Review: Spherical Harmonics $Y_\ell^m(\theta,\phi)$ (angular solutions to TISE for $V(r)$ incl. $V_{hyd.}$)

Y_ℓ^m are eigenfunctions of $\hat{L}^2$ and $\hat{L}_z$ are hermitian observables

$$\boxed{\begin{aligned}\hat{L}^2 Y_\ell^m &= \hbar^2 \ell(\ell+1) Y_\ell^m \\ \hat{L}_z Y_\ell^m &= \hbar m Y_\ell^m\end{aligned}}$$

$\ell = 0, 1, 2 \cdots$

$m = -\ell, \cdots, +\ell$

explains why these are orthogonal

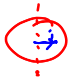
$\vec{L} = \vec{r}_{cm} \times \vec{p}_{cm}$ (motion of cm)

Classically we can split orbital motion from spinning motion.

$\vec{S} = I_{cm} \vec{\omega}$ (about the cm)

The Y_ℓ^m describe only the orbital motion of electrons in atoms.

Q. Can the electron spin?



Classically $\cancel{\sum_i \vec{r}_i \times \vec{p}_i}$ $\sim \infty$ for a nonzero $\vec{S}$

$\hat{L} = 0$

doesn't work for spin

Spin is an intrinsic and unchangeable property of point particles.

nothin changes it!

this is not built from external or spacetime d.o.f. (no built from x, p)

We have an abstract algebraic approach to angular momentum.

$$\boxed{\begin{aligned}\hat{S}^2 \chi_s^m &= \hbar^2 s(s+1) \chi_s^m \qquad & s &= 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \cdots \\ \hat{S}_z \chi_s^m &= \hbar m \chi_s^m \qquad & m &= -s, \cdots, s\end{aligned}}$$

For $\hat{\vec{L}} = \frac{\hbar}{i}\left[r(\hat{r}\times\hat{r})\frac{\partial}{\partial r} + (\hat{r}\times\hat{\theta})\frac{\partial}{\partial\theta} + (\hat{r}\times\hat{\phi})\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\right]$

from $= \vec{r} \times \vec{p}$

$\Rightarrow Y_\ell^m(\theta,\phi)$ labelled by m and ℓ.

For spin we only have labels m and s!!

We would like to know χ_s^m and $\hat{S}^2$ and $\hat{S}_z$ starting from eigenvalue expression with known eigenvalues.

Contrast: $\vec{L}$ where we knew $\hat{L}^2, \hat{L}_z$ then found eigenfunctions and eigenvalues.

Example: $s = \frac{1}{2} \Rightarrow m = \overset{\text{spin down}}{-\frac{1}{2}}, \underset{\text{spin up}}{\frac{1}{2}}$

$$\boxed{\begin{aligned} \chi_{\frac{1}{2}}^{-\frac{1}{2}} &= |\overset{s}{\tfrac{1}{2}}, \overset{m}{-\tfrac{1}{2}}\rangle = \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ \chi_{\frac{1}{2}}^{\frac{1}{2}} &= |\tfrac{1}{2}, \tfrac{1}{2}\rangle = \chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{aligned}}$$

Spin dictionary

Building $\hat{S}^2$ and $\hat{S}_z$:

a) $\hat{S}^2 \chi_+ = \hbar^2 \frac{1}{2}(\frac{1}{2}+1)\chi_+ = \frac{3}{4}\hbar^2 \chi_+$

b) $\hat{S}^2 \chi_- = \hbar^2 \frac{1}{2}(\frac{1}{2}+1)\chi_- = \frac{3}{4}\hbar^2 \chi_-$

Suppose $\hat{S}^2 = \begin{pmatrix} c & d \\ e & f \end{pmatrix}$ ← complex

a) $\begin{pmatrix} c & d \\ e & f \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 \\ 0 \end{pmatrix} \Rightarrow \begin{pmatrix} c \\ e \end{pmatrix} = \begin{pmatrix} \frac{3}{4}\hbar^2 \\ 0 \end{pmatrix}$

b) $\begin{pmatrix} c & d \\ e & f \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{3}{4}\hbar^2 \begin{pmatrix} 0 \\ 1 \end{pmatrix} \Rightarrow \begin{pmatrix} d \\ f \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{3}{4}\hbar^2 \end{pmatrix}$

$$\Rightarrow \hat{S}^2 = \begin{pmatrix} \frac{3}{4}\hbar^2 & 0 \\ 0 & \frac{3}{4}\hbar^2 \end{pmatrix} = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Now for $\hat{S}_z$: let $\hat{S}_z = \begin{pmatrix} q & r \\ s & t \end{pmatrix}$

