All together now:

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)\, Y_l^m(\theta,\phi)\begin{pmatrix}1\\0\end{pmatrix}$$

↓

Replaced by $nlm_l s m_s$ = $nlm_l \frac{1}{2} \frac{1}{2}$

Now we need 5 quantum numbers to represent the state of one electron in a H atom.

Comment: The total magnetic moment arises from the sum as vectors of **L** and **S**. This will be discussed in P412.

Returning, again!, to the general combination:

$$\chi = \begin{pmatrix} a \\ b \end{pmatrix} = a\chi_+ + b\chi_-$$

What is the probability that the spin points say along the *positive x axis*?

To answer this question, first you have to diagonalize the 2x2 Pauli matrix "x". Turns out the "eigenspinors" are:

$$\chi_+^{(x)} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}, \left(\text{eigenvalue} + \frac{\hbar}{2}\right); \quad \chi_-^{(x)} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix}, \left(\text{eigenvalue} - \frac{\hbar}{2}\right)$$

The general combination ...

$$\chi = \begin{pmatrix} a \\ b \end{pmatrix} = a\chi_+ + b\chi_-$$

... can now be written as:

$$\chi = \left(\frac{a+b}{\sqrt{2}}\right)\chi_+^{(x)} + \left(\frac{a-b}{\sqrt{2}}\right)\chi_-^{(x)}$$

$$(1/2)|a+b|^2$$

is the probability of measuring spin up along x.

$$(1/2)|a-b|^2$$

is the probability of measuring spin down along x.

Review for Test 3 begins:

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)\, Y_l^m(\theta,\phi)$$

$$R_{10} = 2a^{-3/2}\exp(-r/a)$$

$$R_{20} = \frac{1}{\sqrt{2}}a^{-3/2}\left(1-\frac{1}{2}\frac{r}{a}\right)\exp(-r/2a)$$

$$R_{21} = \frac{1}{\sqrt{24}}a^{-3/2}\frac{r}{a}\exp(-r/2a)$$

$$R_{30} = \frac{2}{\sqrt{27}}a^{-3/2}\left(1-\frac{2}{3}\frac{r}{a}+\frac{2}{27}\left(\frac{r}{a}\right)^2\right)\exp(-r/3a)$$

$$R_{31} = \frac{8}{27\sqrt{6}}a^{-3/2}\left(1-\frac{1}{6}\frac{r}{a}\right)\left(\frac{r}{a}\right)\exp(-r/3a)$$

$$R_{32} = \frac{4}{81\sqrt{30}}a^{-3/2}\left(\frac{r}{a}\right)^2\exp(-r/3a)$$

$$R_{40} = \frac{1}{4}a^{-3/2}\left(1-\frac{3}{4}\frac{r}{a}+\frac{1}{8}\left(\frac{r}{a}\right)^2-\frac{1}{192}\left(\frac{r}{a}\right)^3\right)\exp(-r/4a)$$

$$R_{41} = \frac{\sqrt{5}}{16\sqrt{3}}a^{-3/2}\left(1-\frac{1}{4}\frac{r}{a}+\frac{1}{80}\left(\frac{r}{a}\right)^2\right)\frac{r}{a}\exp(-r/4a)$$

$$R_{42} = \frac{1}{64\sqrt{5}}a^{-3/2}\left(1-\frac{1}{12}\frac{r}{a}\right)\left(\frac{r}{a}\right)^2\exp(-r/4a)$$

$$R_{43} = \frac{1}{768\sqrt{35}}a^{-3/2}\left(\frac{r}{a}\right)^3\exp(-r/4a)$$

Already normalized!

