Hydrogen atom

Shell n	orbits	ℓ	m_ℓ	# of orbits	# of $\bar{e}$
K $n=1$	1s	0	0	1	2
L $n=2$	2s 2p	0 1	0 $-1,0,1$	1 3] 4	8
M $n=3$	3s 3p 3d	0 1 2	0 $-1,0,1$ $-2,-1,0,1,2$	1 3 5] 9	18
N $n=4$	4s 4p 4d 4f	0 1 2 3	0 $-1,0,1$ $-2,-1,0,1,2$ $-3,-2,-1,0,1,2,3$	1 3 5 7] 16	32
O $n=5$	5s 5p 5d 5f 5g	0 1 2 3 4	0 $-1,0,1$ $-2,-1,0,1,2$ $-3,-2,-1,0,1,2,3$ $-4,-3,-2,-1,0,1,2,3,4$	1 3 5 7 9] 25	50

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

$\ell = 0, 1, 2, \ldots (n-1)$

$m_\ell = -\ell, \ldots, 0, \ldots \ell$: # : $(2\ell+1)$

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

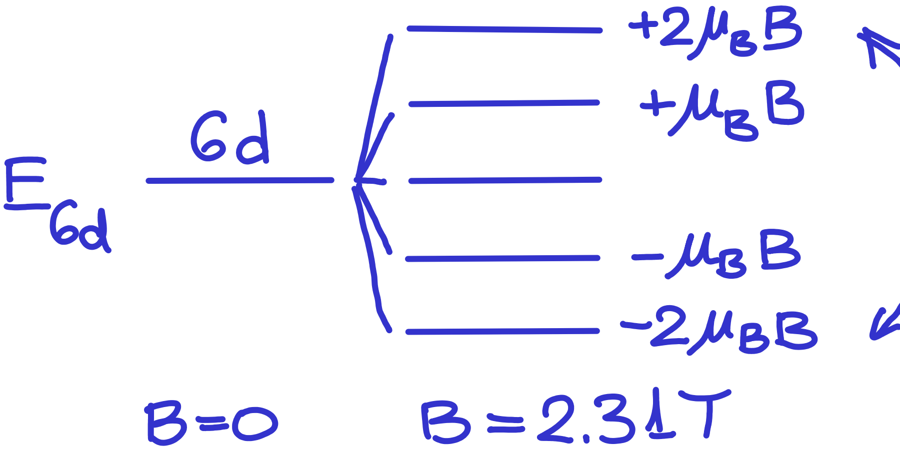
$L = |\vec{L}| = \sqrt{\ell(\ell+1)} \cdot \hbar$

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

Normal Zeeman effect for H

State: 6d $\rightarrow$ $n = 6$

d: $l = 2$: $m_l = \underbrace{-2, -1, 0, 1, 2}_{(2l+1)\text{ orientations}}$

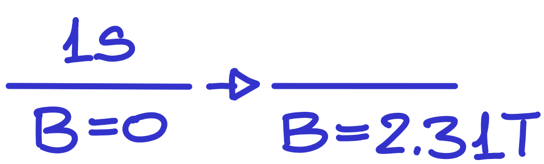


$\Delta E_{max} = 4\mu_B B$

generally

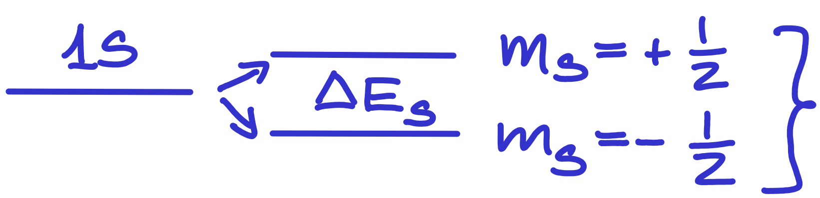
$\Delta E_{max} = 2l\mu_B B$

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



no spin $\Rightarrow$ no split

$n = 1$



doublet

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

Δm_s: $\frac{1}{2} - (-\frac{1}{2}) = 1$

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

Probabilities of finding the electron in the Hydrogen atom

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

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

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

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

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

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

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

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

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

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

If $x_1 = 2.70$, 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 : $R_{32}(r) = \frac{4}{81\sqrt{30a_0^3}} \cdot \frac{r^2}{a_0^2} \cdot e^{-\frac{r}{3a_0}}$

→ $P(r) = r^2 \cdot (R(r))^2$

→ 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 :

$$\left.\begin{array}{ll} 1s & : a_0 \\ 2p & : 4a_0 \\ 3d & : 9a_0 \\ 4f & : 16a_0 \end{array}\right\}$$

most probable radii : $\dfrac{dP(r)}{dr} = 0$

These functions don't wave in the radial direction.