$\hat{S}_z \chi_+ = \frac{\hbar}{2}\chi_+ \Rightarrow \begin{pmatrix} q & r \\ s & t \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{\hbar}{2} \\ 0 \end{pmatrix} = \begin{pmatrix} q \\ s \end{pmatrix}$

$\hat{S}_z \chi_- = -\frac{\hbar}{2}\chi_- \Rightarrow \begin{pmatrix} q & r \\ s & t \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ -\hbar/2 \end{pmatrix} = \begin{pmatrix} r \\ t \end{pmatrix}$

$$\Rightarrow \hat{S}_z = \begin{pmatrix} \hbar/2 & 0 \\ 0 & -\hbar/2 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

2 issues remain

i) With $\vec{L}$ we could also build $\hat{L}_x, \hat{L}_y$ so can we build $\hat{S}_x, \hat{S}_y$?

ii) The cool quantumness of $\vec{S}$ comes in $[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z$.

So building $\hat{S}_x$ and $\hat{S}_y$:

Do not have an eigenvalue eqn. $\cancel{\hat{S}_x \chi_\pm = ?\, \chi_\pm}$

Note: $\hat{S}_x$ will have its own eigenspinors $\chi_\pm^x \neq \chi_\pm$.

Recall: $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y \Rightarrow \begin{cases} \hat{S}_x = \frac{1}{2}(\hat{S}_+ + \hat{S}_-) \\ \hat{S}_y = \frac{1}{2i}(\hat{S}_+ - \hat{S}_-) \end{cases}$

from $\hat{S}_z$ ← 　　from HW

We know: $\hat{S}_- \boxed{\chi_+} = \hbar\, \chi_-$ 　　$\hat{S}_+ \chi_+ = 0$

$\hat{S}_+ \chi_- = \hbar\, \chi_+$ 　　$\hat{S}_- \chi_- = 0$

$$\Rightarrow \hat{S}_+ = \begin{pmatrix} 0 & \hbar \\ 0 & 0 \end{pmatrix}, \quad \hat{S}_- = \begin{pmatrix} 0 & 0 \\ \hbar & 0 \end{pmatrix}$$

$$\Rightarrow \quad \hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

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

Finally: $\hat{\vec{S}} = \frac{\hbar}{2}\hat{\vec{\sigma}}$

$$\hat{\vec{\sigma}} = (\sigma_x, \sigma_y, \sigma_z)$$

$$= \underbrace{\left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right)}_{\text{Pauli spin matrices}}$$

3 things to consider

i) Does $[\hat{S}_x, \hat{S}_y] = i\hbar \hat{S}_z$?

ii) Are eigenspinors of $\hat{S}_x$ $(\chi^x_\pm)$ different from $\chi_\pm$ of $\hat{S}_z$?

iii) Is $\hat{S}^2 \chi^x_\pm = \frac{3\hbar^2}{4} \chi^x_\pm$

$$\text{i)} \quad \frac{\hbar^2}{4}\left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} - \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right) = \frac{\hbar^2}{4}\left(\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} - \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}\right)$$

$$= \frac{\hbar^2}{4}\begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix}$$

$$= i\hbar \underbrace{\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}_{S_z}$$

$$\text{ii)} \quad \hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Rightarrow \chi^x_\pm = \begin{pmatrix} 1/\sqrt{2} \\ \pm 1/\sqrt{2} \end{pmatrix} \neq \chi_\pm$$

$$\text{iii)} \quad \hat{S}^2 \chi^x_\pm = \frac{3}{4}\hbar^2 \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}}_{I} \chi^x_\pm = \frac{3}{4}\hbar^2 \chi^x_\pm$$

We have a spin-$\frac{1}{2}$ particle $\chi = a\chi_+ + b\chi_-$

$$\langle \hat{S}_z \rangle_\chi = \chi^\dagger \hat{S}_z \chi$$

$= ($ More Next time....