Structure of Matter

1D: $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x) + V(x)\Psi(x) = E\Psi(x)$

kinetic energy; potential energy

Schrödinger equation

3D: $-\frac{\hbar^2}{2m}\nabla^2\Psi(x,y,z) + V(x,y,z)\Psi(x,y,z) = E\Psi(x,y,z)$

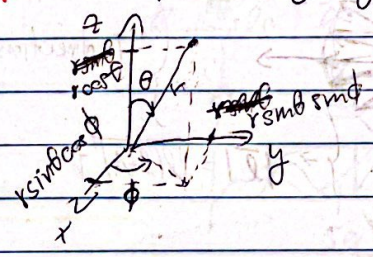
$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$

H-like systems: 1 nucleus, 1 electron

* H, He^+, Ne^{9+}

$V(r) = \frac{-Ze^2}{4\pi\varepsilon_0 r}$

- spherically symmetric ⇒ use spherical coord.



$[0,\pi]$ θ = polar angle wrt $\oplus z$-axis

$[0,2\pi)$ ϕ = azimuthal angle

$$\left\{-\frac{\hbar^2}{2\mu}\nabla^2_{r\theta\phi} + V(r)\right\}\Psi = E\Psi$$

μ = reduced mass

$\mu = \frac{mM}{m+M} \approx m$

m = mass of electron, M = mass of nucleus

$\frac{m_{el}}{m_{proton}} = \frac{1}{1836}$

⇒ H is more than 2000 x larger than m

$$\frac{-\hbar^2}{2\mu}\nabla^2_{r,\varphi} = \underbrace{\frac{-\hbar^2}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)}_{\text{radial part}} + \underbrace{\frac{\hat{l}^2}{2\mu r^2}}_{\text{angular part}}$$

$$\hat{l}^2 = -\hbar^2\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right\}$$

⇒ general solution $\Psi_{nlm} = R_{nl}(r)\,Y_{lm}(\theta,\phi)$

$\hat{l}^2 Y_{lm} = l(l+1)\hbar^2 Y_{lm}$

$\hat{l}_z Y_{lm} = m\hbar Y_{lm}$

↳ spherical harmonics – eigenstates of operators $\hat{l}^2$ and $\hat{l}_z$

$Y_{lm}(\theta,\varphi) = \Theta_{lm}(\theta)\,\Phi_m(\varphi)$

↳ probability to find particle at certain angle θ (from z-axis)

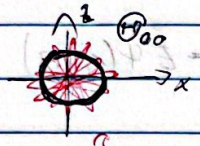
$\Phi_m = \frac{e^{im\varphi}}{\sqrt{2\pi}}$

- sign of m says the ~~rotation~~ direction of rotation about $\hat{z}$

$-l \le m \le l$

$0 \le l \le n-1$

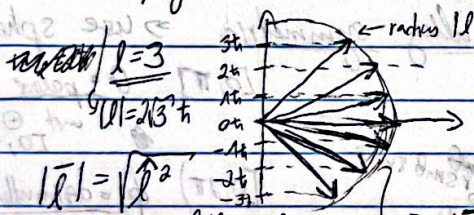
- if m large - Ψ mainly within xy-plane close to
- if $m = 0$ - largest prob. close to z-axis

$\Theta_{lm}(\theta)$: 

equal probability of finding it at all angles
↳ not rotating around

$\vec{l} = \vec{r} \times \vec{p}$ - if rotating along a circle, then $\vec{r} \perp \vec{p}$ and both non-zero, therefore $\vec{l}$ would be non-zero

l_z = "projection of l on to z-axis" - if rotates along a circle ⇒ not the case



7 directions of $\vec{l}$ ⇒ 7 orientations of Ψ
↳ discrete

$|\vec{l}| = \sqrt{\hat{l}^2}$

$\hat{l}^2 Y = l(l+1)\hbar^2 Y$ → $|\vec{l}| = \sqrt{l(l+1)}\,\hbar$

Energy

$E_{nlm} \rightsquigarrow E_n = -\frac{Rhc\,Z^2}{n^2} \approx \frac{-2.2\cdot 10^{-18}}{n^2} Z^2$ (speed of light, 13.6 eV = Z^2/n^2)