$$\psi_{nlm}(r, \theta, \phi) = R_{nl}(r)\, Y_l^m(\theta, \phi)$$

$$Y_0^0 = \left(\frac{1}{4\pi}\right)^{1/2}$$

$$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta$$

$$Y_1^{\pm 1} = \mp\left(\frac{3}{8\pi}\right)^{1/2} \sin\theta e^{\pm i\phi}$$

$$Y_2^0 = \left(\frac{5}{16\pi}\right)^{1/2} (3\cos^2\theta - 1)$$

$$Y_2^{\pm 1} = \mp\left(\frac{15}{8\pi}\right)^{1/2} \sin\theta \cos\theta e^{\pm i\phi}$$

$$Y_2^{\pm 2} = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta e^{\pm 2i\phi}$$

$$Y_3^0 = \left(\frac{7}{16\pi}\right)^{1/2} (5\cos^3\theta - 3\cos\theta)$$

$$Y_3^{\pm 1} = \mp\left(\frac{21}{64\pi}\right)^{1/2} \sin\theta\, (5\cos^2\theta - 1) e^{\pm i\phi}$$

$$Y_3^{\pm 2} = \left(\frac{105}{32\pi}\right)^{1/2} \sin^2\theta \cos\theta e^{\pm 2i\phi}$$

$$Y_3^{\pm 3} = \mp\left(\frac{35}{64\pi}\right)^{1/2} \sin^3\theta e^{\pm 3i\phi}$$

Already normalized!

Consider an electron in the Hydrogen atom potential, located in the state with quantum numbers n=2, l=1, m=-1.

(a) Using the tables of R and Y provided, construct the wave function $\Psi_{2,1,-1}(r,\theta,\phi)$.

(b) Find the expectation value <r> in this state.

(a)

$$R_{21} = \frac{1}{\sqrt{24}} a^{-3/2} \left(\frac{r}{a}\right) e^{-r/2a} \qquad Y_1^{-1} = \sqrt{\frac{3}{8\pi}} \sin\theta \, e^{-i\phi}$$

$$\boxed{\psi_{21-1}(r,\theta,\phi) = \frac{1}{\sqrt{24}} \sqrt{\frac{3}{8\pi}} a^{-5/2} \, r \, e^{-r/2a} \sin\theta \, e^{-i\phi}}$$

(b)

$$\langle r \rangle = \frac{\cancel{3}^{\,1}}{\cancel{24}_{\,8} \cdot 8\pi} a^{-5} \underbrace{\int_0^\infty r^2 e^{-r/a} \, r \, r^2 dr}_{\int_0^\infty r^5 e^{-r/a} dr = 5! \, a^6} \underbrace{\int_0^\pi \sin^3\theta \, d\theta}_{4/3} \underbrace{\int_0^{2\pi} d\phi}_{2\pi} = \frac{2\cancel{\pi}}{64\cancel{\pi}} 5! \, a \, \frac{4}{3} = \boxed{5a}$$

$e^{-i\phi} e^{+i\phi}$ gives 1

Integrals in formula sheet

Check length unit "a" is correct

Consider an electron in the Hydrogen atom potential, located in the state n=2, l=0, m=0.

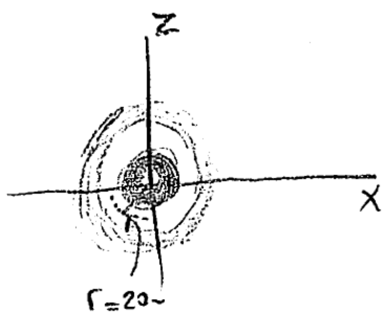
(a) Using the formula sheet tables, construct the wave function $\Psi_{2,0,0}(r,\theta,\phi)$.

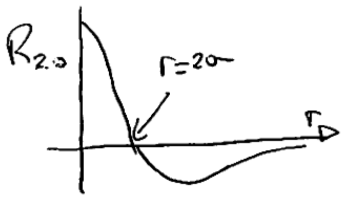
(b) Make a crude sketch by hand, as in the book and as in one of the lectures, of the probability $|\Psi_{2,0,0}(r,\theta,\phi)|^2$ describing the nodes and the angular dependence in the plane (x,z).

