Phys 506 lecture 1 Spin and Pauli matrices

Recall the spin operators and eigenstates
$\hat{S}_z$, $|\uparrow;z\rangle$ and $|\downarrow;z\rangle$

$$\left.\begin{aligned} \hat{S}_z|\uparrow;z\rangle &= \tfrac{\hbar}{2}|\uparrow;z\rangle \\ \hat{S}_z|\downarrow;z\rangle &= -\tfrac{\hbar}{2}|\downarrow;z\rangle \end{aligned}\right\} \text{eigenstates}$$

Raising and lowering operators: define $\hat{S}_+$ and $\hat{S}_-$ to connect these states

$$\hat{S}_+|\uparrow;z\rangle = 0 \qquad \hat{S}_+|\downarrow;z\rangle = \hbar|\uparrow;z\rangle$$
$$\hat{S}_-|\uparrow;z\rangle = \hbar|\downarrow;z\rangle \qquad \hat{S}_-|\downarrow;z\rangle = 0$$

Compute their commutators:

$$(\hat{S}_+\hat{S}_- - \hat{S}_-\hat{S}_+)|\uparrow;z\rangle = \hbar^2|\uparrow;z\rangle = 2\hbar\hat{S}_z|\uparrow;z\rangle$$
$$(\hat{S}_+\hat{S}_- - \hat{S}_-\hat{S}_+)|\downarrow;z\rangle = -\hbar^2|\downarrow;z\rangle = 2\hbar\hat{S}_z|\downarrow;z\rangle$$

so $\boxed{[\hat{S}_+,\hat{S}_-] = 2\hbar\hat{S}_z}$

similarly

$$(\hat{S}_z\hat{S}_+ - \hat{S}_+\hat{S}_z)|\uparrow;z\rangle = 0 = \hat{S}_+|\uparrow;z\rangle$$
$$(\hat{S}_z\hat{S}_+ - \hat{S}_+\hat{S}_z)|\downarrow;z\rangle = \hbar^2|\uparrow;z\rangle = \hbar\hat{S}_+|\downarrow;z\rangle$$

So $\boxed{[\hat{S}_z,\hat{S}_+] = \hbar\hat{S}_+}$ You can verify that $\boxed{[\hat{S}_z,\hat{S}_-] = -\hbar\hat{S}_-}$

These three commutation relations are the SU(2) algebra.

If we define $\hat{S}_x = \frac{1}{2}(\hat{S}_+ + \hat{S}_-)$ and $\hat{S}_y = \frac{1}{2i}(\hat{S}_+ - \hat{S}_-)$ then $\hat{S}_+ = \hat{S}_x + i\hat{S}_y$ and $\hat{S}_- = \hat{S}_x - i\hat{S}_y$. The algebra of the cartesian spins follows:

$$[\hat{S}_x,\hat{S}_y] = \frac{1}{4i}[\hat{S}_+ + \hat{S}_-, \hat{S}_+ - \hat{S}_-]$$
$$= \frac{1}{4i}\left\{[\hat{S}_+,\hat{S}_+] - [\hat{S}_+,\hat{S}_-] + [\hat{S}_-,\hat{S}_+] - [\hat{S}_-,\hat{S}_-]\right\}$$
$$= \frac{1}{4i}\left[-2\hbar\hat{S}_z - 2\hbar\hat{S}_z\right] = i\hbar\hat{S}_z$$

You can verify (and should) that we have

$$[\hat{S}_i,\hat{S}_j] = i\hbar\sum_k \varepsilon_{ijk}\hat{S}_k$$

which is the standard form for angular momentum commutators.

ε_{ijk} is the completely antisymmetric tensor

$\varepsilon_{123} = \varepsilon_{231} = \varepsilon_{312} = 1 \quad \varepsilon_{132} = \varepsilon_{321} = \varepsilon_{213} = -1$ all others $= 0$

From this relation, we find that

$$[\hat{S}^2, \hat{S}_j] = 0$$

Proof! $\hat{S}^2 = \sum_i \hat{S}_i \hat{S}_i$ so

$$[\hat{S}^2, \hat{S}_j] = \sum_i [\hat{S}_i \hat{S}_i, \hat{S}_j] = \sum_i \left(\hat{S}_i [\hat{S}_i, \hat{S}_j] + [\hat{S}_i, \hat{S}_j]\hat{S}_i\right)$$

$$= i\hbar \sum_i \sum_k \left(\hat{S}_i \varepsilon_{ijk} \hat{S}_k + \varepsilon_{ijk} \hat{S}_k \hat{S}_i\right)$$

$$= i\hbar \sum_{ik} \varepsilon_{ijk}\left(\hat{S}_i \hat{S}_k + \hat{S}_k \hat{S}_i\right)$$

