

Hydrogen atom

Shell n	Subshell (n, l)	l	m_l	# of orbitals	# of e^-
K $n=1$	1s	0	0	1	2
L $n=2$	2s 2p	0 1	0 -1, 0, 1	$\left. \begin{smallmatrix} 1 \\ 3 \end{smallmatrix} \right] 4$	8
M $n=3$	3s 3p 3d	0 1 2	0 -1, 0, 1 -2, -1, 0, 1, 2	$\left. \begin{smallmatrix} 1 \\ 3 \\ 5 \end{smallmatrix} \right] 9$	18
N $n=4$	4s 4p 4d 4f	0 1 2 3	0 -1, 0, 1 -2, -1, 0, 1, 2 -3, -2, -1, 0, 1, 2, 3	$\left. \begin{smallmatrix} 1 \\ 3 \\ 5 \\ 7 \end{smallmatrix} \right] 16$	32
O $n=5$	5s 5p 5d 5f 5g	0 1 2 3 4	0 -1, 0, 1 -2, -1, 0, 1, 2 -3, -2, -1, 0, 1, 2, 3 -4, -3, -2, -1, 0, 1, 2, 3, 4	$\left. \begin{smallmatrix} 1 \\ 3 \\ 5 \\ 7 \\ 9 \end{smallmatrix} \right] 25$	50

$$n = 1, 2, 3, \dots ; (K, L, M, N, O, P, \dots)$$

$$l = 0, 1, 2, \dots (n-1) ; (s, p, d, f, g, h, \dots)$$

$$m_l = -l, \dots, 0, \dots, l : \# : (2l+1)$$

$$m_s = \pm \frac{1}{2}$$

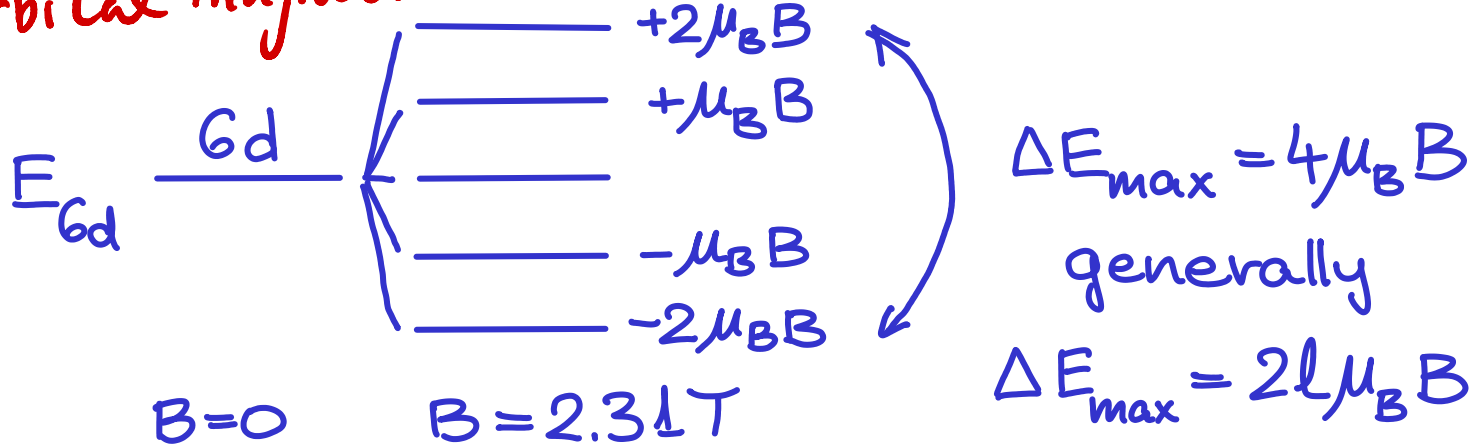
$$L = |\vec{L}| = \sqrt{l(l+1)} \cdot \hbar$$

Shell n has n different subshells,
 n^2 orbitals and $2n^2$ electrons.

Normal Zeeman effect for H

State: $6d \rightarrow n=6$

Due to electron orbital magnetic moment
 $d: l=2: m_l = \underbrace{-2, -1, 0, 1, 2}_{(2l+1) \text{ orientations}}$



$$\mu_B = \frac{e\hbar}{2m_e} = 5.7884 \cdot 10^{-5} \frac{\text{eV}}{\text{T}}$$

$\frac{1s}{B=0} \rightarrow \frac{1s}{B=2.31 \text{ T}} \quad n=1$

$\frac{1s}{B=0} \rightarrow \frac{1s}{B=2.31 \text{ T}} \quad \left. \begin{array}{l} m_s = +\frac{1}{2} \\ m_s = -\frac{1}{2} \end{array} \right\} \text{doublet}$

Due to electron spin magnetic moment

$$\Delta E_s = g_s \cdot \Delta m_s \cdot \mu_B \cdot B$$

$$\rightarrow \frac{1}{2} - (-\frac{1}{2}) = 1$$

$\rightarrow g_s = 2$ is ok! (instead of 2.002)