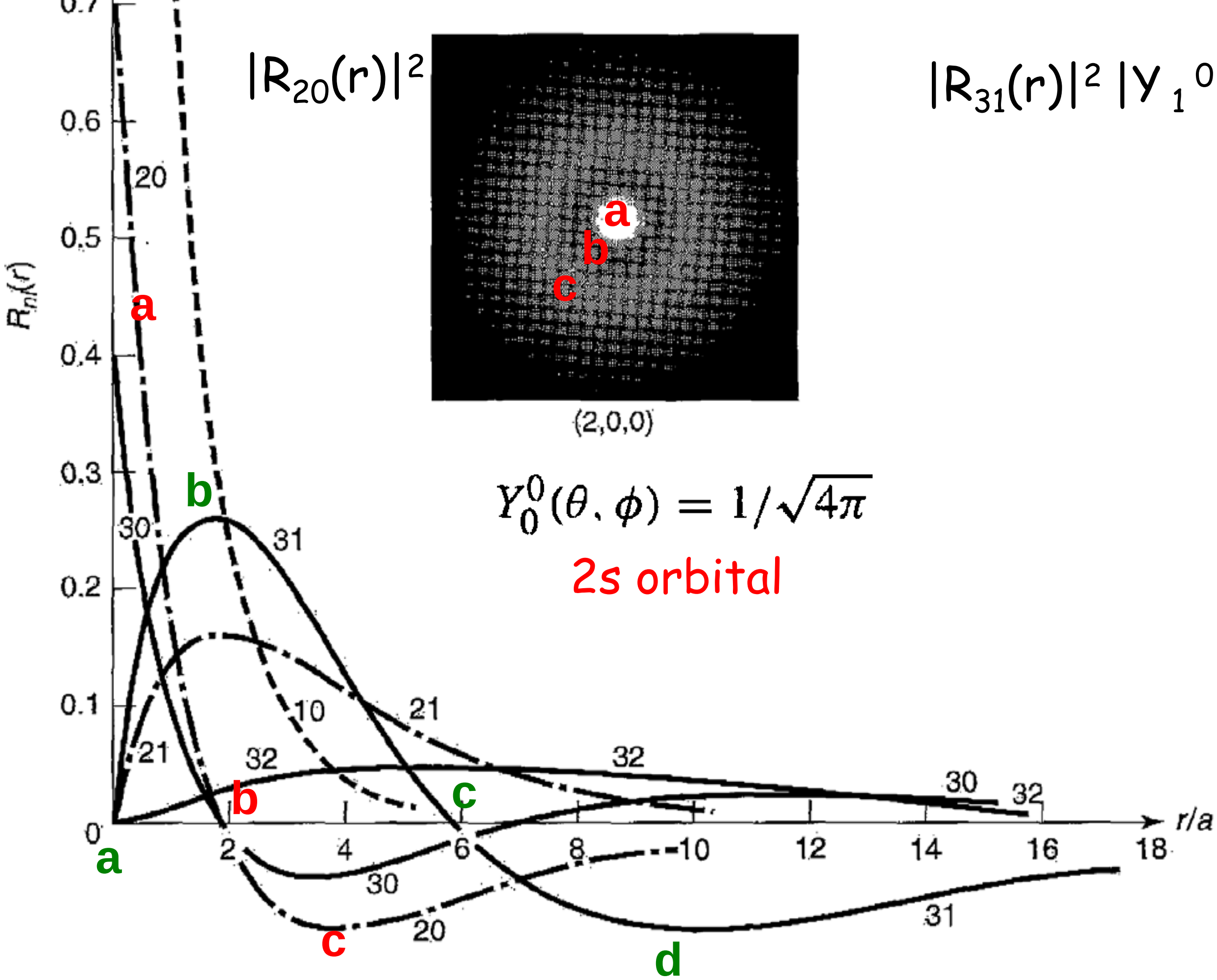
(a) $$\psi_{200} = R_{20}(r)\, Y_0^0(\theta,\phi) = \frac{1}{\sqrt{2}}\, a^{-3/2}\left(1-\frac{r}{2a}\right) e^{-r/2a}\, \frac{1}{\sqrt{4\pi}}$$

(b) Because $l=0$, then ψ_{200} at the origin is non zero.

It only has a node at $r=2a$ and then an exponential decay. Thus, $|\psi|^2$ will have a bright spot centered at $r=0$, a weak region near $r=2a$, and then another soft maximum before dropping exponentially to 0. No angular dependence because $l=m=0$.