The claim is that this is zero. To see this let $i \to k'$ and $k \to i'$

$$= i\hbar \sum_{i'k'} \varepsilon_{k'ji'} \left(\hat{S}_{k'} \hat{S}_{i'} + \hat{S}_{i'} \hat{S}_{k'}\right)$$

$$= i\hbar \sum_{i'k'} \left(-\varepsilon_{i'jk'}\right)\left(\hat{S}_{i'} \hat{S}_{k'} + \hat{S}_{k'} \hat{S}_{i'}\right)$$

since $\varepsilon_{ijk} = -\varepsilon_{kji}$. Now drop the primes

$$= -i\hbar \sum_{ik} \varepsilon_{ijk} \left(\hat{S}_i \hat{S}_k + \hat{S}_k \hat{S}_i\right)$$

Anything equal to its negative must vanish so $[\hat{S}^2, \hat{S}_j] = 0$.

Let's compute $\hat{S}^2 |\sigma; z\rangle$ $\quad \sigma = \uparrow$ or $\downarrow$.

$$\hat{S}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2 = \frac{1}{4}(\hat{S}_+ + \hat{S}_-)^2 - \frac{1}{4}(\hat{S}_+ - \hat{S}_-)^2 + \hat{S}_z^2$$

$$= \frac{1}{2}\left(\hat{S}_+ \hat{S}_- + \hat{S}_- \hat{S}_+\right) + \hat{S}_z^2$$

So $\hat{S}^2 |\uparrow; z\rangle = \frac{1}{2}\left(\hat{S}_+ \hat{S}_- + \hat{S}_- \hat{S}_+\right)|\uparrow; z\rangle + \hat{S}_z^2 |\uparrow; z\rangle$

$$= \left(\frac{1}{2}\hbar^2 + \frac{1}{4}\hbar^2\right)|\uparrow; z\rangle = \frac{3}{4}\hbar^2 |\uparrow; z\rangle$$

$$\hat{S}^2 |\downarrow; z\rangle = \frac{1}{2}\left(\hat{S}_+ \hat{S}_- + \hat{S}_- \hat{S}_+\right)|\downarrow; z\rangle + \hat{S}_z^2 |\downarrow; z\rangle$$

$= \frac{3}{4}\hbar^2 |\downarrow; z\rangle$ as well.

$|\sigma; z\rangle$ is an eigenstate of both $\hat{S}^2$ and $\hat{S}_z$!

Assume we have an arbitrary superposition of states

$$|\psi\rangle = \alpha |\uparrow; z\rangle + \beta |\downarrow; z\rangle$$

We let the column vector $\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ denote the state $|\psi\rangle$.
The operators $\hat{S}_i$ are represented by two-dimensional matrices in this space.

$$\hat{S}_z |\uparrow; z\rangle = \frac{\hbar}{2} |\uparrow; z\rangle \qquad \Leftrightarrow \qquad \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\hat{S}_z |\downarrow; z\rangle = -\frac{\hbar}{2} |\downarrow; z\rangle \qquad \qquad \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The matrix representing the operator is

$$M_{\sigma\sigma'} = \langle \sigma; z | \hat{S}_i | \sigma'; z\rangle$$

Let's compute the matrix for $\hat{S}_y$

$$S^y_{\sigma\sigma'} = \langle \sigma; z | \hat{S}^y | \sigma'; z\rangle = \frac{1}{2i} \langle \sigma; z | \hat{S}_+ - \hat{S}_- | \sigma'; z\rangle$$

$$\sigma' = \uparrow \; : \; (\hat{S}_+ - \hat{S}_-) |\uparrow; z\rangle = -\hbar |\downarrow; z\rangle \Rightarrow S^y_{\uparrow\uparrow} = 0 \quad S^y_{\downarrow\uparrow} = \frac{i\hbar}{2}$$

$$\sigma' = \downarrow \; : \; (\hat{S}_+ - \hat{S}_-) |\downarrow; z\rangle = \hbar |\uparrow; z\rangle \Rightarrow S^y_{\uparrow\downarrow} = -\frac{i\hbar}{2} \quad \hat{S}^y_{\downarrow\downarrow} = 0$$

so $\hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

Similary $\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

We call σ_i the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Note that $\sigma_i^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \Rightarrow S^2_{\sigma\sigma'} = \frac{\hbar^2}{4} \times 3 \times \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

