G. Learning the Mathematical Structure of QM from Spin

$\boxed{\text{▪ All information of a system is given by the wavefunction}}$

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 $\psi(x_1), \psi(x_2), \ldots, \psi(x_n), \ldots$ infinitely many values! So it is like a vector with infinitely many components (& we have infinitely many allowed energies).

▪ Physical Quantities are represented by Hermitian Operators

<u>In context of Spin</u>

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

$$(M_{nm} = M^*_{mn}) \qquad (30)$$

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>

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

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

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

orthogonal

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

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

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

orthogonal

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

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

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

orthogonal

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

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

In context of Spin

$$\begin{pmatrix} c \\ d \end{pmatrix} = c\begin{pmatrix} 1 \\ 0 \end{pmatrix} + d\begin{pmatrix} 0 \\ 1 \end{pmatrix} = c\cdot\alpha_z + d\cdot\beta_z \qquad (31)$$

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 <u>basis vectors</u> in Eq.(31)

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))
- $$|\psi\rangle = \underset{\uparrow}{c} \cdot \alpha_z + \underset{\nearrow}{d} \cdot \beta_z \quad \text{OR} \quad |\psi\rangle = c\,|\uparrow\rangle_z + d\,|\downarrow\rangle_z \quad (32)$$

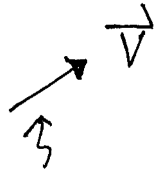
  read out coefficients
- The abstract $|\psi\rangle$ becomes $\begin{pmatrix} c \\ d \end{pmatrix}$ ← stacking up coefficients in expanding $|\psi\rangle$ in the chosen basis (33)

  general spin-½ state (general wave function)

$\therefore$ 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

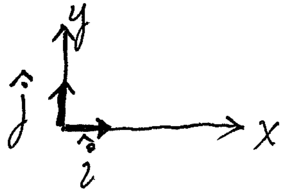
<u>An analogy : a vector</u>



a general vector (abstract)

[there is a length
there is a direction]

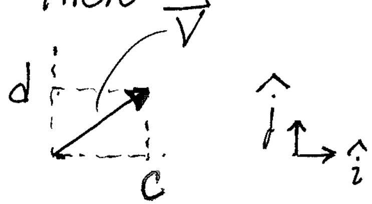
To describe it



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.

Change of Basis

- We saw that $\begin{pmatrix}1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\1\end{pmatrix}$ form a complete set
- But there are other choices that are also complete

E.g. we saw (see Eq.(27)) that

$$|\psi\rangle = \underset{\uparrow}{c_1 \alpha_x} + \underset{\uparrow}{c_2 \beta_x} \qquad (34)$$

using α_x, β_x as the basis set to expand any $|\psi\rangle$

Eq.(27) reads:

$$\begin{pmatrix}c\\d\end{pmatrix} = \overbrace{\frac{c+d}{\sqrt{2}}}^{c_1} \cdot \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \overbrace{-\frac{(c-d)}{\sqrt{2}}}^{c_2} \frac{1}{\sqrt{2}}\begin{pmatrix}-1\\1\end{pmatrix} \qquad (27)$$

$\therefore$ $\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$ & $\frac{1}{\sqrt{2}}\begin{pmatrix}-1\\1\end{pmatrix}$ also form a complete set!

If we announce (choose) the basis set is $\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$ and $\frac{1}{\sqrt{2}}\begin{pmatrix}-1\\1\end{pmatrix}$,
the abstract $|\psi\rangle = c_1 \cdot \alpha_x + c_2\beta_x$ OR $|\psi\rangle = c_1|\uparrow\rangle_x + c_2|\downarrow\rangle_x$.

- Read out coefficients c_1 & c_2, stack them up, then the general state $|\psi\rangle$ is described by the state vector ("wavefunction")

$$\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} \frac{c+d}{\sqrt{2}} \\ \frac{c-d}{\sqrt{2}} \end{pmatrix} \quad \text{in the basis of } \alpha_x \text{ and } \beta_x$$

Other choices?

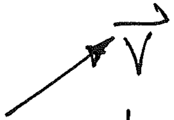
- Of course, we could use α_y and β_y, they also form a complete set
- OR we could use the eigenstates α_ϕ and β_ϕ of $\hat{S}_\phi$ (in Eq. (29))
- Therefore, a general spin-half state $|\psi\rangle$ can be expressed in many different basis sets. (But they describe the same $|\psi\rangle$).

