PHY456H1F: Quantum Mechanics II. Lecture 14 (Taught by Prof J.E. Sipe). Representation of two state kets and Pauli spin matrices.

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Contents

1. Disclaimer.

Peeter's lecture notes from class. May not be entirely coherent.

2. Representation of kets.

Reading: §5.1 - §5.9 and §26 in [1].
We found the representations of the spin operators

$$S_x \rightarrow \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{1}$$

$$S_y \rightarrow \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \tag{2}$$

$$S_z \rightarrow \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{3}$$

How about kets? For example for $\left|{\chi}\right\rangle \in H_s$

$$\left|{\chi}\right\rangle \rightarrow \begin{bmatrix} \left\langle{+}\middle|{\chi}\right\rangle \\ \left\langle{-}\middle|{\chi}\right\rangle \end{bmatrix}, \tag{4}$$

and

$$|+\rangle \to \begin{bmatrix}1\\0\end{bmatrix} \tag{5}$$

$$|0\rangle \to \begin{bmatrix}0\\1\end{bmatrix} \tag{6}$$

So, for example

$$S_y\,|+\rangle \to \frac{\hbar}{2}\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} = \frac{i\hbar}{2}\begin{bmatrix}0\\1\end{bmatrix} \tag{7}$$

Kets in $H_o \otimes H_s$

$$|\psi\rangle \to \begin{bmatrix}\langle \mathbf{r}+|\psi\rangle\\ \langle \mathbf{r}-|\psi\rangle\end{bmatrix} = \begin{bmatrix}\psi_+(\mathbf{r})\\ \psi_-(\mathbf{r})\end{bmatrix}. \tag{8}$$

This is a "spinor"
Put

$$\begin{aligned}\langle \mathbf{r}\pm|\psi\rangle &= \psi_\pm(\mathbf{r})\\ &= \psi_+\begin{bmatrix}1\\0\end{bmatrix} + \psi_-\begin{bmatrix}0\\1\end{bmatrix}\end{aligned} \tag{9}$$

with

$$\langle\psi|\psi\rangle = 1 \tag{10}$$

Use

$$\begin{aligned}I &= I_o \otimes I_s\\ &= \int d^3\mathbf{r}\,|\mathbf{r}\rangle\langle\mathbf{r}| \otimes (|+\rangle\langle+| + |-\rangle\langle-|)\\ &= \int d^3\mathbf{r}\,|\mathbf{r}\rangle\langle\mathbf{r}| \otimes \sum_{\sigma=\pm}|\sigma\rangle\langle\sigma|\\ &= \sum_{\sigma=\pm}\int d^3\mathbf{r}\,|\mathbf{r}\sigma\rangle\langle\mathbf{r}\sigma|\end{aligned} \tag{11}$$

So

$$\begin{aligned}\langle\psi|\,I\,|\psi\rangle &= \sum_{\sigma=\pm}\int d^3\mathbf{r}\,\langle\psi|\mathbf{r}\sigma\rangle\langle\mathbf{r}\sigma|\psi\rangle\\ &= \int d^3\mathbf{r}\left(|\psi_+(\mathbf{r})|^2 + |\psi_-(\mathbf{r})|^2\right)\end{aligned} \tag{12}$$

Alternatively

$$
\begin{aligned}
|\psi\rangle &= I\,|\psi\rangle \\
&= \int d^3\mathbf{r} \sum_{\sigma=\pm} |\mathbf{r}\sigma\rangle \langle \mathbf{r}\sigma|\psi\rangle \\
&= \sum_{\sigma=\pm} \left(\int d^3\mathbf{r}\psi_\sigma(\mathbf{r}) \right) |\mathbf{r}\sigma\rangle \\
&= \sum_{\sigma=\pm} \left(\int d^3\mathbf{r}\psi_\sigma(\mathbf{r})\,|\mathbf{r}\rangle \right) \otimes |\sigma\rangle
\end{aligned}
\tag{13}
$$

In braces we have a ket in H_o, let's call it

$$
|\psi_\sigma\rangle = \int d^3\mathbf{r}\psi_\sigma(\mathbf{r})\,|\mathbf{r}\rangle\,, \tag{14}
$$

then

$$
|\psi\rangle = |\psi_+\rangle\,|+\rangle + |\psi_-\rangle\,|-\rangle \tag{15}
$$

where the direct product $\otimes$ is implied.

