Operators on disjoint Hilbert spaces

An electron in hydrogen has: $\psi_{tot} = \psi_{n\ell m_\ell} \chi_s^{m_s}$

actually $\chi_{\frac{1}{2}}^{\pm\frac{1}{2}} = \chi_{\pm}$

$\psi_{tot} \in \mathcal{H} = H_\infty^{space} \otimes H_2^{spin}$

$\psi_{n\ell m_\ell} \in H_\infty^{space}$

$\chi_s^{m_s} \in H_2^{spin}$

Example: $\psi_{tot} = \psi_{321}\chi_+$

Suppose we want to calculate:

a) E: $\langle \psi_{tot} | \hat{H}\psi_{tot}\rangle = \int \psi_{321}^* \underbrace{(\hat{H}\psi_{321})}_{E_3\psi_{321}} dV \underbrace{\langle \chi_+ | \chi_+ \rangle}_{(1\ 0)\binom{1}{0}}$

$= E_3 \cancel{\int \psi_{321}^*\psi_{321}\, dV}^{\,1} \cancel{\langle \chi_+ | \chi_+\rangle}^{\,1}$

$= E_3 = -\frac{13.6}{9}\,eV$

b) S_z: $\langle \psi_{tot} | \hat{S}_z \psi_{tot}\rangle = \cancel{\int \psi_{321}^*\psi_{321}\, dV}_{\,1} \langle \chi_+ | \underbrace{\hat{S}_z\chi_+}_{+\frac{\hbar}{2}\chi_+}\rangle$ $\quad \frac{\hbar}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix}\binom{1}{0}$

$= \frac{\hbar}{2}$

c) $L_z + S_z$: $\langle \psi_{tot} | (\hat{L}_z + \hat{S}_z)\psi_{tot}\rangle = \int \psi_{321}^* \underbrace{(\hat{L}_z\psi_{321})}_{\hbar\psi_{321}} dV \langle \chi_+ | \chi_+\rangle$

$+ \int \psi_{321}^*\psi_{321}\, dV \langle \chi_+ | \underbrace{\hat{S}_z\chi_+}_{\frac{\hbar}{2}\chi_+}\rangle$

$= \hbar + \frac{\hbar}{2}$

$= \frac{3}{2}\hbar$

d) ES_z: $\langle \psi_{tot} | \hat{H}\hat{S}_z\psi_{tot}\rangle = \int \psi_{321}^* \underbrace{(\hat{H}\psi_{321})}_{E_3\psi_{321}} dV \langle \chi_+ | \underbrace{\hat{S}_z\chi_+}_{\frac{\hbar}{2}\chi_+}\rangle$

$= E_3\frac{\hbar}{2}$

Note: ψ_{tot} is an eigenstate of every operator we considered.

i.e. $\hat{H}\psi_{tot} = E_3\psi_{tot}$

$\hat{H}\psi_{321}\chi_+ = E_3\psi_{321}\chi_+$

Suppose we have 2 electrons and ignore everything but spin.

We know that for each electron we can have $\chi^{\pm\frac{1}{2}} = \uparrow$ or $\downarrow$

$\chi_+ \quad \chi_-$

$\in H_2^{spin}$

But their spin wavefunctions <u>lives on 2 disjoint copies of H_2^{spin}</u>!

!!!!

4 possibilities: $\uparrow\uparrow, \uparrow\downarrow, \downarrow\uparrow, \downarrow\downarrow$

What could we measure? $S_{1z}, S_{2z}, S_1^2, S_2^2$

Example: $\uparrow\uparrow = \chi_{tot}$

$S_{1z}: \langle \chi_+ | \hat{S}_{1z} \chi_+ \rangle \langle \chi_+ | \chi_+ \rangle = \frac{\hbar}{2}$

$S_1^2: \langle \chi_+ | \underbrace{\hat{S}_1^2 \chi_+}_{\hbar^2 s(s+1)\chi_+} \rangle \langle \chi_+ | \chi_+ \rangle = \frac{3}{4}\hbar^2$

Consider: S_z, S^2 where $\hat{S}_z = \hat{S}_{1z} + \hat{S}_{2z}$, $\hat{S}^2 = \hat{\vec{S}} \cdot \hat{\vec{S}}$