These matrices also anticommute. To see this go back to our spin commutators

$$\hat{S}_x \hat{S}_y - \hat{S}_y \hat{S}_x = i\hbar \hat{S}_z$$

multiply on left by $\hat{S}_x$ and on right by $\hat{S}_x$

$$\hat{S}_x^2 \hat{S}_y - \hat{S}_x \hat{S}_y \hat{S}_x = i\hbar \hat{S}_x \hat{S}_z$$

$$\hat{S}_x \hat{S}_y \hat{S}_x - \hat{S}_y \hat{S}_x^2 = i\hbar \hat{S}_z \hat{S}_x$$

Now substitute in the Pauli matrices

$$\frac{\hbar^3}{8}\left[\sigma_x^2 \sigma_y - \sigma_x \sigma_y \sigma_x\right] = i\frac{\hbar^3}{4} \sigma_x \sigma_z$$

$$\frac{\hbar^3}{8}\left[\sigma_x \sigma_y \sigma_x - \sigma_y \sigma_x^2\right] = i\frac{\hbar^3}{4} \sigma_z \sigma_x$$

add (and recall $\sigma_x^2 = \mathbb{I}$):

$$\frac{\hbar^3}{8}\left[\sigma_y - \sigma_y\right] = i\frac{\hbar^3}{4}\left(\sigma_x \sigma_z + \sigma_z \sigma_x\right)$$

$$0 = \sigma_x \sigma_z + \sigma_z \sigma_x$$

and it is obvious this holds for other permutations. Hence, we have derived that

$$\sigma_i \sigma_j = \frac{1}{2}\left[\sigma_i \sigma_j + \sigma_j \sigma_i + \sigma_i \sigma_j - \sigma_j \sigma_i\right]$$

$$= \frac{1}{2} \delta_{ij} \times 2\mathbb{I} + \frac{1}{2} i \; 2 \varepsilon_{ijk} \sigma_k$$

or $\boxed{\sigma_i \sigma_j = \delta_{ij} \mathbb{I} + i \varepsilon_{ijk} \sigma_k}$

Another interesting identity is the product of all 3

$$\sigma_x \sigma_y \sigma_z = i \; \varepsilon_{123} \sigma_z \sigma_z = i \; \mathbb{I}$$

$$\boxed{\sigma_x \sigma_y \sigma_z = i \mathbb{I}}$$

Any 2x2 matrix can be expressed in terms of the identity and the 3 Pauli matrices.

Check! $\alpha \mathbb{I} + \beta \sigma_x + \gamma \sigma_y + \delta \sigma_z = \begin{pmatrix} \alpha+\delta & \beta - i\gamma \\ \beta + i\gamma & \alpha - \delta \end{pmatrix}$

So to find $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$ set $a = \alpha+\delta$ $b = \beta - i\gamma$ $c = \beta + i\gamma$ $d = \alpha - \delta$

or $\alpha = \frac{a+d}{2}$ $\beta = \frac{b+c}{2}$ $\gamma = \frac{i}{2}(b-c)$ $\delta = \frac{a-d}{2}$

We often write this as $M = \alpha \mathbb{I} + \vec{v} \cdot \vec{\sigma}$ $\vec{v} = \left(\frac{b+c}{2}, \frac{i}{2}(b-c), \frac{a-d}{2} \right)$

Let's get some practice working with these objects

$$(\vec{A} \cdot \vec{\sigma})(\vec{B} \cdot \vec{\sigma}) = \sum_{ij} A_i B_j \sigma_i \sigma_j$$

$$= \sum_{ij} A_i B_j \left(\delta_{ij} \mathbb{I} + i \varepsilon_{ijk} \sigma_k \right)$$

$$= \vec{A} \cdot \vec{B}\, \mathbb{I} + i\, \varepsilon_{ijk} A_i B_j \sigma_k$$

$$= \vec{A} \cdot \vec{B}\, \mathbb{I} + i\, (\vec{A} \times \vec{B}) \cdot \vec{\sigma}$$

Note that if $\vec{A}$ is parallel to $\vec{B}$, then $(\vec{A} \cdot \vec{\sigma})(\vec{B} \cdot \vec{\sigma}) = \vec{A} \cdot \vec{B}\, \mathbb{I}$.
This identity is a useful one to remember.

