Illustrative example

Consider an operator $\hat{M}$ whose matrix elements in a given basis are given by

$$M = \begin{pmatrix} 2 & 0 & -2 \\ -2i & i & 2i \\ 1 & 0 & -1 \end{pmatrix}$$

(Note: M is neither unitary nor Hermitian.)

The characteristic equation is

$$\det(\hat{M} - \omega \hat{I}) = \begin{vmatrix} 2-\omega & 0 & -2 \\ -2i & i-\omega & 2i \\ 1 & 0 & -1-\omega \end{vmatrix} = -\omega^3 + (1+i)\omega^2 - i\omega$$
$$= -\omega(\omega^2 - (1+i)\omega + i) = 0$$

- Its root are $\boxed{\omega_1 = 0,\ \omega_2 = 1,\ \omega_3 = i.}$

- To find the eigenvector corresponding to ω_1, we must solve

$$\begin{pmatrix} 2 & 0 & -2 \\ -2i & i & 2i \\ 1 & 0 & -1 \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = 0 \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\Rightarrow \begin{array}{ll} 2a_1 - 2a_3 = 0 & \Rightarrow a_1 = a_3 \\ -2ia_1 + ia_2 + 2ia_3 = 0 & \Rightarrow a_2 = 0 \\ a_1 - a_3 = 0 & \Rightarrow a_1 = a_3 \text{ (redundant)} \end{array}$$

Pick $a_1 = 1$: $\Rightarrow \boxed{\vec{a}^{(1)} = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \text{ for } \omega_1 = 0}$

- To find the second eigenvector, solve:

$$\begin{pmatrix} 2 & 0 & -2 \\ -2i & i & 2i \\ 1 & 0 & -1 \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = 1 \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

$$\Rightarrow \quad 2a_1 - 2a_3 = a_1 \qquad \Rightarrow \quad a_1 = 2a_3$$
$$-2ia_1 + ia_2 + 2ia_3 = a_2 \qquad \Rightarrow \quad a_2 = \frac{1-i}{2} a_1$$
$$a_1 - a_3 = a_3 \qquad \Rightarrow \quad a_1 = 2a_3 \ \text{(redundant)}$$

Pick $a_1 = 2$: $\boxed{\vec{a}^{(2)} = \begin{pmatrix} 2 \\ 1-i \\ 1 \end{pmatrix} \text{ for } \omega_2 = 1}$

(Of course, you can normalize the eigenvectors, if you want.)

Similarly, the third eigenvector is found as $a_3 = a_1 = 0$, a_2 arbitrary. Pick $a_2 = 1 \Rightarrow$ $\boxed{\vec{a}^{(3)} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \text{ for } \omega_3 = i}$

More conventionally the eigenvectors are labelled by their eigenvalues:

$$|\omega_1 = 0\rangle \leftrightarrow \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$$

$$|\omega_2 = 1\rangle \leftrightarrow \begin{pmatrix} 1 \\ \frac{1}{2}(1-i) \\ \frac{1}{2} \end{pmatrix}$$

$$|\omega_3 = i\rangle \leftrightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

If two or more root of the characteristic polynomial coincide, we say that the corresponding eigenvalue is degenerate. If this happens, the procedure to find the eigenvectors must be modified (see below).

<u>Theorem</u> The eigenvalues of a Hermitian operator are real

<u>Proof</u>: Let $\hat{\Omega}|\omega\rangle = \omega|\omega\rangle \Rightarrow \langle\omega|\hat{\Omega}|\omega\rangle = \omega\langle\omega|\omega\rangle$

and $\langle\omega|\Omega^+|\omega\rangle = \langle\hat{\Omega}\omega|\omega\rangle = \langle\omega|\hat{\Omega}\omega\rangle^* = \omega^*\langle\omega|\omega\rangle$

Since $\hat{\Omega}^+ = \hat{\Omega}$, $(\omega-\omega^*)\underbrace{\langle\omega|\omega\rangle}_{\neq 0} = 0 \Rightarrow \omega^* = \omega$ ◇

<u>Theorem</u> The normalized eigenvectors of a Hermitian operator form an orthonormal basis, and in this eigenbasis it is diagonal, with its eigenvalues as its diagonal elements.

<u>Proof</u> Let $|\omega_1\rangle, |\omega_2\rangle$ be normalized eigenvectors of a Hermitian operator $\hat{\Omega}$ with different (real) eigenvalues $\omega_1 \neq \omega_2$ (we assume non-degenerate eigenvalues for simplicity).

$$\langle\omega_1|\hat{\Omega}|\omega_2\rangle = \omega_2\langle\omega_1|\omega_2\rangle$$

$$= \langle\omega_1|\Omega^+|\omega_2\rangle = \langle\hat{\Omega}\omega_1|\omega_2\rangle = \langle\omega_1|\omega_1^*|\omega_2\rangle$$

$$= \omega_1\langle\omega_1|\omega_2\rangle$$

Since $\omega_1 \neq \omega_2$, it follows that $\langle\omega_1|\omega_2\rangle = 0$

This proves that eigenvectors to different eigenvalues of a Hermitian operator are mutually orthogonal.

