Diagonalizing $\hat{H}$

If a matrix is diagonal $\Rightarrow$ all elements on the diagonal, then the eigenvalues are on the diagonal.

If

$$\hat{H} = \begin{pmatrix} E_1 & 0 & 0 \\ 0 & E_2 & 0 \\ 0 & 0 & E_3 \end{pmatrix}$$

then the eigenvalues are

$$\lambda = E_1, E_2, E_3$$

and the eigenvectors

$$|E_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad |E_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad |E_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

Matrices are profoundly easier to deal with if they are diagonal, so it is periodically convenient to change the basis to the basis that makes the matrix diagonal.

To change basis, we use a <u>unitary</u> operator $\hat{S}$ that performs a rotation.

$$\hat{H}_{diag} = \hat{S}\hat{H}\hat{S}^{-1}$$

The eigenvectors of $\hat{H}$ give us $\hat{S}$.

Let $\vec{a}^{j}$ be an eigenvector with components a^{j}_{i}.

$$\left(\hat{S}^{-1}_{ij}\right) = a^{j}_{i}$$

$\Longrightarrow$ The colums of $\hat{S}^{-1}$ are the eigenvectors.

$$\overleftrightarrow{S}^{-1} = \left(\underbrace{\begin{bmatrix} a^1_1 \\ a^1_2 \\ a^1_3 \end{bmatrix}}_{\text{Eigenvector 1}} \begin{bmatrix} a^2_1 \\ a^2_2 \\ a^2_3 \end{bmatrix} \begin{bmatrix} a^3_1 \\ a^3_2 \\ a^3_3 \end{bmatrix} \right)$$

Block Diagonal Form - Suppose the matrix can be separated into squares about the diagonal.

$$\begin{pmatrix} a_1 & a_2 & 0 & 0 & 0 \\ b_1 & b_2 & 0 & 0 & 0 \\ 0 & 0 & c_3 & 0 & 0 \\ 0 & 0 & 0 & d_4 & 0 \\ 0 & 0 & 0 & 0 & e_4 \end{pmatrix}$$

Ex

The matrix has eigenvalues, c_3, d_4, e_5

and $\det \begin{vmatrix} a_1-\lambda & a_2 \\ b_1 & a_2-\lambda \end{vmatrix} = 0 \Rightarrow \lambda_1, \lambda_2$

with eigenvectors

$$|c_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \qquad |d_4\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \qquad |e_5\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

$$|\lambda_1\rangle = \alpha_1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \alpha_2 \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$|\lambda_2\rangle = B_1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} + B_2 \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Commutation Relations

In classical mechanics, numbers commute

$$x p_x = p_x x$$

but in QM numbers are replaced by operators which do not in general commute.

$$\hat{x}\hat{p}_x \neq \hat{p}_x \hat{x}$$

To characterize, this we report the commutator or commutation relation of the operators.

Commutation Relation (Commutator)

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

$\Longrightarrow$ If $[\hat{A}, \hat{B}] = 0$, the operators commute.

Example

$$[\hat{x}, \hat{p}_x] = i\hbar = \hat{x}\hat{p}_x - \hat{p}_x\hat{x}$$

Unitary Operators

Dfn <u>Unitary Operator</u>

$$\hat{U}^{+} = \hat{U}^{-1}$$

$$\Rightarrow \hat{U}^{+} U = \hat{1} \quad \text{the identity operator}$$

$$\hat{1}\,|a\rangle = |a\rangle$$

Consider, $|a'\rangle = U|a\rangle$

$$\Rightarrow \langle a'| = \langle a|U^{+}$$

$$\langle a'|a'\rangle = \langle a|U^{+}U|a\rangle = \langle a|a\rangle$$

$\Rightarrow$ Unitary operators preserve the norm of the vector.

$\Rightarrow$ The operator that moves quantum systems forward in time will be unitary.

Thm If $\hat{A}$ is ~~h~~ hermition, $e^{i\hat{A}}$ is unitary

Proof We define a function of an operator by using the power series of the normal function

$$e^{x} = 1 + x + \frac{1}{2}x^2 + \frac{1}{6}x^3 \dots$$

$$e^{\hat{A}} = 1 + \hat{A} + \frac{1}{2}\hat{A}\hat{A} + \frac{1}{6}\hat{A}\hat{A}\hat{A} + \dots$$

therefore, if $\hat{T} = e^{i\hat{A}}$, $\hat{T}^{+} = e^{-i\hat{A}^{+}}$

by observing power series.

$$\hat{T}^{+}\hat{T} = e^{-i\hat{A}} \cdot e^{i\hat{A}} = e^{-i\hat{A}+i\hat{A}} = \hat{1}$$

$$\Rightarrow \hat{T}^{+} = \hat{T}^{-1} \Rightarrow \hat{T} \text{ unitary}$$

Eigenvectors of Unitary Operator are $\lambda = e^{i\theta}$

Proof $\hat{U}|a\rangle = \lambda|a\rangle$

$$\langle a|\hat{U}^{+} = \langle a|U^{-1} = \lambda^{*}\langle a|$$

$$\langle a|U^{+}U|a\rangle = \lambda\lambda^{*}\langle a|a\rangle$$

$$\langle a|a\rangle = \lambda\lambda^{*}\langle a|a\rangle \Rightarrow \lambda\lambda^{*} = 1$$