The matrix exponential:

$$\mathrm{EXP}\left[i \vec{v} \cdot \vec{\sigma} \right] = \sum_{n=0}^{\infty} \frac{(i)^n}{n!} (\vec{v} \cdot \vec{\sigma})^n$$

Separate out into even and odd powers

$$e^{i \vec{v} \cdot \vec{\sigma}} = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} (\vec{v} \cdot \vec{\sigma})^{2n} + i \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} (\vec{v} \cdot \vec{\sigma})^{2n+1}$$

But recall $(\vec{v} \cdot \vec{\sigma})(\vec{v} \cdot \vec{\sigma}) = v^2 \mathbb{I}$ so

$$e^{i \vec{v} \cdot \vec{\sigma}} = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} (v^2)^n \mathbb{I} + i\, \vec{v} \cdot \vec{\sigma} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} (v^2)^n$$

$$\boxed{e^{i \vec{v} \cdot \vec{\sigma}} = \cos|v|\, \mathbb{I} + i \frac{\vec{v} \cdot \vec{\sigma}}{|v|} \sin|v|}$$

Let's compute

$$e^{i\vec{v}\cdot\vec{\sigma}}\,\sigma_j\,e^{-i\vec{v}\cdot\vec{\sigma}}$$

In general, such terms can involve an infinite series as we will show in a later lecture via the Hadamard lemma, but in this case, we can explicitly calculate it. Just use our identity for the exponential

$$e^{i\vec{v}\cdot\vec{\sigma}}\,\sigma_j\,e^{-i\vec{v}\cdot\vec{\sigma}} = \left(\cos|v|\,\mathbb{I} + i\frac{\vec{v}\cdot\vec{\sigma}}{|v|}\sin|v|\right)\sigma_j\left(\cos|v|\,\mathbb{I} - i\frac{\vec{v}\cdot\vec{\sigma}}{|v|}\sin|v|\right)$$

$$= \cos^2|v|\,\sigma_j - i\frac{\cos|v|\sin|v|}{|v|}\left(\sigma_j\,\vec{v}\cdot\vec{\sigma} - \vec{v}\cdot\vec{\sigma}\,\sigma_j\right) + \frac{\sin^2|v|}{|v|^2}\,\vec{v}\cdot\vec{\sigma}\,\sigma_j\,\vec{v}\cdot\vec{\sigma}$$

$$= \cos^2|v|\,\sigma_j - i\frac{\cos|v|\sin|v|}{|v|}\sum_i[\sigma_j,\sigma_i]\,v_i + \frac{\sin^2|v|}{|v|^2}\sum_{ik}v_i v_k\,\sigma_i\sigma_j\sigma_k$$

$$= \cos^2|v|\,\sigma_j + \frac{\cos|v|\sin|v|}{v}\sum_{ik}2\varepsilon_{jik}\,v_i\sigma_k + \frac{\sin^2|v|}{|v|^2}\sum_{ik}v_i v_k\,\sigma_i\sigma_j\sigma_k$$

But

$$\sum_{ik}v_i v_k\,\sigma_i\sigma_j\sigma_k = \sum_{ik}v_i v_k\left[\delta_{ij}\mathbb{I} + i\varepsilon_{ijl}\sigma_l\right]\sigma_k$$

$$= v_j\,\vec{v}\cdot\vec{\sigma} + i\sum_{ikl}v_i v_k\,\varepsilon_{ijl}\left(\overset{0}{\delta_{lk}} + i\varepsilon_{lkm}\sigma_m\right)$$

$$= v_j\,\vec{v}\cdot\vec{\sigma} - \sum_{iklm}v_i v_k\,\varepsilon_{ijl}\,\varepsilon_{lkm}\,\sigma_m$$

$$= v_j\,\vec{v}\cdot\vec{\sigma} - \sum_{ikm}v_i v_k\left(\delta_{ik}\delta_{jm} - \delta_{im}\delta_{jk}\right)\sigma_m$$

$$= v_j\,\vec{v}\cdot\vec{\sigma} - v^2\sigma_j + \vec{v}\cdot\vec{\sigma}\,v_j$$

$$= \cos^2|v|\,\sigma_j + 2\frac{\cos|v|\sin|v|}{|v|}\left(\vec{v}\times\vec{\sigma}\right)_j + \frac{\sin^2|v|}{|v|^2}\left(2\,\vec{v}\cdot\vec{\sigma}\,v_j - v^2\sigma_j\right)$$

Our last topic is on exponential disentangling.