$= (\hat{\vec{S}}_1 + \hat{\vec{S}}_2) \cdot (\hat{\vec{S}}_1 + \hat{\vec{S}}_2)$

$$\langle \chi_+ | \underbrace{\hat{S}_{1z} \chi_+}_{\frac{\hbar}{2}\chi_+} \rangle \langle \chi_+ | \chi_+ \rangle + \langle \chi_+ | \chi_+ \rangle \langle \chi_+ | \underbrace{\hat{S}_{2z} \chi_+}_{\frac{\hbar}{2}\chi_+} \rangle = \hbar$$

$$\hat{S}^2 = \hat{S}_1^2 + \hat{S}_2^2 + 2\hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2$$

$$\langle \chi_+ | \underbrace{\hat{S}_1^2 \chi_+}_{\frac{3}{4}\hbar^2\chi_+} \rangle \langle \chi_+ | \chi_+ \rangle + \langle \chi_+ | \chi_+ \rangle \langle \chi_+ | \overbrace{\hat{S}_2^2 \chi_+}^{\frac{3}{4}\hbar^2\chi_+} \rangle$$
$$+ 2 \langle \chi_{tot} | \underbrace{(\hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2)}_{\hat{S}_{1x}\hat{S}_{2x} + \hat{S}_{1y}\hat{S}_{2y} + \hat{S}_{1z}\hat{S}_{2z}} \chi_{tot} \rangle$$

$$= \frac{3}{2}\hbar^2 + 2\langle \chi_+ | \hat{S}_{1x}\chi_+ \rangle \langle \chi_+ | \hat{S}_{2x}\chi_+ \rangle \longleftarrow \text{need } \hat{S}_x\chi_+ = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{\hbar}{2}\chi_-$$
$$+ 2\langle \chi_+ | \hat{S}_{1y}\chi_+ \rangle \langle \chi_+ | \hat{S}_{2y}\chi_+ \rangle$$
$$+ 2\langle \chi_+ | \underbrace{\hat{S}_{1z}\chi_+}_{\frac{\hbar}{2}\chi_+} \rangle \langle \chi_+ | \underbrace{\hat{S}_{2z}\chi_+}_{\frac{\hbar}{2}\chi_+} \rangle$$

need $\hat{S}_y\chi_+ = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{i\hbar}{2}\chi_-$

$\hat{S}_x\chi_- = \frac{\hbar}{2}\chi_+$

$\hat{S}_y\chi_- = -\frac{i\hbar}{2}\chi_+$

$$= \frac{3}{2}\hbar^2 + \frac{1}{2}\hbar^2 + 2\langle \chi_+ | \tfrac{\hbar}{2}\chi_- \rangle \langle \chi_+ | \tfrac{\hbar}{2}\chi_- \rangle$$
$$+ 2\langle \chi_+ | \tfrac{i\hbar}{2}\chi_- \rangle \langle \chi_+ | \tfrac{i\hbar}{2}\chi_- \rangle$$

$\langle \chi_+ | \chi_- \rangle = 0$

$= 2\hbar^2$

Is $\uparrow\uparrow = \chi_{tot}$ an eigenstate?

$\hat{S}_z \psi_{tot} \stackrel{?}{=} \hbar \psi_{tot}$

$(\hat{S}_{1z} + \hat{S}_{2z})\uparrow\uparrow = (\hat{S}_{1z}\uparrow)\uparrow + \uparrow(\hat{S}_{2z}\uparrow) = \frac{\hbar}{2}\uparrow\uparrow + \frac{\hbar}{2}\uparrow\uparrow$

$= \hbar\uparrow\uparrow$ ✓

$\cancel{2\frac{\hbar}{2}\frac{\hbar}{2}\downarrow\downarrow} - \cancel{2\frac{\hbar}{2}\frac{\hbar}{2}}\downarrow\downarrow$

$\hat{S}^2 \psi_{tot} \stackrel{?}{=} (\ )\psi_{tot}$

$$(\hat{S}_1^2 + \hat{S}_2^2 + 2\hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2)\uparrow\uparrow = \underbrace{(\hat{S}_1^2\uparrow)\uparrow}_{\frac{3}{4}\hbar^2\uparrow\uparrow} + \underbrace{\uparrow(\hat{S}_2^2\uparrow)}_{\frac{3}{4}\hbar^2\uparrow\uparrow} + 2(\hat{S}_{1x}\uparrow)(\hat{S}_{2x}\uparrow)$$
$$+ 2(\hat{S}_{1y}\uparrow)(\hat{S}_{2y}\uparrow)$$
$$+ 2(\hat{S}_{1z}\uparrow)(\hat{S}_{2z}\uparrow)$$

$+ \frac{\hbar^2}{2}\uparrow\uparrow$

✓

Awesome!!!