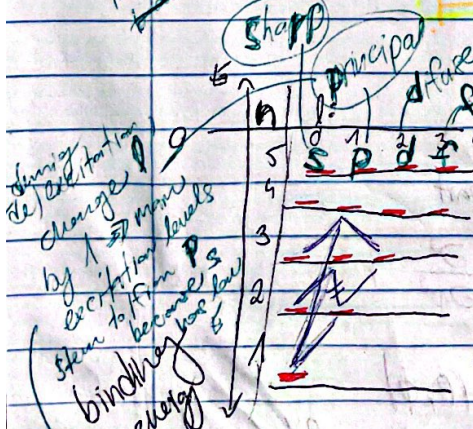
Bohr Model

Rydberg constant $R = \frac{1}{1+\frac{m}{M}}$, $R \approx 1.1 \cdot 10^7\,m^{-1}$

$E_n = -13.6\,\frac{Z^2}{n^2}\,eV$

↳ binding energy (positive means $E<0$)

only these light transitions are seen ⇒ very sharp S-orbitals



decay between levels $\Delta l = \pm 1$

↳ $-1 \gg +1$ more likely for decay

↳ for excitation: $+1 \gg -1$

electric dipole/optical transitions

2 ↳ p-type transitions are most common

$$\left\{-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} - \frac{Ze^2}{4\pi\varepsilon_0 r}\right\} P_{nl} = E P_{nl}$$

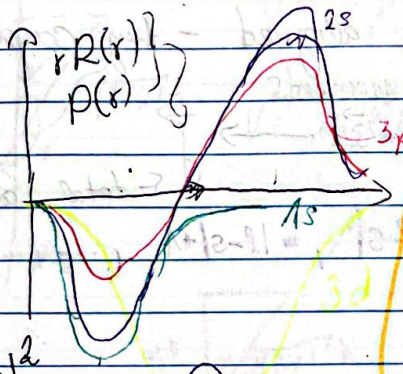
Radial part of Ψ

$r \cdot R_{nl}$ – remove singularity at $r=0$ ~~for $l=0$~~

$$dP(r,\theta,\phi) = |\Psi|^2 dV$$
$$= |\Psi|^2 r^2 \sin\theta \, dr \, d\theta \, d\phi$$

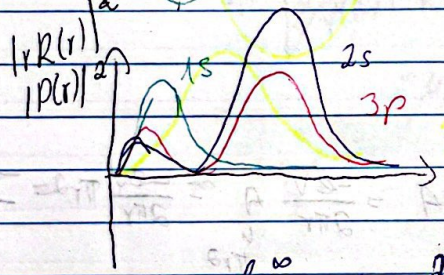
$$dP(r) = r^2 |R_{nl}|^2 dr \underbrace{\int_0^\pi \sin\theta \, |\Theta_{lm}|^2 d\theta}_{=1} \underbrace{\int_0^{2\pi} |\Phi_m|^2 d\phi}_{=1}$$

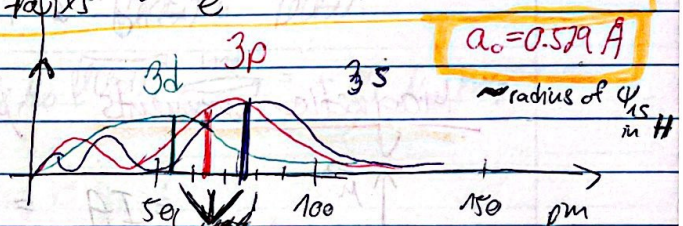
$$dP(r) = r^2 |R_{nl}|^2 dr = |P_{nl}|^2 dr \Rightarrow P(r) = |P_{nl}|^2$$



- first lobe negative by convention
- ✱ first P_{nl} (or R_{nl}) goes down
- ✱ $n-l-1$ = # crossings with r-axis
  - ↳ higher l, less crossings
- ✱ first lobe smallest, last largest
- ✱ tails $\propto e^{-2r/na_0}$

#zeros





$a_0 = 0.529$ Å ~ radius of Ψ_{1s} in H

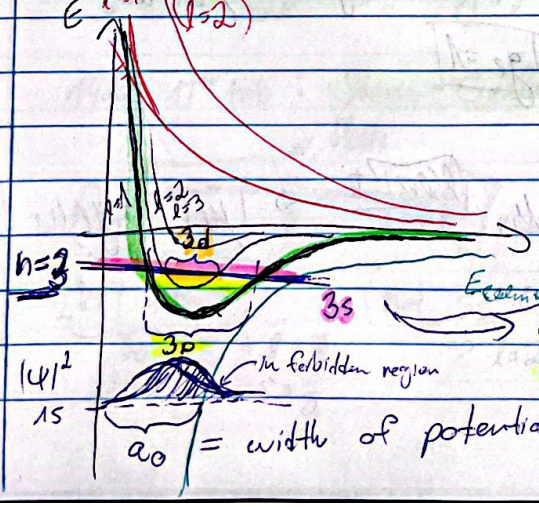
↳ 3d is on avg closest and 3s furthest!