We saw:

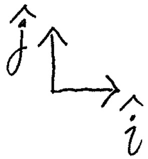
$$|\psi\rangle \nearrow \begin{pmatrix} c \\ d \end{pmatrix} \text{ in basis set formed by } \begin{pmatrix} 1 \\ 0 \end{pmatrix} \,\&\, \begin{pmatrix} 0 \\ 1 \end{pmatrix} \text{ [eigenstates of } \hat{S}_z]$$

$$|\psi\rangle \searrow \begin{pmatrix} \frac{c+d}{\sqrt{2}} \\ \frac{c-d}{\sqrt{2}} \end{pmatrix} \text{ in basis set formed by } \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \text{ and } \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \end{pmatrix} \text{ [eigenstates of } \hat{S}_x]$$

An analogy: A vector



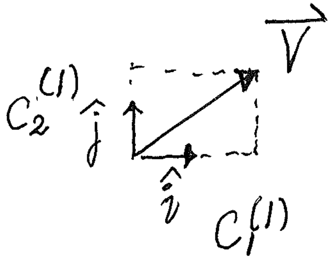
a vector (general)



basis set #1

basis set #2

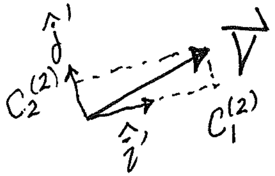
(35)



basis #1 basis set #1

$$\vec{V} = c_1^{(1)}\,\hat{i} + c_2^{(1)}\,\hat{j}$$

$\vec{V}$ described by $\begin{pmatrix} c_1^{(1)} \\ c_2^{(1)} \end{pmatrix}$

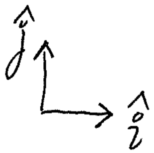


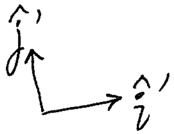
basis set #2 basis set #2

$$\vec{V} = c_1^{(2)}\,\hat{i}' + c_2^{(2)}\,\hat{j}'$$

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

What is "Wavefunction" after all?

- There is an abstract state $|\psi\rangle$
- There is a basis set $|\varphi_n\rangle$ that is complete (or labelled $|n\rangle$)
- Wavefunction of an abstract state $|\psi\rangle$ is given by the projectors (inner products) of the state and each member of the basis set.

[This is the meaning of "Wavefunction".]

- Since different basis sets can be used to represent the state $|\psi\rangle$, there can be different wavefunctions (representations) of the same state $|\psi\rangle$.

$$|\psi\rangle = \sum_i c_i |\varphi_i\rangle \qquad \text{(A1)}$$

$c_i = \langle \varphi_i | \psi \rangle$ ($\because$ φ_i's are orthogonal)

$$\therefore |\psi\rangle = \sum_i \underbrace{\langle \varphi_i | \psi \rangle}_{} |\varphi_i\rangle \qquad \text{(A2)}$$

these inner products (OR projecting $|\psi\rangle$ onto $|\varphi_i\rangle$) collectively give the wavefunction

c.f. Same state $|\psi\rangle$

$\rightarrow \begin{pmatrix} c \\ d \end{pmatrix}$ in $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ & $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ basis set

$\rightarrow \begin{pmatrix} \frac{c+d}{\sqrt{2}} \\ \frac{-(c-d)}{\sqrt{2}} \end{pmatrix}$ in $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ & $\frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \end{pmatrix}$ basis set

So far, we assumed the basis can be labelled by a discrete number, and so summing over i.

But there are commonly used basis set(s) with members that cannot be labelled by a discrete number.

E.g. Basis set of momentum eigenstates

$$e^{i\frac{px}{\hbar}} \qquad \text{(definite } p\text{)}$$

But all p (continuous values) are allowed.

Cannot count allowed p's by $1, 2, 3, \cdots$

Sum over i $\rightarrow$ integrate over p

Beyond Spin : Back to Wavefunction $\psi(x)$

What is the corresponding wavefunction $\phi(p)$ in momentum representation?

- Expand in eigenstates of $\hat{p}$ and read out coefficients

$$\underbrace{\psi(x)}_{\substack{\text{State} \\ \text{in position representation} \\ \text{[Wavefunction in} \\ \text{position representation]}}} = \frac{1}{\sqrt{2\pi\hbar}} \int \underbrace{\phi(p)}_{} \underbrace{e^{i\frac{px}{\hbar}}}_{\text{eigenstates of } \hat{p}} \, dx$$

Read Out $\phi(p) =$ Wavefunction in momentum representation

$|\phi(p)|^2 dp =$ Prob. of finding momentum in $p \to p+dp$

It is just the Fourier Transform.
We did this before.