(For n-fold degenerate eigenvalues, we can find n mutually orthogonal eigenvectors by Gram-Schmidt orthonormalization.)

Now consider the basis $|\omega_1\rangle, |\omega_2\rangle, \ldots |\omega_n\rangle$.

The matrix elements of $\hat{\Omega}$ in this basis are

$\langle \omega_i | \hat{\Omega} | \omega_j \rangle = \langle \omega_i | \omega_j | \omega_j \rangle = \omega_j \langle \omega_i | \omega_j \rangle = \omega_j \delta_{ij}$

i.e. the matrix representing $\hat{\Omega}$ in this basis is diagonal, with the eigenvalues ω_j as its diagonal elements.

What happens in the degenerate case?

Suppose $\omega_1 = \omega_2 = \dots \omega_m = \omega$. In this case we have m linearly independent eigenvectors ~~to~~ the same, m-fold degenerate eigenvalue. We can use Gram-Schmidt to pick one of them and orthogonalise all others relative to it and to each other. But instead of starting with this particular eigenvector, we could start Gram-Schmidt from any other linear combination of these m eigenvectors. In each case we obtain a different m-dimensional set of orthonormal eigenvectors, all with eigenvalue ω.

So, for Hermitian operators with degenerate eigenvalues, there are in general many different possible choices of orthonormalized eigenvectors which diagonalize the operator.

Remember, however, that eigenvectors to different eigenvalues are always orthogonal on each other for Hermitian operators.

Degenerate example:

Consider $\hat{\Omega} \leftrightarrow \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix}$

Characteristic equation is $(\omega-2)^2\omega = 0 \Rightarrow \omega_1 = 0$, $\omega_{2/3} = 2$

$|\omega_1 = 0\rangle \leftrightarrow \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$

$|\omega_2 = 2\rangle$: $\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = 2\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$

$$\Rightarrow \begin{aligned} a_1 + a_3 &= 2a_1 & & a_1 = a_3 \\ 2a_2 &= 2a_2 & \Rightarrow \;& a_2 \text{ arbitrary} \\ a_1 + a_3 &= 2a_3 & & a_1 = a_3 \end{aligned}$$

$\Rightarrow$ now we have 2 arbitrary components!

These conditions define a 2-dimensional ensemble of vectors that are perpendicular to $|\omega_1 = 0\rangle$, i.e. lie in a plane perpendicular to $|\omega_1\rangle$.

Choosing arbitrarily $a_1 = 1$ and $a_2 = 1$, we get $|\omega_2 = 2\rangle \Leftrightarrow \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$ (after normalization)

The second vector in the plane $a_1 = a_3$, a_2 arbitrary that is orthogonal to $|\omega_2 = 2\rangle$ is

$$|\omega_3 = 2\rangle \leftrightarrow \frac{1}{\sqrt{6}}\begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}$$

<u>Theorem</u> The eigenvalues of a unitary operator lie on the unit circle in $\mathbb{C}$, i.e. are complex numbers with unit modulus; their eigenvectors are mutually orthogonal (for degenerate situations, this will be achieved in the same way as for Hermitian operators).

<u>Proof</u> (assuming no degeneracy for simplicity)

$$\hat{U}|u_i\rangle = u_i|u_i\rangle \quad , \quad \hat{U}|u_j\rangle = u_j|u_j\rangle$$

$$\langle u_j|\underbrace{U^+U}_{=\hat{I}}|u_i\rangle = u_i u_j^* \langle u_j|u_i\rangle$$

$$\Rightarrow (1-u_iu_j^*)\langle u_j|u_i\rangle = 0$$

For $i=j$: $1-u_iu_i^*=0$ since $\langle u_i|u_i\rangle \neq 0 \Rightarrow |u_i|^2=1$

For $i\neq j$: Since $|u_i\rangle \neq |u_j\rangle \Rightarrow u_i \neq u_j \Rightarrow u_iu_j^* \neq u_iu_i^* = 1$
hence $u_iu_j^* \neq 1$ and therefore $\langle u_j|u_i\rangle = 0$ ◇

Diagonalization of Hermitian or unitary matrices:

Consider an orthonormal basis
$|1\rangle, |2\rangle \ldots |n\rangle$ in $\mathbb{V}^n(\mathbb{C})$

The orthonormalized eigenstates $|\omega_1\rangle, \ldots, |\omega_n\rangle$ of a Hermitian or unitary operator $\hat{\Omega}$ can be expanded in this basis as

$$|\omega_i\rangle = \sum_k u_{ik}|k\rangle$$

where u_{ik} is the k^{th} component of $|\omega_i\rangle$ in the basis $\{|k\rangle, k=1,\ldots n\}$.