Linear transformation (continued)

1 Linear transformation was defined as

$$\psi \to \psi' = A\psi$$

and is explicitly seen in

$$
\begin{aligned}
(\phi, A\psi) &= (e_i x_i, A e_j y_j) \\
&= x_i^* y_j (e_i, A e_j) \\
&= x_i^* y_j (e_i, e_k A_{kj}) \\
&= x_i^* y_j A_{kj} (e_i, e_k) \\
&= x_i^* y_j A_{kj} \delta_{ik} \\
&= x_i^* A_{ij} y_j
\end{aligned}
$$

$A e_i = e_k A_{ki}$

2 Adjoint operator : $(\phi, A\psi) = (A^\dagger \phi, \psi)$

Hermitian operator : $(\phi, A\psi) = (A\phi, \psi) \Rightarrow A = A^\dagger$

Unitary operator : $(U\phi, U\psi) = (\phi, \psi) \Rightarrow UU^\dagger = 1$

Projection operator : $P_\phi \psi = \phi(\phi, \psi)$

(3) <u>Theorem:</u>

Hermitian operator have real eigenvalues. If the eigenvalues are distinct, the associated eigenvector are orthogonal.

<u>Proof:</u> $\underline{i} \rightarrow$ no summation

$$A\,\psi_i = \lambda_{\underline{i}}\,\psi_i$$

$$(\psi_j, A\,\psi_i) = \lambda_{\underline{i}}\,(\psi_j, \psi_i)$$

$$(A\,\psi_i, \psi_j)^* = \lambda_{\underline{i}}\,(\psi_j, \psi_i)$$

$$(\psi_i, A\,\psi_j)^* = \lambda_{\underline{i}}\,(\psi_j, \psi_i)$$

$$(\psi_i, \lambda_{\underline{j}}\,\psi_j)^* = \lambda_{\underline{i}}\,(\psi_j, \psi_i)$$

$$\lambda_{\underline{j}}^*\,(\psi_j, \psi_i) = \lambda_{\underline{i}}\,(\psi_j, \psi_i)$$

$$(\lambda_{\underline{j}}^* - \lambda_{\underline{i}})\,(\psi_j, \psi_i) = 0$$

if $i = j$ $\quad \lambda_i = \lambda_j^* \Rightarrow \lambda_i$ is real.

if $i \neq j$ $\quad (\psi_j, \psi_i) = 0 \Rightarrow$ eigenvector are orthogonal.

(4) What if the eigenvalues are degenerate?

Let λ_i be degenerate with d independent eigenvectors, $\psi_1, \psi_2, \ldots, \psi_d$. Thus, a vector

$$\phi = \sum_{n=1}^{d} x_i\,\psi_i$$

will also be an eigenvector. This allows us to choose an orthogonal set of base vectors.

(5) <u>Schmidt orthogonalization</u>

Let $\psi_1, \psi_2, \psi_3, \ldots$ be independent vectors.

→ Construct $\phi_1 = N_1 \psi_1$

Choose N_1 such that $(\phi_1, \phi_1) = 1$.

→ Construct $\phi_2 = N_2 \left[\psi_2 - P_{\phi_1} \psi_2 \right]$

$= N_2 \left[\psi_2 - \phi_1 (\phi_1, \psi_2) \right]$

Choose N_2 such that $(\phi_2, \phi_2) = 1$.

Note that $(\phi_1, \phi_2) = N_2 \left[(\phi_1, \psi_2) - (\phi_1, \phi_1)(\phi_1, \psi_2) \right] = 0$

→ Construct $\phi_3 = N_3 \left[\psi_3 - P_{\phi_1} \psi_3 - P_{\phi_2} \psi_3 \right]$

$= N_3 \left[\psi_3 - \phi_1 (\phi_1, \psi_3) - \phi_2 (\phi_2, \psi_3) \right]$

Choose N_3 such that $(\phi_3, \phi_3) = 1$

Note that $(\phi_1, \phi_3) = (\phi_2, \phi_3) = 0$.

→ ...

(6) Thus, we can always find an orthonormal set of eigenvectors as a base set of vectors for our linear vector space.