Probabilities of finding the electron in the Hydrogen atom

$$R_{10}(r) = \frac{2}{\sqrt{a_0^3}} \cdot e^{-\frac{r}{a_0}}$$

$$P(r) = r^2 (R(r))^2 = r^2 \cdot \frac{4}{a_0^3} \cdot e^{-\frac{2r}{a_0}} =$$
$$= \frac{1}{a_0} \cdot 4 \left(\frac{r}{a_0} \right)^2 \cdot e^{-2\left(\frac{r}{a_0}\right)}$$

$$P(x) = \frac{1}{a_0} \cdot 4x^2 \cdot e^{-2x}$$

$$\text{where } x = \frac{r}{a_0}$$

$$\Rightarrow dx = \frac{1}{a_0} \cdot dr$$

Probability of finding the electron at a distance greater than x_1 (i.e. $r > x_1 \cdot a_0$):

$$\int_{x_1}^{\infty} P(x) dx = 4 \int_{x_1}^{\infty} x^2 \cdot e^{-2x} dx = \textcircled{*}$$

$$\text{Calculus: } \int e^{cx} \cdot x^2 dx = e^{cx} \cdot \left(\frac{x^2}{c} - \frac{2x}{c^2} + \frac{2}{c^3} \right)$$

$$\textcircled{*} = 4 \left[e^{-2x} \left(\frac{x^2}{-2} - \frac{2x}{4} + \frac{2}{-8} \right) \right]_{x_1}^{\infty} =$$

$$= e^{-2x_1} (2x_1^2 + 2x_1 + 1)$$

$$\text{If } x_1 = 2.70, \text{ then } P(x > x_1) = 0.09476$$

Probabilities of finding... 2.

Probability of finding the electron between $1.40a_0$ and $2.50a_0$ i.e
 $1.40 < x < 2.50$:

$$P(1.40 < x < 2.50) = P(1.40 < x < \infty) \\ - P(2.50 < x < \infty)$$

With the $x_1 = 1.40$ and $x_2 = 2.50$ notation:

$$P(x_1 < x < x_2) = \\ = e^{-2x_1} \cdot (2x_1^2 + 2x_1 + 1) \\ - e^{-2x_2} \cdot (2x_2^2 + 2x_2 + 1)$$

Most probable radii

Radial wave functions:

$$1s: R_{10}(r) = \frac{2}{\sqrt{a_0^3}} \cdot e^{-\frac{r}{a_0}}$$

$$2s: R_{20}(r) = \frac{1}{\sqrt{(2a_0)^3}} \cdot \left(2 - \frac{r}{a_0}\right) \cdot e^{-\frac{r}{2a_0}}$$

$$2p: R_{21}(r) = \frac{1}{\sqrt{3(2a_0)^3}} \cdot \frac{r}{a_0} \cdot e^{-\frac{r}{2a_0}}$$

$$3d: R_{32}(r) = \frac{4}{81\sqrt{30a_0^3}} \cdot \frac{r^2}{a_0^2} \cdot e^{-\frac{r}{3a_0}}$$

$$\rightarrow P(r) = r^2 \cdot (R(r))^2$$

$\rightarrow$ most probable: $P(r)$ is maximum

$$\frac{dP(r)}{dr} = 0$$

$$\boxed{1s}: P_{10}(r) = \frac{4}{a_0^3} \cdot r^2 \cdot e^{-\frac{2r}{a_0}}$$

$$\frac{dP_{10}(r)}{dr} = 0$$

Most probable radii 2.

$$1s: \frac{4}{a_0^3} \left(2r \cdot e^{-\frac{2r}{a_0}} + r^2 \cdot e^{-\frac{2r}{a_0}} \cdot \left(-\frac{2}{a_0} \right) \right) = 0$$

$$2r \cdot e^{-\frac{2r}{a_0}} = \frac{2}{a_0} r^2 \cdot e^{-\frac{2r}{a_0}}$$

$$1 = \frac{r}{a_0}$$

$\Rightarrow \boxed{r = a_0}$ most probable
radius for 1s

$$\boxed{2p}: P_{21}(r) = \frac{1}{24a_0^3} \cdot \frac{r^4}{a_0^2} \cdot e^{-\frac{r}{a_0}} = K \cdot r^4 \cdot e^{-\frac{r}{a_0}}$$

$$\frac{dP_{21}(r)}{dr} = K \left(4r^3 \cdot e^{-\frac{r}{a_0}} - \frac{1}{a_0} \cdot r^4 \cdot e^{-\frac{r}{a_0}} \right) = 0$$

$$4r^3 \cdot e^{-\frac{r}{a_0}} = \frac{1}{a_0} \cdot r^4 \cdot e^{-\frac{r}{a_0}}$$

$$4 = \frac{r}{a_0}$$

$\boxed{r = 4a_0}$ most probable
radius for 2p

Most probable radii 3.

$$\boxed{3d} : P_{32}(r) = K \cdot r^6 \cdot e^{-\frac{2r}{3a_0}}$$

↑ different constant

$$\frac{dP_{32}(r)}{dr} = K \left(6r^5 \cdot e^{-\frac{2r}{3a_0}} - \frac{2}{3a_0} \cdot r^6 \cdot e^{-\frac{2r}{3a_0}} \right) = 0$$

$$6r^5 \cdot e^{-\frac{2r}{3a_0}} = \frac{2}{3a_0} \cdot r^6 \cdot e^{-\frac{2r}{3a_0}}$$

$$9 = \frac{r}{a_0}$$

$\boxed{r = 9a_0}$ most probable
radius for 3d

Summary : Bohr's $r_n = n^2 \cdot a_0$
result somehow survives, but
but with an extra twist:

$$\left. \begin{array}{l} 1s : a_0 \\ 2p : 4a_0 \\ 3d : 9a_0 \\ \underbrace{4f : 16a_0} \end{array} \right\} \text{most probable radii : } \frac{dP(r)}{dr} = 0$$

These functions don't wave in the
radial direction.