$$\langle f(r)\rangle = \int_0^\infty f(r) \underbrace{|P_{nl}|^2}_{P(r)} dr$$

$$\langle r\rangle = \frac{a_0}{2Z}\{3n^2 - l(l+1)\}$$

$$\langle r\rangle_{1s}^{H} = \frac{3}{2}a_0 \neq a_0$$

$$E_{Coulomb} = \frac{-Ze^2}{4\pi\varepsilon_0 r}$$
$$E_{centrifugal} = \frac{\hbar^2 l(l+1)}{2\mu r^2}$$
(μ: mass) } sum



$r_{n=3}$ can't have $l=3$ because the well is above $n=3$ energy

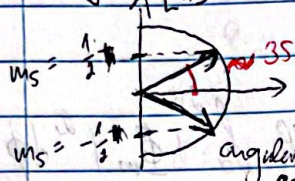
all have same binding energy but different spread in options.

(?!)

Spin

$s = \frac{1}{2}$, $m_s = \pm\frac{1}{2}$ for electron

$$\Rightarrow \psi_{n\ell m_\ell m_s} = R_{n\ell} Y_{\ell m_\ell} \chi_{m_s}$$



"spin up/down" but not actually in $\hat{z}$ direction, - actually close to the midplane

(2.) ~~are~~ angular momenta and $\vec{l}$ and $\vec{s}$?

↳ not independently aligned - they couple together because of magnetic moments

$$\vec{l} + \vec{s} \longrightarrow \vec{j}$$

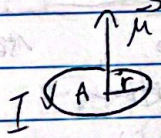
← total angular momentum

$3p$: $l = 1$, $m_s = \frac{1}{2}$

$$j = |l-s|, |l-s|+1, \ldots, l+s-1, l+s$$

↳ $j = \frac{1}{2}, \frac{3}{2}$

Magnetic moments μ



$$\mu = IA = \frac{-e}{T} A = \frac{-eV}{2\pi r} A = \frac{-eV}{2\pi r} \pi r^2 = \frac{-evr}{2}$$

($A = \pi r^2$, $T = \frac{2\pi r}{V}$)

$$\mu = \frac{-evr}{2}$$

$$\vec{l} = \vec{r} \times \vec{p} = m(\vec{r} \times \vec{v}) = mrv \Rightarrow \vec{\mu}_l = \frac{-e}{2m}\vec{l}$$

↳ always perpendicular

in opposite direction

$$\Rightarrow \vec{\mu}_l = \frac{-e\hbar}{2m}\frac{\vec{l}}{\hbar} \equiv -\mu_B \frac{\vec{l}}{\hbar}$$

↳ Bohr magneton: $\mu_B = \frac{e\hbar}{2m_e} \approx 9.27 \cdot 10^{-24}\ A m^2$

$$\boxed{\vec{\mu}_l = -g_l \mu_B \frac{\vec{l}}{\hbar}}, \quad \boxed{g_l = 1}$$

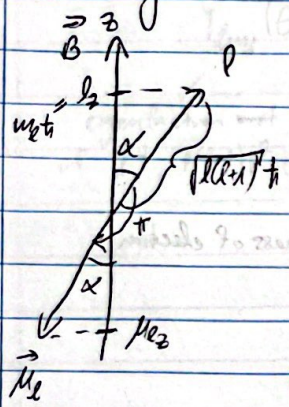
$$|\vec{\mu}_l| = -g_l \mu_B \frac{|\vec{l}|}{\hbar} = -g_l \mu_B \frac{\sqrt{l(l+1)}\hbar}{\hbar} \Rightarrow \boxed{|\vec{\mu}_l| = -g_l \mu_B \sqrt{l(l+1)}}$$

"spin is angular momentum" ⇒ "l" $\propto s = \frac{1}{2}\hbar$

$\vec{\mu}_s = -g_s \mu_B \frac{\vec{s}}{\hbar} =$

↳ $g_s \approx 2$ Einstein - de Haas (1915) - experimental
↳ explained by Dirac with Relat. QM (1928)
⇒ $g_s = 2.0023\ldots$ - by QED

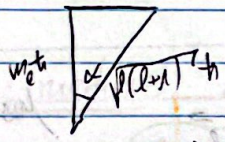
• magnetic moment in external magnetic field



