G. Learning the Mathematical Structure of QM from Spin

▪ All information of a system is given by the wavefunction

In context of spin

▪ All information of a spin-½ system† is given by its state expressed as a state vector

$$\begin{pmatrix} c \\ d \end{pmatrix}$$

For $s=\frac{1}{2}$ spin, it has two entries just like a vector [but entries can be complex]

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† For particle-in-a-box, $\psi(x)$ is more complicated because we need to know $\psi(x_1), \psi(x_2), \cdots, \psi(x_n), \cdots$ infinitely many values! So it is like a vector with infinitely many components (& we have infinitely many allowed energies).

- $\boxed{\text{Physical Quantities are represented by Hermitian Operators}}$

In context of spin

- $\hat{S}_x$, $\hat{S}_y$, $\hat{S}_z$, $\hat{S}^2$ are Hermitian
- $\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ is a Hermitian Matrix

$$(M_{nm} = M^*_{mn}) \qquad (33)$$

Same for other quantities.

$\hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ has $M_{12} = M^*_{21}$ (also $M_{mn} = M^*_{nm}$)

▪ Eigenstates of Hermitian Operator are orthogonal

<u>In context of Spin</u>

$\hat{S}_z$: $\frac{\hbar}{2}$ $\quad \alpha_z = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$\quad -\frac{\hbar}{2}$ $\quad \beta_z = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Inner product $\langle \alpha_z | \beta_z \rangle$

orthogonal

$$(1^* \quad 0^*) \begin{pmatrix} 0 \\ 1 \end{pmatrix} = (1 \quad 0) \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0$$

$\hat{S}_y$: $\frac{\hbar}{2}$ $\quad \alpha_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}$

$\quad -\frac{\hbar}{2}$ $\quad \beta_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$

orthogonal

$$\langle \alpha_y | \beta_y \rangle = \frac{1}{2} (1^* \quad i^*) \begin{pmatrix} 1 \\ -i \end{pmatrix} = \frac{1}{\sqrt{2}} (1 \quad -i) \begin{pmatrix} 1 \\ -i \end{pmatrix} = 0$$

$\hat{S}_x$: $\frac{\hbar}{2}$ $\quad \alpha_z = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

$\quad -\frac{\hbar}{2}$ $\quad \beta_z = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix}$

orthogonal

$$\langle \alpha_x | \beta_x \rangle = \frac{1}{2} (1 \quad 1) \begin{pmatrix} -1 \\ 1 \end{pmatrix} = 0$$

▪ Eigenstates of an Operator can be used to express a general state

In context of Spin

$\hat{S}_z$'s eigenstates

$$\begin{pmatrix} c \\ d \end{pmatrix} = c\begin{pmatrix} 1 \\ 0 \end{pmatrix} + d\begin{pmatrix} 0 \\ 1 \end{pmatrix} = c\cdot\alpha_z + d\cdot\beta_z \qquad (34)$$

general state

[in general, c & d can be complex]

Why can this be done?

Mathematics: $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ form a complete set in the (mathematical) space of spin-½ problems

OR $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ span the space

$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ are used as basis vectors in Eq.(34)

With a choice of basis, what does a general state $|\psi\rangle$ mean?

- General state $|\psi\rangle$, it is free from a choice of basis (i.e. free from representation)
- Make a choice of basis of α_z and β_z (eigenstates of $\hat{S}_z$)
- The abstract $|\psi\rangle$ becomes $\begin{pmatrix} c \\ d \end{pmatrix}$ (see Eq.(31))
- $$|\psi\rangle = c \cdot \alpha_z + d \cdot \beta_z \quad \text{OR} \quad |\psi\rangle = c\,|\uparrow\rangle_z + d\,|\downarrow\rangle_z \qquad (34)$$

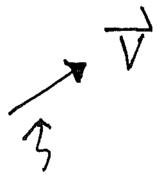
  read out coefficients
- The abstract $|\psi\rangle$ becomes $\begin{pmatrix} c \\ d \end{pmatrix}$ ← stacking up coefficients in expanding $|\psi\rangle$ in the chosen basis (35)

  general spin-½ state (general wavefunction)

$\therefore$ When we say the general state is $\begin{pmatrix} c \\ d \end{pmatrix}$, it is accompanied by a choice of basis [$\therefore$ you should look for the basis set being used]

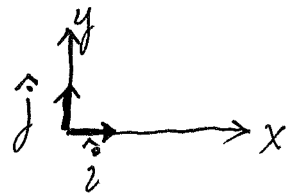
A useful analogy to make things less abstract

<u>An analogy : a vector</u>



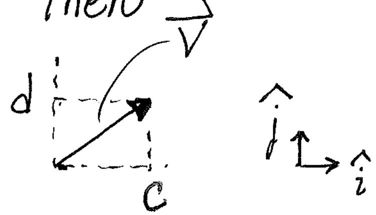
a general vector (abstract)
[there is a length
there is a direction]

To describe it



Choose a basis set, e.g
$\hat{i}$, $\hat{j}$ unit vectors

Then



$$\vec{V} = c\,\hat{i} + d\,\hat{j}$$
(c.f. Eq. (32))

then $\vec{V}$ can be expressed as $\begin{pmatrix} c \\ d \end{pmatrix}$ or $(c \;\; d)$

QM is slightly more complicated, as c & d can be complex.

