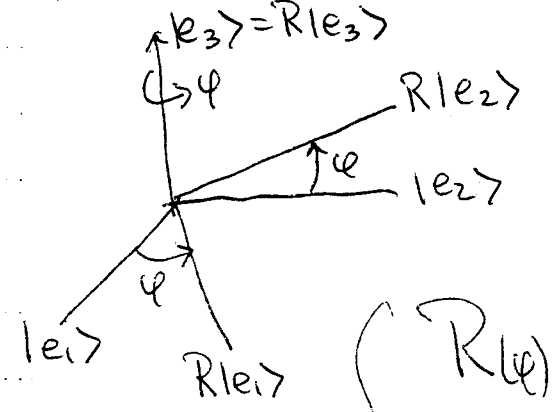
examples 1.) Recall the position and momentum operators in wavemechanics

$$\vec{X}\,\psi(\vec{r}) = \vec{r}\,\psi(\vec{r}) \quad \text{and}$$

$$\vec{P}\,\psi(\vec{r}) = -i\hbar\vec{\nabla}\psi(\vec{r}) \,, \Rightarrow$$

$$[X_i, P_j] = i\hbar\delta_{ij} \,.$$

2) Rotations about the z-axis in $\mathbb{R}^3$



Let $R(\varphi)$ be the rotation operator by $\measuredangle\varphi$ about the z-axis

R maps vectors into vectors according to

$$\begin{cases} R(\varphi)|e_1\rangle = \cos\varphi\,|e_1\rangle + \sin\varphi\,|e_2\rangle \\ R(\varphi)|e_2\rangle = -\sin\varphi\,|e_1\rangle + \cos\varphi\,|e_2\rangle \\ R(\varphi)|e_3\rangle = |e_3\rangle \end{cases},$$

that is $\quad R|e_i\rangle = \sum_{j=1}^{3} R_{ji}\,|e_j\rangle$

$$R_{ij}(\varphi) = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

given any vector $|v\rangle = \sum_{i=1}^{3} v_i |e_i\rangle$, we find

$$R(\varphi)|v\rangle = \sum_i^{} v_i R(\varphi)|e_i\rangle$$

$$= \sum_{ij} R(\varphi)_{ji} v_i |e_j\rangle .$$

Calling the transformed vector $|v'\rangle \equiv R(\varphi)|v\rangle$

we have $\quad |v'\rangle = \sum_j v_j' |e_j\rangle \Rightarrow$

$$v_j' = R(\varphi)_{ji} v_i$$ as usual this is

$$\begin{pmatrix} v_1' \\ v_2' \\ v_3' \end{pmatrix} = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} .$$

Comment about Dirac Notation:

Recall a closed (or complete) bracket $\langle \, | \, \rangle$ is a complex number

an open (or incomplete) bracket is a vector
bra $\langle \, |$, ket $| \, \rangle$, this is said

to be open on one side, $\langle\,|$ is open on the right $\langle\ ,\ |\rangle$ is open on the left $\rangle$.

An operator is open on both sides $|\,\rangle\langle\,|$ in this notation. That is, any operator A, given an orthonormal basis $\{|\phi_k\rangle\}$, can be written as

$$A = \sum_{i,j} |\phi_i\rangle A_{ij} \langle\phi_j|$$

$$= \sum_{i,j} A_{ij}\, |\phi_i\rangle\langle\phi_j|$$

where the operator $|\phi_i\rangle\langle\phi_j|$ is defined by

$$\left(|\phi_i\rangle\langle\phi_j|\right) |\psi\rangle \equiv |\phi_i\rangle\left(\langle\phi_j|\psi\rangle\right)$$

$$= \langle\phi_j|\psi\rangle\, |\phi_i\rangle$$

and likewise

$$\langle\psi|\left(|\phi_i\rangle\langle\phi_j|\right) \equiv \langle\psi|\phi_i\rangle \langle\phi_j| .$$

Hence

$$A|\psi\rangle = \sum_{i,j} A_{ij} \langle\phi_j|\psi\rangle |\phi_i\rangle$$

$$= \sum_{ij} A_{ij} \psi_j |\phi_i\rangle = \sum_i \psi_i' |\phi_i\rangle$$

as required. Hence we can view the complex number

$$\langle\psi|A|\phi\rangle\langle\chi|B|\omega\rangle$$

$$= \underbrace{\left(\langle\psi|\right)}_{\text{bra}} \underbrace{\left(A|\phi\rangle\langle\chi|\right)}_{\text{operator}} \underbrace{\left(B|\omega\rangle\right)}_{\text{ket}}$$

or

$$= \underbrace{\left(\langle\psi|A\right)}_{\text{bra}} \underbrace{\left(|\phi\rangle\langle\chi|\right)}_{\text{operator}} \underbrace{\left(B|\omega\rangle\right)}_{\text{ket}}$$

etc.