Buttt!!!

Consider: $\psi_{tot} = \uparrow\downarrow$

$\hat{S}_z \psi_{tot} \overset{?}{=} (\ )\psi_{tot}$

$(\hat{S}_{1z} + \hat{S}_{2z})\uparrow\downarrow = (\hat{S}_{1z}\uparrow)\downarrow + \uparrow(\hat{S}_{2z}\downarrow) = \frac{\hbar}{2}\uparrow\downarrow - \frac{\hbar}{2}\uparrow\downarrow$

$= 0 \cdot \uparrow\downarrow$ ✓

$\hat{S}^2 \psi_{tot} \overset{?}{=} (\ )\psi_{tot}$

$(\hat{S}_1^2 + \hat{S}_2^2 + 2\hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2)\uparrow\downarrow = (\hat{S}_1^2\uparrow)\downarrow + \uparrow(\hat{S}_2^2\downarrow) + 2(\hat{S}_{1x}\uparrow)(\hat{S}_{2x}\downarrow)$

$+ 2(\hat{S}_{1y}\uparrow)(\hat{S}_{2y}\downarrow)$

$+ 2(\hat{S}_{1z}\uparrow)(\hat{S}_{2z}\downarrow)$

$= \frac{3}{4}\hbar^2\uparrow\downarrow + \frac{3}{2}\hbar^2\uparrow\downarrow + 2\frac{\hbar^2}{4}\downarrow\uparrow + 2\frac{\hbar^2}{4}\downarrow\uparrow$

$+ 2\frac{\hbar^2}{4}\uparrow\downarrow$

$= 2\hbar^2\uparrow\downarrow + \hbar^2\downarrow\uparrow$ ✗

Does $\vec{S}$ have the angular mom. algebraic structure?

$\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y = (\hat{S}_{1x} + \hat{S}_{2x}) \pm i(\hat{S}_{1y} + \hat{S}_{2y})$

$\boxed{\hat{S}_{1-} = \hat{S}_{1x} - i\hat{S}_{1y} \Rightarrow \hat{S}_- = \hat{S}_{1-} + \hat{S}_{2-}}$

Start: $\uparrow\uparrow$

Then: $\hat{S}_-\uparrow\uparrow = (\hat{S}_{1-}\uparrow)\uparrow + \uparrow(\hat{S}_{2-}\uparrow)$

$= \hbar\downarrow\uparrow + \hbar\uparrow\downarrow$

$= \hbar(\downarrow\uparrow + \uparrow\downarrow)$ $\quad \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow)$

Then: $\hat{S}_- \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow) \propto \downarrow\downarrow$

Then: $\hat{S}_-\downarrow\downarrow = 0$

Also: $\hat{S}_+\uparrow\uparrow = 0$

$\hat{S}_z\chi_+ = \hbar\chi_+$

$\hat{S}_z\chi_0 = 0\,\chi_0$

$\hat{S}_z\chi_- = -\hbar\chi_-$

$\downarrow$

$\left.\begin{array}{l} \chi_+ \quad \uparrow\uparrow \\ \chi_0 \quad \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow) \\ \chi_- \quad \downarrow\downarrow \end{array}\right\}$ triplet

connected by $\hat{S}_\pm$

are eigenspinors of $\hat{S}_z$, $\hat{S}^2$

$\uparrow$

$\hat{S}^2\chi_{\substack{+\\0\\-}} = 2\hbar^2\chi_{\substack{+\\0\\-}}$

$\frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)$: $\left.\begin{array}{l} \hat{S}_\pm \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow) = 0 \\ \hat{S}^2 \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow) = 0 \end{array}\right\}$ singlet

Generally any time we have more than one angular momentum (including a single electron in hydrogen which has $\vec{L}$ and $\vec{S}$) and we want to describe things in terms of <u>total ang. mom.</u> we get led to various linear combinations w/ Clebsch-Gordon coefficients (hard!!)