First note that $\sigma_+ = \sigma_x + i\sigma_y = \begin{pmatrix}0 & 2\\ 0 & 0\end{pmatrix}$ so

$$\exp(\alpha\sigma_+) = 1 + \alpha\sigma_+ + \frac{1}{2}\alpha^2\underbrace{(\sigma_+)^2}_{0} + \cdots$$

$$= \begin{pmatrix}1 & 2\alpha\\ 0 & 1\end{pmatrix}$$

$$\exp(\alpha\sigma_-) = \begin{pmatrix}1 & 0\\ 2\alpha & 1\end{pmatrix}$$

Now, let's consider the following exponential

$$\exp\left(i\vec{v}\cdot\vec{\sigma}\right) = \begin{pmatrix}\cos|v| + i\frac{v_z}{|v|}\sin|v| & \left(i\frac{v_x}{|v|} + \frac{v_y}{|v|}\right)\sin|v|\\ \left(\frac{iv_x}{|v|} - \frac{v_y}{|v|}\right)\sin|v| & \cos|v| - i\frac{v_z}{|v|}\sin|v|\end{pmatrix}$$

We want to rewrite it as

$$\exp[\alpha\sigma_+]\exp[\beta\sigma_z]\exp[\gamma\sigma_-]$$

$$\begin{pmatrix}1 & 2\alpha\\ 0 & 1\end{pmatrix}\begin{pmatrix}e^{\beta} & 0\\ 0 & e^{-\beta}\end{pmatrix}\begin{pmatrix}1 & 0\\ 2\gamma & 1\end{pmatrix}$$

$$= \begin{pmatrix}e^{\beta} & 2\alpha e^{-\beta}\\ 0 & e^{-\beta}\end{pmatrix}\begin{pmatrix}1 & 0\\ 2\gamma & 1\end{pmatrix} = \begin{pmatrix}e^{\beta}+4\alpha\gamma e^{-\beta} & 2\alpha e^{-\beta}\\ 2\gamma e^{-\beta} & e^{-\beta}\end{pmatrix}$$

Comparing to the exponential, we have

$$\cos|\sigma| + i\frac{\sigma_z}{|\sigma|}\sin|\sigma| = e^{\beta} + 4\alpha\gamma e^{-\beta}$$

$$\left(i\frac{\sigma_x}{|\sigma|} + \frac{\sigma_y}{|\sigma|}\right)\sin|\sigma| = 2\alpha e^{-\beta}$$

$$\left(i\frac{\sigma_x}{|\sigma|} - \frac{\sigma_y}{|\sigma|}\right)\sin|\sigma| = 2\gamma e^{-\beta}$$

$$\cos|\sigma| - i\frac{\sigma_z}{|\sigma|}\sin|\sigma| = e^{-\beta}$$

First note that $e^{\beta}\left(1+4\alpha\gamma e^{-2\beta}\right) = \dfrac{1}{\cos|\sigma| - i\frac{\sigma_z}{|\sigma|}\sin|\sigma|}\left(1+\sin^2|\sigma|\left(\dfrac{-\sigma_x^2-\sigma_y^2}{|\sigma|^2}\right)\right)$

$$= \frac{\cos|\sigma| + i\frac{\sigma_z}{|\sigma|}\sin|\sigma|}{\cos^2|\sigma| + \frac{\sigma_z^2}{|\sigma|^2}\sin^2|\sigma|}\left(1+\sin^2|\sigma|\left(\frac{\sigma_z^2}{|\sigma|^2}-1\right)\right)$$

$$= \cos|\sigma| + i\frac{\sigma_z}{|\sigma|}\sin|\sigma|$$

So if we solve the bottom 3 eq'ns, the top automatically holds!

$$\Rightarrow \boxed{\begin{aligned}\beta &= -\ln\left[\cos|\sigma| - i\frac{\sigma_z}{|\sigma|}\sin|\sigma|\right]\\ \alpha &= \frac{1}{2}\left(\frac{i\sigma_x}{|\sigma|} + \frac{\sigma_y}{|\sigma|}\right)\frac{\sin|\sigma|}{\cos|\sigma| - i\frac{\sigma_z}{|\sigma|}\sin|\sigma|}\\ \gamma &= \frac{1}{2}\left(\frac{i\sigma_x}{|\sigma|} - \frac{\sigma_y}{|\sigma|}\right)\frac{\sin|\sigma|}{\cos|\sigma| - i\frac{\sigma_z}{|\sigma|}\sin|\sigma|}\end{aligned}}$$

An important special case is when $\boxed{\sigma_x = \sigma_z = 0}$

then

$$\boxed{\beta = \ln\sec\sigma_y \qquad \alpha = \tfrac{1}{2}\tan\sigma_y \qquad \gamma = -\tfrac{1}{2}\tan\sigma_y}$$

This is your first taste of exponential disentangling.

We will see more of it soon.