Consider 2 operators A and B, if for all $|\psi\rangle$ and $|\phi\rangle$ in the vector space we find

$$\langle\psi|A|\phi\rangle = \langle\phi|B|\psi\rangle^*,$$

then B is called the <u>adjoint</u> of A and we denote $B = A^\dagger$. Thus

$$\langle \psi | A | \phi \rangle = \langle \phi | A^\dagger | \psi \rangle^*,$$

$A^\dagger$ is the adjoint of A.

(Old notation $(\psi, A\phi) = (B\psi, \phi) \Rightarrow B = A^\dagger$)

Taking the complex conjugate of this equation we find

$$\left(\langle \psi | A | \phi \rangle = \langle \phi | B | \psi \rangle^* \right)^*$$

$\Rightarrow$

$$\langle \psi | A | \phi \rangle^* = \langle \phi | B | \psi \rangle$$ from B's point of view $\Rightarrow B^\dagger = A$. However $B = A^\dagger$, so

$$\boxed{(A^\dagger)^\dagger = A}.$$

The matrix elements of $A^\dagger$ in the $\{|\phi_k\rangle\}$ orthonormal bases are

$$(A^\dagger)_{ij} = \langle \phi_i | A^\dagger | \phi_j \rangle = \langle \phi_j | A | \phi_i \rangle^*$$
$$= (A_{ji})^* = A_{ji}^*$$ just

hermitean conjugation in matrix notation.

Note that the adjoint operation is <u>anti-linear</u>

$$\langle\phi|(A+B)^\dagger|\psi\rangle \equiv \langle\psi|(A+B)|\phi\rangle^*$$

$$= \langle\psi|A|\phi\rangle^* + \langle\psi|B|\phi\rangle^*$$

$$= \langle\phi|A^\dagger|\psi\rangle + \langle\phi|B^\dagger|\psi\rangle$$

$$\Rightarrow \quad (A+B)^\dagger = A^\dagger + B^\dagger$$

but

$$\langle\phi|(\lambda A)^\dagger|\psi\rangle = \langle\psi|(\lambda A)|\phi\rangle^*$$

$$= \lambda^* \langle\psi|A|\phi\rangle^*$$

$$= \lambda^* \langle\phi|A^\dagger|\psi\rangle$$

$$= \langle\phi|\lambda^* A^\dagger|\psi\rangle$$

$$\Rightarrow \quad (\lambda A)^\dagger = \lambda^* A^\dagger \,.$$

(This anti-linearity is clear from the matrix element formula for $A^\dagger$).

Another Comment on Dirac Notation: By definition, $A|\psi\rangle$ can also be written as the vector $|A\psi\rangle$; $A|\psi\rangle \equiv |A\psi\rangle$. We may also view A as operating on bra vectors as

$$\langle\phi|A = \langle A^\dagger\phi| \text{ not } \langle A\phi| \, !$$

That is consider

$$\langle\phi|A|\psi\rangle \equiv \langle\phi|A\psi\rangle$$
$$= \left(\langle\psi|A^\dagger|\phi\rangle\right)^* \equiv \left(\langle\psi|A^\dagger\phi\rangle\right)^*$$
$$= \langle A^\dagger\phi|\psi\rangle$$
$$\Rightarrow \boxed{\langle A^\dagger\phi|\psi\rangle = \langle\phi|A\psi\rangle} \, .$$
$$\boxed{= \langle\phi|A|\psi\rangle}$$

* footnote

So we have the adjoint of the product of operators is the reverse ordered product of adjoints

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* footnote (By Riesz's Thm. $|\psi\rangle$ and $\langle\psi|$ are conjugate, if $|\psi'\rangle = A|\psi\rangle = |A\psi\rangle$ then $|\psi'\rangle$ and $\langle\psi'|$ are conjugate ; $\langle\psi'| = \langle A\psi| = \langle\psi|A^\dagger$)

$$\langle\phi|(AB)^\dagger|\psi\rangle = \langle\psi|AB|\phi\rangle^*$$
$$= \langle\psi|A|B\phi\rangle^*$$
$$= \langle A^\dagger\psi|B\phi\rangle^*$$
$$= \langle B\phi|A^\dagger\psi\rangle$$
$$= \langle\phi|B^\dagger|A^\dagger\psi\rangle$$
$$= \langle\phi|B^\dagger A^\dagger|\psi\rangle$$
$$\Rightarrow \boxed{(AB)^\dagger = B^\dagger A^\dagger}$$

