[This Section also goes into Ch. X]

H. Why are QM, Eigenvalue Problems closely related to Matrices?

QM: TISE $\hat{H}\psi = E\psi$ (eigenvalue problem of $\hat{H}$)

General Eigenvalue Problem

$$\hat{A}\psi = a\psi \quad (38)$$

> Key Point: Eigenvalue Problem can be turned into a Matrix problem. (39)

Consider the space involved in problem, choose a complete set of orthonormal functions $\{\phi_i\}$

ψ can be expanded in $\{\phi_i\}$

i.e. $\psi = \sum_i c_i \phi_i$ (40) 1/. $\{\phi_i\}$ is complete
2/. know $\{c_i\} \Rightarrow$ know ψ

Substitute into Eq. (38):

$$\sum_i c_i \hat{A} \phi_i = a \sum_i c_i \phi_i$$

Left multiply ϕ_j^* and $\int \cdots d\tau$:

$$\sum_i c_i \int \phi_j^* \hat{A} \phi_i d\tau = a \sum_i c_i \int \phi_j^* \phi_i d\tau = a \sum_i c_i \delta_{ji} = a c_j$$

$$\Rightarrow \boxed{\sum_i \left(\int \phi_j^* \hat{A} \phi_i d\tau \right) c_i = a c_j} \qquad (40)$$

Eq. (40) and Eq. (38) are <u>equivalent</u>.

Eq. (40) <u>is</u> a Matrix Equation! Let's see.

$$\underbrace{A_{ji}}_{\uparrow} \equiv \int \phi_j^* \hat{A} \phi_i \, d\tau$$

the $(ji)^{th}$ matrix element of $\hat{A}$

e.g. $A_{13,4} \equiv \int \phi_{13}^* \hat{A} \phi_4 \, d\tau$

With $\hat{A}$ and $\{\phi_i\}$,
all A_{ji} can be calculated!

1/. coordinate integrated over $\int \cdots d\tau$
$\Rightarrow$ not a function of coordinate (just a number)

2/. <u>Not</u> to confuse it with expectation value. Here ϕ_j may not be equal to ϕ_i.

3/. It gives a value for a pair ϕ_j, ϕ_i. Thus its value is labelled by "ji".

4/. A_{ji} depends on choice of complete set (basis) $\{\phi_i\}$

Eq. (40) reads $\boxed{\sum_i A_{ji} C_i = a C_j}$ (41)

Meaning:

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \underbrace{\begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix}}_{\text{eigenvector}} = \underset{\substack{\uparrow \\ \text{eigenvalue}}}{a} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix} \qquad \text{(41) in long form}$$

Wrote $\hat{A}\psi = a\psi$ into a Matrix Eigenvalue Problem!

TISE: Need H_{ji}, same form as Eq. (41) with "a" becomes E

For a <u>Hermitian</u> Operator $\hat{A}$:

$$A_{ji} = \int \phi_j^* \hat{A} \phi_i \, d\tau = \int \phi_i (\hat{A} \phi_j)^* \, d\tau = \left(\phi_i^* \hat{A} \phi_j \, d\tau \right)^*$$

definition of Hermitian Operator

$$\therefore \boxed{A_{ji} = A_{ij}^*} \qquad (42)$$

defines <u>Hermitian Matrix</u>

Real Eigenvalues

Orthogonal Eigenvectors

- In general, Matrix in Eq. (41) is $\underbrace{\infty \times \infty}$!

($\because$ $\{\phi_i\}$ has infinitely many functions)

<u>e.g.</u> e^{ikx} for all k

"plane wave" expansion

Recipe: QM TISE Problem is one Big Matrix Eigenvalue Problem

1/. Write down $\hat{H}$ for QM problem in hand

2/. Take your favorite set of $\{\phi_i\}$

3/. Evaluate H_{ji} (save time by Hermitian Property)

4/. $$\begin{pmatrix} H_{11} & H_{12} & H_{13} & \cdots \\ H_{21} & H_{22} & H_{23} & \cdots \\ H_{31} & H_{32} & H_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$ Hamiltonian Matrix

5/. Call Subroutine to find eigenvalues (allowed energies E) and corresponding eigenvectors (energy eigenstates). Done!

Remarks

- Learning some Computational Techniques helps!
- What if $\{\phi_i\}$ are <u>NOT</u> orthogonal to each other?
  [Sometimes (in Molecular Physics) such choice is convenient]
  How is Eq. (41) modified?
- Many existing algorithms of finding eigenvalues of big matrix
  (e.g. Matlab, Mathematica, Numerical Recipe)
- The recipe provides a way to solve QM problems that cannot be solved analytically

<u>One particular choice of $\{\phi_i\}$ that makes A_{ji} simply</u>

- $\hat{A}\psi = a\psi$ is the problem
- If one <u>so clever</u> or <u>insightful</u> that $\{\phi_i\}$ chosen happened to be the set of <u>$\hat{A}$'s eigenstates</u> $\{\varphi_i\}$: $\hat{A}\varphi_i = a_i\varphi_i$

then $A_{ji} = \int \varphi_j^* \hat{A} \varphi_i d\tau = \int \varphi_j^* a_i \varphi_i d\tau = a_i \delta_{ji}$

$\therefore A_{ii} = a_i$, $A_{ij} = 0 \quad (i \neq j)$

The $\hat{A}$ Matrix is:

$$\begin{pmatrix} a_1 & 0 & 0 & \cdots \\ 0 & a_2 & 0 & \\ 0 & 0 & a_3 & \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

is <u>diagonal</u>

[diagonal elements are eigenvalues]

I. Closer look at Spin's Matrices

- In handling Spin-half problems, the nature of spin makes us clever and full of insight!
  - Any direction: Only $+\frac{\hbar}{2}$, $-\frac{\hbar}{2}$ projections
- Take $\hat{S}_z$
- Choose Basis that are eigenstates of $\hat{L}_z$

$$\therefore \quad \hat{S}_z = \begin{pmatrix} \frac{\hbar}{2} & 0 \\ 0 & -\frac{\hbar}{2} \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The chosen basis is $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$

See last page

$${}_z\langle \tfrac{1}{2},\tfrac{1}{2} | \hat{S}_z | \tfrac{1}{2}\tfrac{1}{2}\rangle_z = \frac{\hbar}{2} \; ; \quad {}_z\langle \tfrac{1}{2},-\tfrac{1}{2} | \hat{S}_z | \tfrac{1}{2},\tfrac{1}{2}\rangle_z = \frac{\hbar}{2} \underbrace{{}_z\langle \tfrac{1}{2}-\tfrac{1}{2} | \tfrac{1}{2}\tfrac{1}{2}\rangle_z}_{=0} = 0$$

- It is a choice to intentionally make $\hat{S}_z$ diagonal
- Other $\hat{S}_x$, $\hat{S}_y$ Matrices can then be constructed (e.g. via $\hat{S}_+$, $\hat{S}_-$)
- But $\hat{z}$-direction is nothing special. We could develop a representation in which $\hat{S}_x$ is diagonal (then $\hat{S}_z$ is not diagonal).