$V = -\vec{\mu}\cdot\vec{B}$ ($\mu = \mu_l \propto \mu_s$)

$V = \mu_{lz}|\vec{B}|$ for $\vec{B}$ in z-direction

$\mu_{lz} = |\mu_l|\cos(\pi+\alpha) = -|\mu_l|\cos(\alpha)$ ($+g_l \mu_B \sqrt{l(l+1)}$)



$\Rightarrow \cos\alpha = \frac{m_l\hbar}{\sqrt{l(l+1)}\hbar} = \frac{m_l}{\sqrt{l(l+1)}}$

$\Rightarrow \mu_{lz} = -g_l \mu_B \sqrt{l(l+1)} \frac{m_l}{\sqrt{l(l+1)}} = -g_l \mu_B m_l$

$\Rightarrow$ **$V_l = -g_l \mu_B m_l B$** ?

↳ discrete potential energies

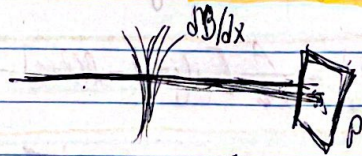
m_l states $= 2l+1$

for spin:

$V_s = -g_s \mu_B m_s B$

$F = -\frac{\partial V}{\partial x} = +g_s \mu_B m_s \frac{\partial B}{\partial x}$

1922 17th Feb: Stern-Gerlach



no $\vec{B}$: 

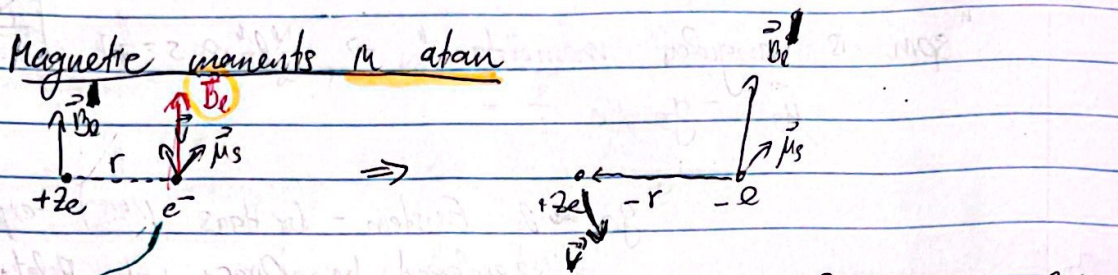
w/ $\vec{B}$ field: 

$s = \frac{1}{2} \Rightarrow m_s = \pm\frac{1}{2}$ ↓ two options ↓ split by spin

$[Kr]\ 4d^{10}\ 5s^1$ (not $5s^2\ 4d^9$ as would be expected ↳ $l=2 \rightarrow m_l = \pm2, \pm1, 0$)

$L=0$, $S=0$ ↓ $l=0$, $S=\frac{1}{2}$

Magnetic moments in atom



Biot-Savart law $\vec{B}_l = \frac{Ze\mu_0}{4\pi r^3}[\vec{v} \times -\vec{r}] = \frac{Ze\mu_0}{4\pi r^3}[\vec{r} \times \vec{v}]$

$\vec{l} = \vec{r} \times \vec{p} = m[\vec{r} \times \vec{v}]$

$\Rightarrow \vec{B}_l' = \frac{Ze\mu_0}{4\pi r^3}\frac{\vec{l}}{m}$

back transformation to coordinate system with nucleus at origin

by $\vec{B}_l = \frac{1}{2}\frac{Ze\mu_0}{4\pi r^3}\frac{\vec{l}}{m}$ ← mass of electron

↓ Thomas factor

$V_{so} = -\vec{\mu}_s \cdot \vec{B}_l = g_s \mu_B \frac{\vec{s}\cdot\vec{B}_l}{\hbar}$

Spin Orbit

$V_{so} = \frac{g_s}{2}\frac{\mu_B}{m_e \hbar}\frac{Ze\mu_0}{4\pi r^3}\vec{s}\cdot\vec{l} = A\hbar^2\,\vec{s}\cdot\vec{l}$

$\mu_B = \frac{e\hbar}{2m}$ $\quad \varepsilon_0 = \frac{1}{c^2\mu_0}$

mass of electron $\quad \xi = \frac{A}{\hbar^2}$

$\Rightarrow A = \xi\hbar^2$ = Spin Orbit constant

Fine structure

↳ commonly energy in cm^{-1} $\quad 8065\,cm^{-1} = 1eV$

↑ λ of photon with energy 1eV

$A \propto \left\langle \frac{1}{r^3} \right\rangle \propto \left\langle \frac{1}{r^3} \right\rangle \propto \frac{Z^3}{n^6}$