Of course we could have obtained this relation, as all relations for linear operators, by considering the corresponding matrix representations. For example

$$[(AB)^\dagger]_{kl} = (AB)^*_{lk} = \sum_m A^*_{lm} B^*_{mk}$$
$$(B^\dagger A^\dagger)_{kl} = \sum_m (B^\dagger)_{km}(A^\dagger)_{ml} = \sum_m B^*_{mk} A^*_{lm}$$

which indeed $= [(AB)^\dagger]_{kl}$.

An operator A is said to be <u>Hermitian</u> if

$$A^{\dagger} = A.$$ This implies that

$$\langle \psi | A | \phi \rangle = \langle \psi | A^{\dagger} | \phi \rangle = \langle \phi | A | \psi \rangle^{*},$$

or for matrix elements $(A^{\dagger})_{k\ell} = A^{*}_{\ell k} = A_{k\ell}$.

examples 1) The identity operator is a trivial example of an hermitian operator

$$\langle \psi | \phi \rangle = \langle \phi | \psi \rangle^{*}$$

2) The momentum operator in wave mechanics

$$\langle \phi | \vec{P} | \psi \rangle = \int d^3r\, \phi^{*}(\vec{r})(-i\hbar\vec{\nabla})\psi(\vec{r})$$

$$= \cancel{\int d^3r\,(-i\hbar\vec{\nabla})(\phi^{*}\psi)}^{\,0}$$

$$+ \int d^3r\,(i\hbar\vec{\nabla}\phi^{*})\psi$$

$$= \int d^3r\,(-i\hbar\vec{\nabla}\phi)^{*}\psi$$

$$= \langle \vec{P}\phi | \psi \rangle$$

but

$\langle \phi | \vec{P} | \psi \rangle = \langle \vec{P}^{\dagger}\phi | \psi \rangle$ by definition, Thus $\vec{P}^{\dagger} = \vec{P}$, $\vec{P}$ is Hermitian

If $AB = 1$ and $BC = 1$, then $C = (AB)C = A(BC) = A$ and so $BA = 1$ and B is said to be the inverse of A denoted by $B = A^{-1}$. Moreover it follows that $A = B^{-1}$, that is $(A^{-1})^{-1} = A$. If A and B have inverses A^{-1} and B^{-1}, respectively, then

$$B^{-1}A^{-1}(AB) = B^{-1}(A^{-1}A)B = B^{-1}B = 1$$

$$\Rightarrow \quad \boxed{(AB)^{-1} = B^{-1}A^{-1}}\,.$$

Finally, a linear operator U is unitary if $U^{\dagger} = U^{-1}$. Note that for a unitary operator

$$\langle U\phi | U\psi\rangle = \langle \phi | U^{\dagger}U | \psi\rangle = \langle \phi | \psi\rangle.$$

If $\{|\phi_k\rangle\}$ and $\{|\phi'_k\rangle\}$ are two different complete orthonormal bases, then the mapping $|\phi'_k\rangle = U|\phi_k\rangle$ defines a unitary operator U.

<u>Proof</u>: If $|\psi\rangle$ and $|\omega\rangle$ are arbitrary kets with the expansions

$$|\psi\rangle = \sum_k{}' \psi_k |\phi_k\rangle$$

$$|\omega\rangle = \sum_k{}' \omega_k |\phi_k\rangle ,$$

then

$$\langle\psi|U^\dagger U|\omega\rangle = \langle U\psi|U\omega\rangle$$

$$= \langle \sum_k{}' \psi_k U\phi_k | \sum_l{}' \omega_l U\phi_l\rangle$$

$$= \sum_{k,l}{}' \psi_k^* \omega_l \langle U\phi_k | U\phi_l\rangle$$

$$= \sum_{k,l}{}' \psi_k^* \omega_l \underbrace{\langle \phi'_k | \phi'_l\rangle}_{=\delta_{kl}}$$