We can form a ket in H_s as

$$
\langle \mathbf{r}|\psi\rangle = \psi_+(\mathbf{r})\,|+\rangle + \psi_-(\mathbf{r})\,|-\rangle \tag{16}
$$

An operator O_o which acts on H_o alone can be promoted to $O_o \otimes I_s$, which is now an operator that acts on $H_o \otimes H_s$. We are sometimes a little cavalier in notation and leave this off, but we should remember this.

$$
O_o\,|\psi\rangle = (O_o\,|\psi+\rangle)\,|+\rangle + (O_o\,|\psi+\rangle)\,|+\rangle \tag{17}
$$

and likewise

$$
O_s\,|\psi\rangle = |\psi+\rangle\,(O_s\,|+\rangle) + |\psi-\rangle\,(O_s\,|-\rangle) \tag{18}
$$

and

$$
O_o O_s\,|\psi\rangle = (O_o\,|\psi+\rangle)(O_s\,|+\rangle) + (O_o\,|\psi-\rangle)(O_s\,|-\rangle) \tag{19}
$$

Suppose we want to rotate a ket, we do this with a full angular momentum operator

$$
e^{-i\theta\hat{\mathbf{n}}\cdot\mathbf{J}/\hbar}\,|\psi\rangle = e^{-i\theta\hat{\mathbf{n}}\cdot\mathbf{L}/\hbar} e^{-i\theta\hat{\mathbf{n}}\cdot\mathbf{S}/\hbar}\,|\psi\rangle \tag{20}
$$

(recalling that $\mathbf{L}$ and $\mathbf{S}$ commute)

So

$$
e^{-i\theta\hat{\mathbf{n}}\cdot\mathbf{J}/\hbar}\,|\psi\rangle = (e^{-i\theta\hat{\mathbf{n}}\cdot\mathbf{L}/\hbar}\,|\psi+\rangle)(e^{-i\theta\hat{\mathbf{n}}\cdot\mathbf{S}/\hbar}\,|+\rangle) + (e^{-i\theta\hat{\mathbf{n}}\cdot\mathbf{L}/\hbar}\,|\psi-\rangle)(e^{-i\theta\hat{\mathbf{n}}\cdot\mathbf{S}/\hbar}\,|-\rangle) \tag{21}
$$

2.1. *A simple example.*

$$|\psi\rangle = |\psi_+\rangle |+\rangle + |\psi_-\rangle |-\rangle \tag{22}$$

Suppose

$$|\psi_+\rangle = \alpha |\psi_0\rangle \tag{23}$$
$$|\psi_-\rangle = \beta |\psi_0\rangle \tag{24}$$

where

$$|\alpha|^2 + |\beta|^2 = 1 \tag{25}$$

Then

$$|\psi\rangle = |\psi_0\rangle |\chi\rangle \tag{26}$$

where

$$|\chi\rangle = \alpha |+\rangle + \beta |-\rangle \tag{27}$$

for

$$\langle\psi|\psi\rangle = 1, \tag{28}$$

$$\langle\psi_0|\psi_0\rangle \langle\chi|\chi\rangle = 1 \tag{29}$$

so

$$\langle\psi_0|\psi_0\rangle = 1 \tag{30}$$

We are going to concentrate on the unentagled state of 26.

- How about with

  $$|\alpha|^2 = 1, \beta = 0 \tag{31}$$

  $|\chi\rangle$ is an eigenket of S_z with eigenvalue $\hbar/2$.

- $$|\beta|^2 = 1, \alpha = 0 \tag{32}$$

  $|\chi\rangle$ is an eigenket of S_z with eigenvalue $-\hbar/2$.

- What is $|\chi\rangle$ if it is an eigenket of $\hat{\mathbf{n}} \cdot \mathbf{S}$?

FIXME: F1: standard spherical projection picture, with $\hat{\mathbf{n}}$ projected down onto the x, y plane at angle ϕ and at an angle θ from the z axis.

The eigenvalues will still be $\pm\hbar/2$ since there is nothing special about the z direction.

$$\begin{aligned}
\hat{\mathbf{n}} \cdot \mathbf{S} &= n_x S_x + n_y S_y + n_z S_z \\
&\rightarrow \frac{\hbar}{2} \begin{bmatrix} n_z & n_x - i n_y \\ n_x + i n_y & -n_z \end{bmatrix} \\
&= \frac{\hbar}{2} \begin{bmatrix} \cos\theta & \sin\theta e^{-i\phi} \sin\theta e^{i\phi} & -\cos\theta \end{bmatrix}
\end{aligned} \tag{33}$$

To find the eigenkets we diagonalize this, and we find representations of the eigenkets are

$$|\hat{\mathbf{n}}+\rangle \rightarrow \begin{bmatrix} \cos\left(\frac{\theta}{2}\right) e^{-i\phi/2} \\ \sin\left(\frac{\theta}{2}\right) e^{i\phi/2} \end{bmatrix} \tag{34}$$

$$|\hat{\mathbf{n}}-\rangle \rightarrow \begin{bmatrix} -\sin\left(\frac{\theta}{2}\right) e^{-i\phi/2} \\ \cos\left(\frac{\theta}{2}\right) e^{i\phi/2} \end{bmatrix}, \tag{35}$$

with eigenvalues $\hbar/2$ and $-\hbar/2$ respectively.