Could expand $|\psi\rangle$ using another basis set [e.g. $[\sigma_x]$ eigenvectors]

$$\begin{pmatrix} c \\ d \end{pmatrix} = \frac{c+d}{\sqrt{2}} \cdot \underbrace{\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}}_{\alpha_x} - \frac{(c-d)}{\sqrt{2}} \cdot \underbrace{\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}}_{\beta_x} \qquad (30)$$

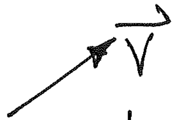
$$|\psi\rangle = c' \alpha_x + d' \beta_x \qquad (36)$$

If we announce (choose) the basis set is $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$, then the general state $|\psi\rangle$ is described by the state vector ("wavefunction")

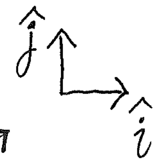
$$\begin{pmatrix} c' \\ d' \end{pmatrix} = \begin{pmatrix} \frac{c+d}{\sqrt{2}} \\ -\frac{(c-d)}{\sqrt{2}} \end{pmatrix} \qquad (37)$$

in the basis of α_x and β_x

An analogy: A vector



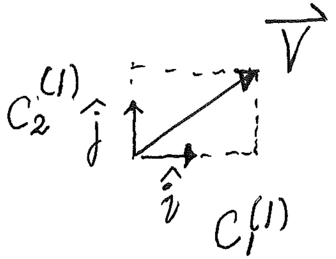
a vector (general)
[direction, magnitude]



basis set #1

basis set #2

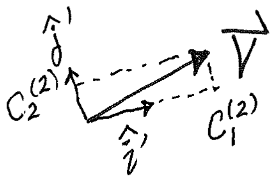
(38)



basis #1 basis set #1

$$\vec{V} = C_1^{(1)}\hat{i} + C_2^{(1)}\hat{j}$$

$\vec{V}$ described by $\begin{pmatrix} C_1^{(1)} \\ C_2^{(1)} \end{pmatrix}$

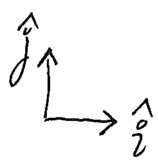


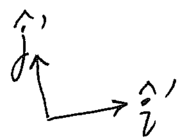
basis set #2 basis set #2

$$\vec{V} = C_1^{(2)}\hat{i}' + C_2^{(2)}\hat{j}'$$

Same $\vec{V}$ described by $\begin{pmatrix} C_1^{(2)} \\ C_2^{(2)} \end{pmatrix}$

How to relate $(C_1^{(2)}, C_2^{(2)})$ and $(C_1^{(1)}, C_2^{(1)})$?





Of course, we can express $\left.\begin{matrix}\hat{i} \\ \hat{j}\end{matrix}\right\}$ in terms of $\left\{\begin{matrix}\hat{i}' \\ \hat{j}'\end{matrix}\right.$

i.e. Transformation (change basis)

What for?

- Given $|\psi\rangle$, measure $[\hat{S}_z]$

$$|\psi\rangle = c \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} + d \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$|d|^2$ = prob. of getting $S_z = -\frac{\hbar}{2}$

$|c|^2$ = prob. of getting $S_z = +\frac{\hbar}{2}$

$$\langle S_z \rangle = |c|^2 \frac{\hbar}{2} - |d|^2 \frac{\hbar}{2}$$

expectation value

- Given $|\psi\rangle$, measure $[\hat{S}_x]$

$$|\psi\rangle = c' \cdot \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + d' \cdot \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$|d'|^2$ = prob. of getting $S_x = -\frac{\hbar}{2}$

$|c'|^2$ = prob. of getting $S_x = +\frac{\hbar}{2}$

$$\therefore \langle S_x \rangle = \underbrace{\frac{(c+d)(c^*+d^*)}{2}}_{|c'|^2} \left(\frac{\hbar}{2}\right) + \underbrace{\frac{(c-d)(c^*-d^*)}{2}}_{|d'|^2} \left(\frac{-\hbar}{2}\right) = \frac{\hbar}{2} [cd^* + dc^*]$$

expectation value

These expectation values can be found by plugging in formula

$$\langle \hat{A} \rangle = \int \Psi^* \hat{A} \Psi \, d\tau$$

$$\Psi \to \begin{pmatrix} c \\ d \end{pmatrix} \; ; \quad \hat{A} \nearrow \hat{S}_z, \; \hat{A} \searrow \hat{S}_x \; ; \quad \int \Psi^* \hat{A} \Psi \, d\tau \to (c^* \; d^*) \begin{pmatrix} 2\times 2 \\ \text{operator} \end{pmatrix} \begin{pmatrix} c \\ d \end{pmatrix}$$

Check: $\langle S_z \rangle = (c^* \;\; d^*) \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} c \\ d \end{pmatrix} = (c^* \; d^*) \begin{pmatrix} c \\ -d \end{pmatrix} \frac{\hbar}{2} = (|c|^2 - |d|^2) \frac{\hbar}{2}$

$$\langle S_x \rangle = (c^* \; d^*) \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} c \\ d \end{pmatrix} = (c^* \; d^*) \begin{pmatrix} d \\ c \end{pmatrix} \frac{\hbar}{2} = (cd^* + dc^*) \frac{\hbar}{2}$$

[Same results as on last page]

Behind these manipulations are the <u>QM</u> <u>postulates</u>...

- In any measurement of the observable quantity represented by $\hat{A}$, the only values that will ever be observed are the eigenvalues a_n of operator $\hat{A}$
- Given a normalized state Ψ, the average value (expectation value) of the observable quantity represented by $\hat{A}$ is given by

$$\langle \hat{A} \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{A} \Psi \, d\tau$$