$$= \sum_k{}' \psi_k^* \omega_k$$

$$= \langle\psi|\omega\rangle .$$

Since $|\psi\rangle$ and $|\omega\rangle$ were arbitrary, $\Rightarrow$

$$U^\dagger U = 1, \text{ hence } U \text{ is unitary.}$$

The effect of such a change of basis is the same as a change in all operators

$$A \to A' \equiv U A U^{-1}.$$

That is the matrix element of A' in the $\{|\phi_k'\rangle\}$ basis are

$$\begin{aligned} A'_{ij} &= \langle \phi_i' | A' | \phi_j' \rangle \\ &= \langle U\phi_i | U A U^{-1} | U\phi_j \rangle \\ &= \langle \phi_i | \underbrace{(U^\dagger U)}_{=1} A \underbrace{(U^{-1} U)}_{=1} | \phi_j \rangle \\ &= \langle \phi_i | A | \phi_j \rangle \\ &= A_{ij}. \end{aligned}$$

Thus A' has the same matrix elements in the $\{|\phi_k'\rangle\}$ basis as A has in the $\{|\phi_k\rangle\}$ basis.

Consider the eigenvalue problem for an operator A acting on $\mathcal{H}$. The operator A has an eigenvalue a if there exists a vector $|\psi\rangle$ such that

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

that is

$$(A - a\mathbb{1})|\psi\rangle = 0 .$$

Expanding $|\psi\rangle$ in terms of an orthonormal basis $\{|\phi_k\rangle\}$ (we consider explicit discrete bases of $\mathcal{H}$, analogously the continuous basis case can be treated)

$$|\psi\rangle = \sum_k \psi_k |\phi_k\rangle ,$$

The eigenvalue equation becomes

$$0 = \sum_k (A - a\mathbb{1})\psi_k|\phi_k\rangle$$

$$= \sum_k \psi_k (A - a\mathbb{1})|\phi_k\rangle$$

$$= \sum_k \psi_k \Big(\sum_l (A_{lk} - a\delta_{lk})|\phi_l\rangle\Big)$$

$$0 = \sum_l{}' \sum_k{}' (A_{lk} - a\delta_{lk}) \psi_k |\phi_l\rangle$$

since recall $A|\phi_k\rangle = \sum_l{}' A_{lk}|\phi_l\rangle$.

Taking the inner product with $|\phi_i\rangle$ this yields

$$0 = \langle\phi_i| \sum_l{}' \sum_k{}' (A_{lk} - a\delta_{lk}) \psi_k |\phi_l\rangle$$

$$= \sum_l{}' \sum_k{}' (A_{lk} - a\delta_{lk}) \psi_k \underbrace{\langle\phi_i|\phi_l\rangle}_{=\delta_{il}}$$

$$\boxed{0 = \sum_k{}' (A_{ik} - a\delta_{ik}) \psi_k}$$

Consider the case of a finite dimensional space with dimension N. The eigenvalue equation becomes a finite N×N matrix relation

$$\sum_{j=1}^{N}{}' (A_{ij} - a\delta_{ij}) \psi_j = 0 .$$

The only way for a non-trivial solution to exist is if the determinant of the $N \times N$ matrix vanishes

$$\det(A - a\mathbb{1}) = 0$$

(here A is the $N \times N$ matrix A_{ij}, not the abstract A operator). The determinant is a N^{th} degree polynomial in a. It follows from the fundamental theorem of algebra that the polynomial has N roots, some or all of which may be degenerate. Thus each linear operator acting on a finite dimensional space has at least one eigenvalue.

For a hermitian operator $H = H^\dagger$, the eigenvalues are real and the eigenvectors for different eigenvalues are orthogonal.

Proof: Let

$$H|\psi_1\rangle = a_1|\psi_1\rangle$$

$$H|\psi_2\rangle = a_2|\psi_2\rangle,$$

then $\langle\psi_2|H|\psi_1\rangle = a_1\langle\psi_2|\psi_1\rangle$

but $\langle\psi_2|H|\psi_1\rangle = \langle\psi_1|H^\dagger|\psi_2\rangle^*$

$$= \langle\psi_1|H|\psi_2\rangle^*$$

Now $\langle\psi_1|H|\psi_2\rangle = a_2\langle\psi_1|\psi_2\rangle$

So $\langle\psi_2|H|\psi_1\rangle = a_1\langle\psi_2|\psi_1\rangle$

$$= \langle\psi_1|H|\psi_2\rangle^*$$

$$= a_2^*\langle\psi_1|\psi_2\rangle^*$$

$$= a_2^*\langle\psi_2|\psi_1\rangle$$

$$\Rightarrow (a_1 - a_2^*)\langle\psi_2|\psi_1\rangle = 0 .$$

If we had chosen $|\psi_2\rangle = |\psi_1\rangle \neq 0$, then

$$(a_1 - a_1^*)\langle\psi_1|\psi_1\rangle = 0$$

$\Rightarrow a_1 = a_1^*$; the eigenvalues of H are real.