$A \propto \frac{Z^4}{n^6}$

$\vec{j} = \vec{l} + \vec{s} \Rightarrow |\vec{j}|^2 = |\vec{l}|^2 + 2\vec{l}\cdot\vec{s} + |\vec{s}|^2$

$2\vec{l}\cdot\vec{s} = j^2 - l^2 - s^2$

$2l+1 = 3$, $2s+1 = 2$, $3 \cdot 2 = 6$

$\Rightarrow V_{so} = \frac{A}{2\hbar^2}(j^2 - l^2 - s^2) = \frac{A}{2}[j(j+1) - l(l+1) - s(s+1)]$

6 states in 3P

#m_j is $2j+1$

6

★ 3p: $l=1,\ s=\frac{1}{2} \rightarrow j = \frac{1}{2}, \frac{3}{2}$

$V_{so}(j=\frac{1}{2}) = -A$

$V_{so}(j=\frac{3}{2}) = +\frac{A}{2}$

} energy wrt 3p energy without coupling effects

binding energy = 6 asymmetric

6 states 3p $\quad j=3/2$ $\quad 4A/2$

2 states $\quad -A$ $\quad j=1/2$

spin & energy = 0

Addition of Angular Momenta

- two angular momenta j_1, m_1 and j_2, m_2

tot ang. momentum: $J = j_1+j_2,\ j_1+j_2-1,\ \dots,\ |j_1-j_2|$

and for each J: azimuthal $M = -J, -J+1, \dots, J$

$Y_{l m_l}(\theta,\phi)\, \chi_{m_s}$ → get definite values for j, m ⇒ coupled states $|(l\tfrac{1}{2})jm\rangle$

$Y_{l m_l}(\theta,\phi)$: eigenfunction wrt. $\hat{l}^2$, $l(l+1)\hbar^2$ eval

χ_{m_s}: eigenfunction of $\hat{s}^2$ wrt eval $\frac{1}{2}(\frac{1}{2}+1)\hbar^2$

↳ eigenfunctions wrt. $\hat{j}^2$ and $\hat{j}_z$ with eval $j(j+1)\hbar^2$, $m\hbar$

and $\hat{l}^2$ and $\hat{s}^2$ with eval $l(l+1)\hbar^2$, $\frac{3}{4}\hbar^2$

Fine structure

ξ

from book: $h_{so} = \frac{1}{2m^2c^2}\frac{1}{4\pi\varepsilon_0}\frac{2e^2}{r^3}\vec{s}\cdot\vec{l} \Rightarrow h_{so} = \xi\, \vec{s}\cdot\vec{l}$

$\xi = \frac{1}{2m^2c^2}\frac{1}{4\pi\varepsilon_0} 2e^2 \left\langle \frac{1}{r^3} \right\rangle$ spin orbit constant

for H: $\left\langle \frac{1}{r^3} \right\rangle = \int_0^\infty \frac{1}{r^3} P_{nl}(r)^2\, dr$

from previous page ⇒ $h_{so} = \frac{\xi}{2}(\vec{j}^2 - \vec{s}^2 - \vec{l}^2)$

$h_{so}\,|(l\tfrac{1}{2})jm\rangle = \frac{\xi\hbar^2}{2}\left[j(j+1) - \frac{1}{2}(\frac{1}{2}+1) - l(l+1)\right]|l(\tfrac{1}{2})jm\rangle$

fine structure const.

$\xi = \frac{\alpha^2}{2} Z^4 \left(\frac{1}{4\pi\varepsilon_0}\frac{e^2}{a_0}\right)\left\langle \left(\frac{a_0}{Zr}\right)^3 \right\rangle$ eigenvalue of h_{so}

$\xi \propto Z^4$

$\alpha \Rightarrow \frac{1}{137}$

↳ spin-orbit interaction is small for light atoms but becomes increasingly important

Zeeman effect

$\mu_j = g_j \frac{\vec{j}}{\hbar} \mu_B$

- interaction of H w/ external $\vec{B}$ → splitting of energy levels

$V_{mag} = -\vec{\mu}_j \cdot \vec{B}$

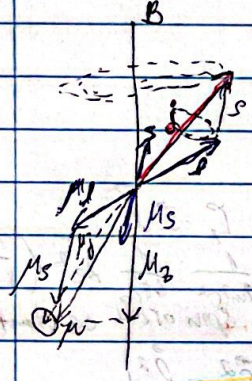
$V_j = -\vec{\mu}_j \cdot \vec{B} = g_j \mu_B \frac{\vec{j}\cdot\vec{B}}{\hbar} = g_j \mu_B m_j B$

$V_{mag} = \frac{e}{2m}(\vec{l} + g_s \vec{s}) \cdot \vec{B} = \frac{e}{2m} B(l_z + g_s s_z)$ for $\vec{B} \parallel \hat{z}$

↳ g_j = ?