7 In the orthonormal basis our matrix is diagonal.

$$(\psi, A\psi) = x_i^* A_{ij} x_j \longrightarrow \lambda_{\underline{i}}\, y_i^* y_i$$

$$A \rightarrow \begin{pmatrix} \lambda_1 & & 0 \\ & \lambda_2 & \\ 0 & & \ddots \ \lambda_n \end{pmatrix}$$

In geometry this is the transformation of a quartic form (a quartic surface) to principal axis, eg:

$$a\, x_1^* x_1 + b\, x_1^* x_2 + c\, x_2^* x_1 + d\, x_2^* x_2 \rightarrow \lambda_1 y_1^* y_1 + \lambda_2 y_2^* y_2 .$$

8 Let $P_i \equiv P_{\varphi_i}$ be the projection operator along an orthonormal base set, $\varphi_1, \varphi_2, \ldots, \varphi_n$ of an operator A. Then,

$$A = \lambda_i P_i$$

Proof. We are given that $A\varphi_i = \lambda_{\underline{i}}\varphi_i$.

We recognize that $\psi = \sum_i \varphi_i (\varphi_i, \psi) = \sum_i P_i \psi$.

$$\begin{aligned} A\psi &= A \sum_i P_i \psi \\ &= A \sum_i \varphi_i (\varphi_i, \psi) \\ &= \sum_i \lambda_i \varphi_i (\varphi_i, \psi) \\ &= \sum_i \lambda_i P_i \psi \\ &= \lambda_i P_i \psi \qquad \text{(summation convention)} \end{aligned}$$

$$\Rightarrow \quad A = \lambda_i P_i$$

9 $A = \lambda_i P_i$ $\qquad\qquad P_i^n = P_i$.

$$A^2 = \lambda_i^2 P_i$$

$$A^n = \lambda_i^n P_i$$

$$f(A) = a_0 + a_1 A + a_2 A^2 + \dots$$

$$= \left[a_0 + a_1 \lambda_i + a_2 (\lambda_i)^2 + \dots \right] P_i$$

$$= \sum_i f(\lambda_i) P_i$$

10 Unitary operator : eigenvalues and eigenvectors

Let $\quad U \psi_i = \lambda_i \psi_i$

Using $\quad (U\psi_i, U\psi_j) = (\psi_i, \psi_j)$

$$(\lambda_i \psi_i, \lambda_j \psi_j) = (\psi_i, \psi_j)$$

$$\lambda_i^* \lambda_j (\psi_i, \psi_j) = (\psi_i, \psi_j)$$

$$(\lambda_i^* \lambda_j - 1)(\psi_i, \psi_j) = 0$$

if $i = j \Rightarrow |\lambda_i|^2 = 1 \Rightarrow \lambda_i^* = \frac{1}{\lambda_i} \Rightarrow \lambda_i = e^{i\phi_i}$

if $i \neq j \Rightarrow (\psi_i, \psi_j) = 0 \Rightarrow$ eigenvectors are orthogonal.

$$U \rightarrow \begin{pmatrix} e^{i\phi_1} & & & 0 \\ & e^{i\phi_2} & & \\ & & \ddots & \\ 0 & & & e^{i\phi_n} \end{pmatrix}$$

11 A unitary operator can be expressed in terms of a Hermitian operator.

$$U = \frac{1 + iA}{1 - iA} = (1+iA)(1-iA)^{-1} = (1-iA)^{-1}(1+iA) \qquad A = A^{\dagger}$$

$$U^{\dagger} = (1+iA)^{-1}(1-iA) = (1-iA)(1+iA)^{-1}.$$

$$U U^{\dagger} = (1+iA)(1-iA)^{-1}(1-iA)(1+iA)^{-1} = 1.$$

$$-\frac{i}{2} \ln U = -\frac{i}{2} \ln \frac{1+iA}{1-iA} = \tan^{-1} A.$$

$$\ln U = i\, 2 \tan^{-1} A$$

$$U = e^{iH} \quad \text{where} \quad H = 2 \tan^{-1} A.$$

(12) Theorem:

$$\left.\begin{array}{l} A\psi_i = a_i \psi_i \\ B\psi_i = b_i\psi_i \end{array}\right\} \Longleftrightarrow [A,B] = 0$$

A & B can be diagonalized simultaneosly.