If $a_1 \neq a_2$, then

$$(a_1 - a_2^*)\langle\psi_2|\psi_1\rangle = 0 = (a_1 - a_2)\langle\psi_2|\psi_1\rangle$$

$$\Rightarrow \langle\psi_2|\psi_1\rangle = 0 ,$$

the eigenvectors for different eigenvalues are orthogonal.

<u>Thm.</u>

Every hermitian operator acting on a finite N-dimensional space has a complete set of N eigenvectors.

<u>Proof</u>: Suppose H has $M<N$ orthonormal eigenvectors $|\psi_k\rangle$. Since this set <u>cannot</u> be complete, there exists another vector $|\phi\rangle$ that cannot be written as a linear combination of the $\{|\psi_k\rangle\}$, $k=1,\dots,M$. Hence

$|\psi_1\rangle, \dots, |\psi_M\rangle, |\phi\rangle$ are independent vectors. We can then construct the vector $|\psi\rangle$ orthogonal to all $|\psi_k\rangle$:

$$|\psi\rangle = |\phi\rangle - \sum_{k=1}^{M} \langle\psi_k|\phi\rangle |\psi_k\rangle ,$$

that is for $l=1,\dots,M$

$$\langle\psi_l|\psi\rangle = \langle\psi_l|\phi\rangle - \sum_{k=1}^{M} \langle\psi_k|\phi\rangle \underbrace{\langle\psi_l|\psi_k\rangle}_{=\delta_{lk}}$$

$$= \langle\psi_l|\phi\rangle - \langle\psi_l|\phi\rangle$$

$$= 0 .$$

Let S be the space spanned by

all such vectors, that is the space spanned by vectors orthogonal to $\{|\psi_k\rangle\}$, $k=1, \ldots, M$. So $|\psi\rangle \in S$.

(Note: S is a space since if $\langle\psi_\ell|\psi\rangle=0$ and $\langle\psi_\ell|\psi'\rangle=0$, then $\langle\psi_\ell|(|\psi\rangle+|\psi'\rangle)=0$. So $|\psi\rangle+|\psi'\rangle$ is orthogonal to $\{|\psi_k\rangle\}$ and hence also an element of S, etc.)

The operator H transforms vectors in S into vectors in S. This follows since if $\langle\psi_\ell|\psi\rangle=0$ then

$$\begin{aligned}\langle\psi_\ell|H|\psi\rangle &= \langle\psi|H^\dagger|\psi_\ell\rangle^* \\ &= \langle\psi|H|\psi_\ell\rangle^* \\ &= a_\ell\langle\psi|\psi_\ell\rangle^* = a_\ell \underbrace{\langle\psi_\ell|\psi\rangle}_{=0} \\ &= 0.\end{aligned}$$

Thus $(H|\psi\rangle) \in S$.

Hence H must have at least one eigenvector in S. That is there is some direction in S that stays fixed under the action of H. Call this direction $|X\rangle$, so $H|X\rangle = a|X\rangle$.

Thus the set $\{|\psi_k\rangle\}$, $k=1,\ldots,M$ and $|\chi\rangle$ are $(M+1)$ mutually orthogonal eigenvectors of H. We can continue this construction until all N eigenvectors are obtained.

Next, consider the case of commuting Hermitian operators. Suppose a is an eigenvalue of A with degeneracy N_a. The set of eigenvectors $|\psi\rangle$ with $A|\psi\rangle = a|\psi\rangle$ spans a space S_a of dimensionality N_a. [As usual if $A|\psi_1\rangle = a|\psi_1\rangle$ and $A|\psi_2\rangle = a|\psi_2\rangle$, then $A(|\psi_1\rangle + \lambda|\psi_2\rangle) = a(|\psi_1\rangle + \lambda|\psi_2\rangle)$. So the set of eigenvectors spans the N_a dimensional space S_a.]

If B commutes with A, then

$(B|\psi\rangle) \in S_a$. This follows from

$$A(B|\psi\rangle) = (AB)|\psi\rangle = (BA)\underbrace{|\psi\rangle}_{=a|\psi\rangle}$$
$$= a(B|\psi\rangle).$$

So $(B|\psi\rangle)$ is an eigenvector of A with eigenvalue a.