So in the abstract notation, tossing the specific representation, we have

$$|\hat{\mathbf{n}}+\rangle \rightarrow \cos\left(\frac{\theta}{2}\right) e^{-i\phi/2} |+\rangle \sin\left(\frac{\theta}{2}\right) e^{i\phi/2} |-\rangle \tag{36}$$

$$|\hat{\mathbf{n}}-\rangle \rightarrow -\sin\left(\frac{\theta}{2}\right) e^{-i\phi/2} |+\rangle \cos\left(\frac{\theta}{2}\right) e^{i\phi/2} |-\rangle \tag{37}$$

3. **Representation of two state kets**

Every ket

$$|\chi\rangle \rightarrow \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \tag{38}$$

for which

$$|\alpha|^2 + |\beta|^2 = 1 \tag{39}$$

can be written in the form 34 for some θ and ϕ, neglecting an overall phase factor.

For any ket in H_s, that ket is "spin up" in some direction.

FIXME: show this.

4. **Pauli spin matrices.**

It is useful to write

$$S_x = \frac{\hbar}{2}\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix} \equiv \frac{\hbar}{2}\sigma_x \tag{40}$$

$$S_y = \frac{\hbar}{2}\begin{bmatrix}0 & -i\\i & 0\end{bmatrix} \equiv \frac{\hbar}{2}\sigma_y \tag{41}$$

$$= \frac{\hbar}{2}\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix} \equiv \frac{\hbar}{2}\sigma_z \tag{42}$$

where

$$\sigma_x = \begin{bmatrix}0 & 1\\1 & 0\end{bmatrix} \tag{43}$$

$$\sigma_y = \begin{bmatrix}0 & -i\\i & 0\end{bmatrix} \tag{44}$$

$$\sigma_z = \begin{bmatrix}1 & 0\\0 & -1\end{bmatrix} \tag{45}$$

These are the Pauli spin matrices.

4.1. ***Interesting properties.***

- $$[\sigma_i, \sigma_j] = \sigma_i\sigma_j + \sigma_j\sigma_i = 0, \qquad \text{if } i < j \tag{46}$$

- $$\sigma_x\sigma_y = i\sigma_z \tag{47}$$

  (and cyclic permutations)

- $$\mathrm{Tr}(\sigma_i) = 0 \tag{48}$$

- $$(\hat{\mathbf{n}} \cdot \boldsymbol{\sigma})^2 = \sigma_0 \tag{49}$$

  where

  $$\hat{\mathbf{n}} \cdot \boldsymbol{\sigma} \equiv n_x\sigma_x + n_y\sigma_y + n_z\sigma_z, \tag{50}$$

  and

  $$\sigma_0 = \begin{bmatrix}1 & 0\\0 & 1\end{bmatrix} \tag{51}$$

  (note $\mathrm{Tr}(\sigma_0) \neq 0$)

- $$\left[\sigma_i, \sigma_j\right] = 2\delta_{ij}\sigma_0 \tag{52}$$
  $$\left[\sigma_x, \sigma_y\right] = 2i\sigma_z \tag{53}$$

  (and cyclic permutations of the latter).

  Can combine these to show that

  $$(\mathbf{A} \cdot \boldsymbol{\sigma})(\mathbf{B} \cdot \boldsymbol{\sigma}) = (\mathbf{A} \cdot \mathbf{B})\sigma_0 + i(\mathbf{A} \times \mathbf{B}) \cdot \boldsymbol{\sigma} \tag{54}$$

  where **A** and **B** are vectors (or more generally operators that commute with the $\boldsymbol{\sigma}$ matrices).

- $$\mathrm{Tr}(\sigma_i\sigma_j) = 2\delta_{ij} \tag{55}$$

- $$\mathrm{Tr}(\sigma_\alpha\sigma_\beta) = 2\delta_{\alpha\beta}, \tag{56}$$

  where $\alpha, \beta = 0, x, y, z$

Note that any complext matrix M can be written as

$$\begin{aligned} M &= \sum_\alpha m_a \sigma_\alpha \\ &= \begin{bmatrix} m_0 + m_z & m_x - im_y \\ m_x + im_y & m_0 - m_z \end{bmatrix} \end{aligned} \tag{57}$$

for any four complex numbers m_0, m_x, m_y, m_z
where

$$m_\beta = \frac{1}{2}\mathrm{Tr}(M\sigma_\beta). \tag{58}$$

References

[1] BR Desai. *Quantum mechanics with basic field theory*. Cambridge University Press, 2009. 2