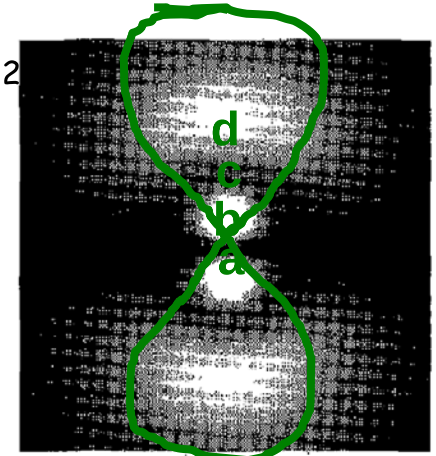
$|R_{20}(r)|^2$

(2,0,0)

$$Y_0^0(\theta, \phi) = 1/\sqrt{4\pi}$$

2s orbital

$|R_{31}(r)|^2 \, |Y_1^{\,0}|^2$



(3,1,0)

$$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta$$

$3p_z$ orbital

Calculate the following two commutators, as in a HW problem.
Do not memorize, because my focus will be on the procedure.

(a) $[L_z, y]$ (b) $[L_z, p_x]$

(a)

$$[L_z, y] = [xp_y - yp_x, y] = [xp_y, y] - [yp_x, y] =$$

$$= x\underbrace{[p_y, y]}_{-i\hbar} - p_x\underbrace{[y, y]}_{=0} = \boxed{-i\hbar x}$$

(b)

$$[L_z, p_x] = [xp_y - yp_x, p_x] = [xp_y, p_x] - [yp_x, p_x] =$$

$$= p_y\underbrace{[x, p_x]}_{i\hbar} - y\underbrace{[p_x, p_x]}_{=0} = \boxed{i\hbar p_y}$$

Consider a hydrogen atom.

(a) What is the degeneracy of the level with quantum number n=3? Provide all the quantum numbers of each degenerate level.

(b) What are the possible values of the angular momentum square, in units of $\hbar^2$, that you could find as an outcome of an experiment if the electron is in an equal-weight mixture of all levels with n=3?

(a) If $n=3$, then $\ell = 2, 1, 0$. $\ell=2$ has $m = -2, -1, 0, +1, +2$
$\ell=1$ has $m = -1, 0, +1$.
$\ell=0$ has $m=0$

Thus, total is $5+3+1 = \boxed{9}$

Not enough to say $n^2=9$

(b) $\langle L^2 \rangle / \hbar^2 \begin{cases} 2(2+1) = \boxed{6} \\ 1(1+1) = \boxed{2} \\ 0(0+1) = \boxed{0} \end{cases}$

Consider the following linear combination of eigenstates of the hydrogen atom:

$\Psi = A\,[\Psi_{3,1,1}(r,\theta,\phi) + i\,\Psi_{2,0,0}(r,\theta,\phi)\,]$. $\quad \Psi = A\,(\psi_{311} + i\,\psi_{200})$

(a) Find the value of A so that Ψ is normalized to 1. **Only** use the orthonormality property of the eigenstates $\Psi_{n,l,m}(r,\theta,\phi)$, not the explicit states.

(b) If Ψ given above is the state at time t=0, write the state at an arbitrary time t. For the energies simple use the notation E_n, not the explicit values.

This entire problem should be done in just a few lines. Do NO write explicitly $\Psi_{3,1,1}(r,\theta,\phi)$ and $\Psi_{2,0,0}(r,\theta,\phi)$, just keep the notation as it is.

(a) $$\int |\psi|^2 d^3r = 1 = A^2 \int (\psi_{311}^* - i\psi_{200}^*)(\psi_{311} + i\psi_{200})\, d^3r =$$

$$= A^2 \Big[\underbrace{\int |\psi_{311}|^2 d^3r}_{1} + \underbrace{\int |\psi_{200}|^2 d^3r}_{1} + i \underbrace{\int \psi_{311}^* \psi_{200}\, d^3r}_{0} - i \underbrace{\int \psi_{200}^* \psi_{311}\, d^3r}_{0} \Big]$$

$$= 2A^2, \quad \text{thus} \quad \boxed{A = 1/\sqrt{2}}.$$

(b) $$\boxed{\psi(r,\theta,\phi,t) = \frac{1}{\sqrt{2}} \left[\psi_{311}\, e^{-iE_3 t/\hbar} + i\,\psi_{200}\, e^{-iE_2 t/\hbar} \right]}$$