If B is Hermitian, then we can find N_a eigenvectors of B in S_a, that is, which are also eigenvectors of A. If A is also Hermitian, then $\sum_a N_a = N$, the dimension of the space. That is S_a is spanned by the simultaneous eigenvectors of A and B, there are N_a of them, the dimensionality of S_a. Since A is hermitian its eigenvectors span the entire Hilbert space $\mathcal{H}$. So $\mathcal{H} = \sum_a S_a$. It has dimension N, so

$$N = \sum_a N_a$$ and from the above argument there are N simultaneous eigenvectors of A and B that span $\mathcal{H}$.

The same reasoning applies to any number of mutually commuting Hermitian operators. If there is a unique eigenvector of a set of commuting Hermitian operators A, B ... corresponding to each set of eigenvalues $\{a, b, \ldots\}$, then the set of commuting operators is said to be complete. (This is "physics" sense of the word complete)

(i.e. this set of eigenvalues has no degeneracy)

As we have seen, all of the above theorems have been rigorously derived in the case of finite dimensional spaces. If the space has infinite dimensionality, we will assume the results to be true. Thus an Hermitian operator A has orthonormal eigenvectors which form a basis for the space $\mathcal{H}$. Such an operator will be called an observable.

Then if only one unique eigenvector of a set of commuting Hermitian operators $\{A, B, \ldots\}$ corresponds to each set of eigenvalues $\{a, b, \ldots\}$, the set of operators is said to be complete. The operators constitute a complete set of commuting observables (CSCO).

Example: In the case of a particle of mass m moving in a central potential, we found that the wavefunctions could be written as the product of eigenvectors for the Hamiltonian H, the orbital angular momentum $\vec{L}^2$ and its z-component L_z.

$$H\psi_{n\ell m} = E_n \psi_{n\ell m}$$

$$\vec{L}^2\psi_{n\ell m} = \ell(\ell+1)\hbar^2\psi_{n\ell m}, \quad \ell=0,1,2,\ldots$$

$$L_z\psi_{n\ell m} = m\hbar\,\psi_{n\ell m}, \quad m=-\ell,\ldots,+\ell$$

These 3 eigenvalues, (n,ℓ,m), uniquely specified which wavefunction we were speaking about, thus the set of Hermitian commuting operators (as $H, \vec{L}^2, L_z$ are) ~~are~~ a CSCO.

In the case of the three dimensional isotropic simple harmonic oscillator,

$V=\frac{1}{2}m\omega^2\vec{r}^{\,2}=\frac{1}{2}m\omega^2(x^2+y^2+z^2)$, $\{H,\vec{L}^2,L_z\}$

were a CSCO with $E_n=\frac{1}{2}\hbar\omega n+\frac{3}{2}\hbar\omega$,

only one unique eigenvector corresponded to the eigenvalues specified by (n,ℓ,m).

On the other hand, we could write the Hamiltonian in this case as

$$H = H_x + H_y + H_z$$

$$H_x = \frac{p_x^2}{2m} + \frac{1}{2} m\omega^2 x^2$$

$$H_y = \frac{p_y^2}{2m} + \frac{1}{2} m\omega^2 y^2$$

$$H_z = \frac{p_z^2}{2m} + \frac{1}{2} m\omega^2 z^2 .$$

The set of mutually commuting Hermitian operators $\{H_x, H_y, H_z\}$ also form a CSCO since all wavefunctions could be written as

$$\psi_{n_x n_y n_z} = \psi_{n_x} \psi_{n_y} \psi_{n_z}$$

$$H_x \psi_{n_x} = \hbar\omega(n_x + \tfrac{1}{2})\psi_{n_x}$$

$$H_y \psi_{n_y} = \hbar\omega(n_y + \tfrac{1}{2})\psi_{n_y}$$

$$H_z \psi_{n_z} = \hbar\omega(n_z + \tfrac{1}{2})\psi_{n_z}$$

$n_x, n_y, n_z = 0, 1, 2, \ldots$ and only one eigenvector $\psi_{n_x n_y n_z}$ corresponds to the eigenvalue (n_x, n_y, n_z).

The CSCO is not unique. It is only required that their simultaneous eigenvectors are unique (no degeneracy for the set of eigenvalues). Since each CSCO has an orthonormal basis of eigenvectors we can expand each set of eigenvectors in terms of the other. In the example we can expand $\{\psi_{n\ell m}\}$ in terms of $\{\psi_{n_x n_y n_z}\}$ and vice versa.

We are now in a position to state the postulates in the abstract formulation of Quantum Mechanics.