What is $\psi(x)$ then?[+]

- $\delta(x)$ = Dirac δ-function $\begin{cases} x \neq 0, & \delta(x) = 0 \\ x = 0, & \delta(x) \to \infty \end{cases}$ but $\int_{-\infty}^{\infty} \delta(x)\,dx = 1$

cover $x=0$ is OK

- $\int_{-\infty}^{\infty} \delta(x) f(x)\,dx = f(0)$ or $\int_{-\infty}^{\infty} \delta(x-a) f(x)\,dx = f(a)$ (taken as definition)

"sum over basis"

$$\psi(x) = \int_{-\infty}^{\infty} \psi(x') \underbrace{\delta(x-x')}_{\text{basis (many members: } \delta(x-x_1),\, \delta(x-x_2),\, \cdots)} dx'$$

(from definition of δ-function)

coefficients: The wavefunction!

+ This is a bit abstract. Don't worry if you couldn't get the point the first time. It needs some math maturity. You can do much QM without this point.

What is this basis set of $\delta(x-x')$?

- $\delta(x-x')$: sharp spike at $x=x'$
- $\delta(x-x'')$: sharp spike at $x=x''$

$\vdots$ $\qquad\qquad$ $\vdots$

Measure position $\downarrow$ these are obviously the possible outcomes

Thus, $\delta(x-x')$ is the function that the state collapses to after a position measurement giving the outcome $x=x'$.

$\therefore$ $\delta(x-x')$ [many x'] are <u>position eigenstates</u>

$\therefore$ The ordinary wavefunction is the description of an abstract state in the basis of position eigenstates, i.e. projecting $|\psi\rangle$ onto basis functions that represent different locations.

Transformation from one basis set to another in Slow Motion

See Eq.(28):

$$\begin{pmatrix}1\\0\end{pmatrix} = \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} - \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}}\begin{pmatrix}-1\\1\end{pmatrix}$$

c.f.

$$\boxed{\alpha_z = \frac{1}{\sqrt{2}} \alpha_x + \left(-\frac{1}{\sqrt{2}}\right) \beta_x} \qquad (36)$$

analogous to $\hat{i} = \frac{1}{\sqrt{2}} \hat{i}' + \left(-\frac{1}{\sqrt{2}}\right) \hat{j}'$

new basis vectors

Relate one basis set (α_z, β_z) to another (α_x, β_x)

Similarly,

$$\begin{pmatrix}0\\1\end{pmatrix} = \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}}\begin{pmatrix}-1\\1\end{pmatrix}$$

c.f.

$$\boxed{\beta_z = \frac{1}{\sqrt{2}} \alpha_x + \frac{1}{\sqrt{2}} \beta_x} \qquad (37)$$

analogous to

$$\hat{j} = \frac{1}{\sqrt{2}} \hat{i}' + \frac{1}{\sqrt{2}} \hat{j}'$$

new basis vectors

Now a general state first expressed in α_z & β_z can be transformed

$$\begin{pmatrix} c \\ d \end{pmatrix} = c\begin{pmatrix} 1 \\ 0 \end{pmatrix} + d\begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad \text{[expressed in } (\alpha_z, \beta_z) \text{ OR } (\hat{i}, \hat{j})]$$

$$= c\left(\frac{1}{\sqrt{2}}\alpha_x - \frac{1}{\sqrt{2}}\beta_x\right) + d\left(\frac{1}{\sqrt{2}}\alpha_x + \frac{1}{\sqrt{2}}\beta_x\right) \qquad \text{[used transformations Eqs.(36),(37)]}$$

$$= \frac{c+d}{\sqrt{2}}\cdot\alpha_x - \frac{c-d}{\sqrt{2}}\cdot\beta_x \qquad \text{[same state expressed in } (\alpha_x, \beta_x) \text{ OR } (\hat{i}', \hat{j}')]$$

$$= \frac{c+d}{\sqrt{2}}\cdot\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} - \frac{c-d}{\sqrt{2}}\cdot\frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \end{pmatrix} \qquad \text{[this is Eq.(27) previously obtained]}$$

$\therefore$ We carried out change of basis in answering measurement questions! ($\because$ Measure S_x, need to expand state (before measurement) in terms of eigenstates of $\hat{S}_x$ to give probabilities)