Proof: (i) Let LHS be true.

$$A\psi_i = a_i\psi_i \quad \Rightarrow \quad BA\psi_i = a_i B\psi_i = a_i b_i \psi_i$$

$$B\psi_i = b_i\psi_i \quad \Rightarrow \quad AB\psi_i = b_i A\psi_i = b_i a_i \psi_i$$

$$\Rightarrow (AB - BA)\psi_i = 0$$

$$\Rightarrow [A,B] = 0.$$

(ii) Let R.H.S. be true, that is $AB = BA$.

Let ψ_i be eigenvector of B, that is $B\psi_i = b_i\psi_i$.

$$B\psi_i = b_i\psi_i$$

$$AB\psi_i = b_i A\psi_i$$

$$B(A\psi_i) = b_i(A\psi_i) \quad \because AB = BA.$$

Thus, $(A\psi_i)$ is an eigenvector of B with eigenvalue b_i. There are two possibilities

(a) b_i are non-degenerate

$$\Rightarrow A\psi_i = a_i\psi_i$$

(b) b_i are degenerate.

13 If b_i is degenerate,

we can construct

$$A \psi_i = \text{linear combination of } \psi_i \text{ belonging to } b_i.$$

$$= \sum_{\beta=1}^{d} \psi_{i,\beta} A^{(i)}_{\beta\alpha}$$

Thus, the matrix representation in this basis set is

$$B = \left[\begin{array}{cc|ccc|c} b_1 & 0 & & 0 & & 0 \\ 0 & b_1 & & & & \\ \hline & & b_2 & 0 & 0 & \\ & 0 & 0 & b_2 & 0 & 0 \\ & & 0 & 0 & b_2 & \\ \hline & 0 & & 0 & & \ddots \end{array}\right]$$

$$A = \left[\begin{array}{cc|ccc|c} A^{(1)}_{11} & A^{(1)}_{12} & & 0 & & 0 \\ A^{(1)}_{21} & A^{(1)}_{22} & & & & \\ \hline & & A^{(2)}_{11} & A^{(2)}_{12} & A^{(2)}_{13} & \\ & 0 & A^{(2)}_{21} & A^{(2)}_{22} & A^{(2)}_{23} & 0 \\ & & A^{(2)}_{31} & A^{(2)}_{32} & A^{(2)}_{33} & \\ \hline & 0 & & 0 & & \ddots \end{array}\right]$$

Thus, we can diagonalize the subspaces of A separately, $S^{(i)}_{\text{subspace}} A^{(i)}_{\text{subsp}} S^{(i)\,-1}_{\text{subspace}} = A^{(i)}_{D}$, which will leave the form of B invariant.

(14) There may still be degeneracy after A and B are diagonalized. Then, find a third operator C

$$[C, A] = [C, B] = 0$$

to make the base set unique.

Example: Hydrogen atom states are made unique by n, l, m, s for $\vec{A}, \vec{L}, L_z$ and spin.

(15) In general we have,

$$S A S^{-1} = A_D$$

S – diagonalising matrix
A_D – diagonalized matrix.

Also, if A is Hermitian, then S is Unitary. That is, Hermitian matrices are diagonalized by Unitary operators.

(16) Secular equation : $\det(A - \lambda 1) = 0$

$$(A' - \lambda 1) = (S A S^{-1} - \lambda 1)$$
$$= S(A - \lambda 1) S^{-1}$$

$$\det(A' - \lambda 1) = (\det S) \det(A - \lambda 1) \det S^{-1}$$
$$= \det(S S^{-1}) \det(A - 1\lambda)$$
$$= \det(A - \lambda 1)$$

Thus, $\det(A - \lambda 1)$ is invariant under diagonalization process.

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$$\det(A - \lambda 1) = (-\lambda)^n + (-\lambda)^{n-1}(\mathrm{tr} A) + \cdots + (\det A)$$

Since $\det(A - \lambda 1)$ is invariant for arbitrary λ, each coefficient in the polynomial has to be zero. Thus, we have $(\mathrm{tr} A)$ and $(\det A)$ to be invariant under the diagonalization process.