- for weak $\vec{B}$: $\vec{l}$ and $\vec{s}$ precess rapidly about $\vec{j}$, while $\vec{j}$ precesses slowly about $\vec{B}$
  ⇒ components of $\vec{l}$ and $\vec{s}$ $\perp \vec{j}$ cancel out over time = many revolutions
  ⇒ replace $\vec{l}$ and $\vec{s}$ with their projection along $\vec{j}$
  → $(\vec{l}\cdot\hat{j})\hat{j}$ → m dir. of $\vec{B}$: $(\vec{l}\cdot\hat{j})\hat{j}_z$
- ⇒ avg l_z for coupled states w/ definite j and m:

$l_z \to (\vec{l}\cdot\hat{j})\hat{j}_z = \frac{(\vec{l}\cdot\vec{j})j_z}{j^2} = \frac{(\vec{l}\cdot\vec{j})j_z}{j(j+1)\hbar^2} \overset{\vec{l}\cdot\vec{j} = \frac{j^2+l^2-s^2}{2}\hbar^2}{=} \frac{(j^2+l^2-s^2)j_z}{2j(j+1)\hbar^2}$



$[\vec{s}\cdot\vec{s} = \vec{j}^2 + \vec{l}^2 - 2\vec{l}\cdot\vec{j}]$

$\Rightarrow l_z \to \frac{j(j+1) + l(l+1) - s(s+1)}{2j(j+1)} j_z$

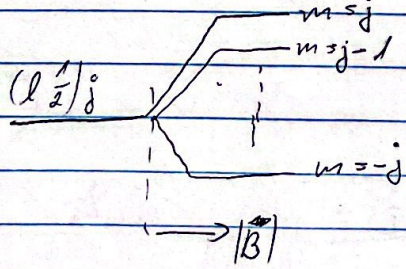
$s_z \to \frac{j(j+1) - l(l+1) + s(s+1)}{2j(j+1)} j_z$

$V_{mag} = \frac{e}{2m} B(l_z + g_s s_z) = \frac{e}{2m} B g_j j_z$ where

$g_j = \frac{j(j+1) + l(l+1) - s(s+1)}{2j(j+1)} + g_s \frac{j(j+1) - l(l+1) + s(s+1)}{2j(j+1)}$

- coupled states = eigenfunctions of j_z corresponding to $m\hbar$
  → splitting of V (m-levels):

$\Delta E = \frac{e}{2m}\hbar B m g_j = g_j \mu_B B m$

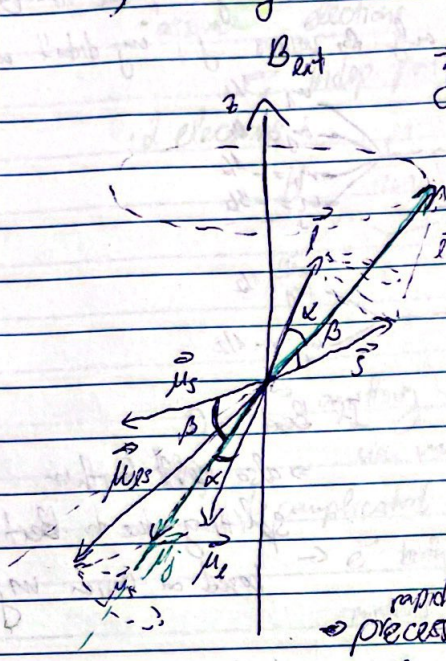


Zeeman effect

↗ spin-orbit coupling

$B_{ext} < B_{int}$ ⇒ How does this change energy levels?

