H-atom
energy eigenfunctions

$$\rho = \kappa r = \sqrt{\frac{-2\mu E}{\hbar}}\, r = \frac{\mu e^2}{\hbar^2 n} r \equiv \frac{r}{n a_0}$$

$$a_0 = \frac{\hbar^2}{\mu e^2} \simeq .53 \cdot 10^{-8}\,\text{cm}$$
← Bohr radius

$$\phi(\vec{r}) = R_{El}(r)\, Y_{lm}(\theta,\phi)$$

labeled by n, l, m

$$\phi_{nlm}(\vec{r}) = R_{nl}(r)\, Y(\theta,\phi)$$

$m = -l, \ldots, l$
$l < n$

ground state $\phi_{1,0,0}(r) = \frac{1}{\sqrt{\pi a_0^3}}\, e^{-r/a_0}$

$$\int d^3r\, |\phi_{nlm}(\vec{r})|^2 = \underline{1}$$

$$\int d\Omega = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta = 4\pi$$

$$\int d\Omega \int dr \cdot r^2\, \frac{1}{\pi a_0^3}\, e^{-2r/a_0} = \frac{4\pi}{\pi a_0^3} \int_0^\infty r^2 e^{-r/a_0}\, dr$$

consider: $I(\alpha) = \int_0^\infty e^{-\alpha r}\, dr \qquad \alpha > 0$

$$= \frac{1}{-\alpha}\, e^{-\alpha r}\Big|_0^\infty = \frac{1}{\alpha}$$

$$\frac{dI}{d\alpha} = \int_0^\infty -r e^{-\alpha r}\, dr$$

$$\frac{d^2 I}{d\alpha^2} = \int_0^\infty r^2 e^{-\alpha r}\, dr = \frac{2}{\alpha^3}$$

$$\rightarrow = \frac{4}{a_0^3}\left(\frac{2}{(2/a_0)^3}\right) = \frac{4}{a_0^3}\left(\frac{1}{4} a_0^3\right) = \underline{1}$$

What about higher n, l?

radial part: $R = \frac{u}{r} \qquad n = k + l + 1$

$$u = e^{-\rho}\left(\rho^{l+1} \sum_{i=0}^{k} c_i \rho^i\right)$$

$$R_{nl} \sim \frac{1}{\rho}\, e^{-\rho} \rho^{l+1}\, (\text{poly of degree } k)$$

$(\text{poly degree of } n-1)\, e^{-\rho} = (\text{poly degree of } n-1)\, e^{-r/n a_0}$

Poly of degree $n-1$ → $n-1$ zeros / nodes @ zeros

$$R_{20} = \frac{1}{\sqrt{2}} a_0^{-3/2} \left(1 - \frac{r}{2a_0}\right) e^{-r/2a_0} \qquad 0 \text{ @ } r = 2a_0$$

$$R_{21} = \frac{1}{\sqrt{24}} a_0^{-3/2} \frac{r}{a_0} e^{-r/2a_0} \qquad 0 \text{ @ } r = 0$$

angular shape $|Y_{lm}(\theta,\phi)|^2$

Y_{00} - constant

$|Y_{10}|^2 \sim (\cos\theta)^2$

$|Y_{11}|^2 \sim (\sin\theta)^2$

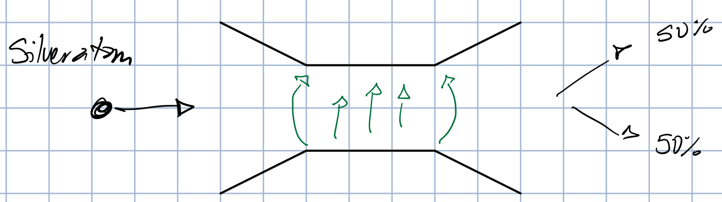
corrections involve:

relativistic corrections : spin-orbit coupling

nuclear spin: hyperfine

QED effects - Lamb shift

Stern Gerlach exp.



Put atoms in $\vec{B}$ field → look @ spectroscopy

shift of spectral lines

can't be solved w/ $|n, l, m\rangle$

Electron - bound to proton has Hilbert space of states

$\mathcal{H} = L^2(\mathbb{R}^3)$ normalizable $\phi(\vec{x})$

Basis $R_{nl}(r)\, Y_{lm}(\theta, \phi)$

Electron w/ spin has Hilbert space $\mathcal{H} = \overbrace{L^2(\mathbb{R}^3)}^{\text{coord. dependence}} \otimes \underbrace{\mathbb{C}^2}_{\text{spin space}}$

If $\chi_+ = \binom{1}{0}$ $\chi_- = \binom{0}{1}$ - basis for $\mathbb{C}^2$ or $|+\rangle, |-\rangle$

A general element of $\mathcal{H}$ is $\phi_+(\vec{x}) \otimes \chi_+ + \phi_-(\vec{x}) \otimes \chi_-$ $\quad \Phi_\pm(\vec{x})$ are normalizable

or as $\begin{pmatrix} \phi_+(\vec{x}) \\ \phi_-(\vec{x}) \end{pmatrix}$

On $\mathcal{H}$,

act on different spaces

$$\vec{J} = \underbrace{\vec{L}}_{\vec{r} \times \vec{p}} \otimes \mathbb{1} + \mathbb{1} \otimes \underbrace{\vec{S}}_{\frac{\hbar}{2}(\sigma_x, \sigma_y, \sigma_z)}$$

$\vec{J}$ - generator of total angular momentum

$[J_i, J_j] = i\hbar\, \epsilon_{ijk} J_k$ $\quad$ b/c $[L_i, S_i] = 0$

similar to $KE + U = E$

systems where $[J_i, H] = 0$ but $[S_i, H] \neq 0$

rotation about $\hat{n}$ axis, by an angle ϵ, there is unitary operator U

$$\mathcal{D}(\hat{n}, \epsilon) = \exp(-i\, \vec{J}\cdot\hat{n}\, \epsilon/\hbar) = \exp(-i\vec{L}\cdot\hat{n}\, \epsilon/\hbar)\, \exp(-i\vec{S}\cdot\hat{n}\, \epsilon/\hbar)$$

to achieve rotational invariance

$$\mathcal{D}_{1/2}(\hat{n}, \epsilon) = \exp(-i\vec{\sigma}\cdot\hat{n}\,\epsilon/2)$$

euler

$$(\vec{\sigma}\cdot\hat{n})^2 = \sigma_i \hat{n}_i \sigma_j \hat{n}_j = \hat{n}_i \hat{n}_j \frac{1}{2}(\sigma_i\sigma_j + \sigma_j\sigma_i) = \hat{n}_i \hat{n}_j \delta_{ij} = 1$$

$$\mathcal{D}(\hat{n}, \epsilon) = \mathbb{1}\cos(\epsilon/2) - i\vec{\sigma}\cdot\hat{n}\sin(\epsilon/2)$$

$$= \begin{pmatrix} \cos(\epsilon/2) - i n_3 \sin(\epsilon/2) & -(n_2 + i n_1)\sin(\epsilon/2) \\ (n_2 - i n_1)\sin\epsilon/2 & \cos(\epsilon/2) + i n_3 \sin(\epsilon/2) \end{pmatrix}$$

$$\mathcal{D}_{1/2}(\hat{n}, 2\pi) = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\mathcal{D}_{1/2}(\hat{n}, 4\pi) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$