$\vec{l} + \vec{s} = \vec{j}$ but $\vec{\mu}_l + \vec{\mu}_s \neq \vec{\mu}_j \parallel \vec{j}$



$\vec{j}$ slowly precessing ~~about~~ around B_{ext}

$\vec{l}, \vec{s}$ precess fast around $\vec{j}$

↳ $B_{int} > B_{ext}$

Consider $\vec{\mu}_{ls} = \vec{\mu}_l + \vec{\mu}_s = -g_l \mu_B \frac{\vec{l}}{\hbar} - g_s \mu_B \frac{\vec{s}}{\hbar}$

$\vec{l}, \vec{s}$ precess around $\vec{j}$

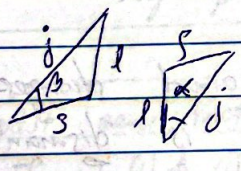
⇒ $\vec{\mu}_{ls}$ precesses around $-\vec{j}$ direction, but doesn't point in $\vec{H}$

(vectors of $\vec{\mu}_l, \vec{\mu}_s$ are different than of $\vec{l}, \vec{s}$ although same angles) ↳ $g_s \neq g_l$

⇒ rapid precession ⇒ averaging out over a whole cycle → component $\perp \vec{j}$ cancels out and only component in $-\vec{j}$ is left → $\vec{\mu}_j$

projection of $\vec{\mu}_{ls}$ onto $\vec{j}$

- $|\vec{\mu}_j| = |\vec{\mu}_l| \cos\alpha + |\vec{\mu}_s| \cos\beta$
- law of cosines



$|\vec{s}|^2 = |\vec{j}|^2 + |\vec{l}|^2 - 2|\vec{j}||\vec{l}|\cos\alpha$

$|\vec{l}|^2 = |\vec{j}|^2 + |\vec{s}|^2 - 2|\vec{j}||\vec{s}|\cos\beta$

$\cos\alpha = \frac{|\vec{j}|^2 + |\vec{l}|^2 - |\vec{s}|^2}{2|\vec{j}||\vec{l}|}$

$\cos\beta = \frac{|\vec{j}|^2 + |\vec{s}|^2 - |\vec{l}|^2}{2|\vec{j}||\vec{s}|}$

⇒ $|\vec{\mu}_j| = \mu_B g_l \frac{|\vec{l}|}{\hbar} \cdot \frac{|\vec{j}|^2 + |\vec{l}|^2 - |\vec{s}|^2}{2|\vec{j}||\vec{l}|} + \mu_B g_s \frac{|\vec{s}|}{\hbar} \cdot \frac{|\vec{j}|^2 + |\vec{s}|^2 - |\vec{l}|^2}{2|\vec{j}||\vec{s}|}$

$g_l = 1$, $g_s = 2$ ↓

$= \frac{\mu_B}{2|\vec{j}|\hbar}\left[3|\vec{j}|^2 - |\vec{l}|^2 + |\vec{s}|^2\right] \frac{|\vec{j}|}{|\vec{j}|} = \frac{\mu_B |\vec{j}|}{\hbar}\left[\frac{3|\vec{j}|^2 + |\vec{s}|^2 - |\vec{l}|^2}{2|\vec{j}|^2}\right] =$

$\vec{\mu}_j = -\frac{\mu_B}{\hbar}\vec{j}\left[1 + \frac{|\vec{j}|^2 - |\vec{l}|^2 + |\vec{s}|^2}{2|\vec{j}|^2}\right] = -\frac{\mu_B}{\hbar} g_j \vec{j}$

g_j

Now for energy:

precession about z-axis ⇒ ~~over~~ over time $\vec{l}$ cancels out

$V = -\vec{\mu}_j \cdot \vec{B}_{ext} = -\vec{\mu}_j \cdot \vec{B}_{ext} = -\vec{\mu}_{jz} \cdot \vec{B}_{ext}$ ~~=~~

$|\vec{\mu}_{jz}| = -\frac{\mu_B}{\hbar} g_j m_j \hbar = -\mu_B g_j m_j$

⇒ $V_{mag} = \mu_B g_j m_j B_{ext}$

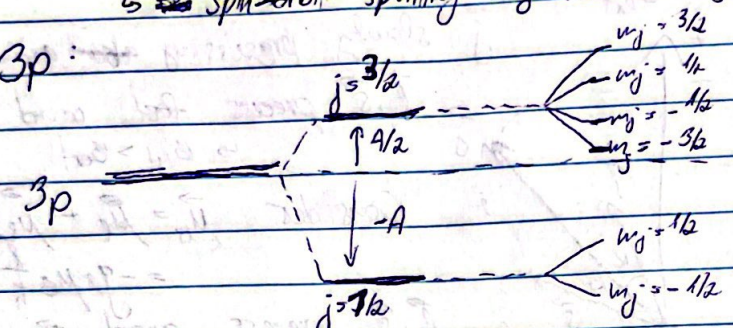
= Zeeman effect

$V_{mj} = \mu_B g_j m_j B_{ext}$

⇒ energy splitting based on various m_j, due to B_{ext}

↳ spin-orbit splitting only for various j, m_j didn't matter

☆ 3p:



Splitting due to spin-orbit coupling based on various values of j

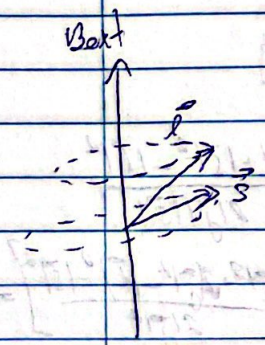
If $B_{ext} \neq 0$ ⇒ also further splitting due to B_{ext} based on various m_j

- 2 types of Zeeman effect
  - normal/ordinary: $S = 0$
  - anomalous: $S \neq 0$ ↳ more common

What if $B_{ext} >> B_{int}$?

- the system will precess around strongest $\vec{B}$ ⇒ spin-orbit coupling is "dismantled" (negligible). and $\vec{l}$, $\vec{s}$ precess around B_{ext} independently

= Paschen-Bach effect



$V = -\vec{\mu}_l \cdot \vec{B}_{ext} - \vec{\mu}_s \cdot \vec{B}_{ext}$

$V = \mu_B g_l m_l B_{ext} + \mu_B g_s m_s B_{ext}$

⇒ $\boxed{V = \mu_B B_{ext} (m_l + 2m_s)}$

Many electron atoms

- assume electrons move independently in avg field of nucleus & e^-'s
  ⇒ indep. particle model ~ good approx.

- 2 electrons:

$$H = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r_1} - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r_2} + \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r_{12}}$$

KE_1 — first e^- — distance from nucleus — KE_2 — second e^- — mutual influence (Coulomb) — distance between e^-

↳ anything influence of spin-spin & spin-orbit interactions via magnetic field

↳ complicated ⇒ use approx. ⇒ independent particle model

⇒ e^- both move in common shared potential $u(\vec{r})$ instead of influencing mutually via Coulomb:

$$H_0 = \underbrace{-\frac{\hbar^2}{2m}\nabla_1^2 - \frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r_1} + u(\vec{r}_1)}_{= h_0(1)} \underbrace{-\frac{\hbar^2}{2m}\nabla_2^2 - \frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r_2} + u(\vec{r}_2)}_{= h_0(2)}$$

$h_0(i)$: single particle Hamiltonian describing motion of ith electron

⇒ simplest wave function description: product: $\Phi = \phi_a(1)\,\phi_b(2)$ — but electrons = fermions ⇒ need odd Ψ

If $h_0(i)\,\phi_{a/b}(i) = \varepsilon_{a/b}\,\phi_{a/b}(i)$ ⇒ $H_0\Phi = E_0\Phi$ — ϕ: eigenfunctions, quantum numbers; $E_0 = \varepsilon_a + \varepsilon_b$; two sols with same energy

⇒ another option: interchange particles ⇒ $\Phi = \phi_b(1)\,\phi_a(2)$

$$H_0\Psi = (h_0(1) + h_0(2))\,\phi_a(1)\,\phi_b(2) = (E_a + E_b)\,\phi_a(1)\,\phi_b(2) = E\,\phi_a(1)\,\phi_b(2)$$

Pauli exclusion principle = no two e^- are in the same state

- product wavefunctions are eigenfunctions but don't satisfy

⇒ instead take: (normalisation)

$$\Psi = \frac{1}{\sqrt{2}}\left[\phi_a(1)\,\phi_b(2) - \phi_a(2)\,\phi_b(1)\right] = \frac{1}{\sqrt{2}}\begin{vmatrix}\phi_a(1) & \phi_a(2)\\ \phi_b(1) & \phi_b(2)\end{vmatrix}$$

$P_{exc}\Psi = -\Psi$

a, b = state (configuration) specified by combination of quantum numbers (n, l, m_l, m_s)

↳ changes sign when switching 1 & 2 ⇒ antisymmetric

0 when $a = b$ ⇒ no two e^- can be in same state

↳ product fns eigenfunctions ⇒ their lin. comb. also eigenfn wrt H_0

⇒ generalise to N electrons: $H_0 = h_0(1) + h_0(2) + \ldots + h_0(N)$

$$\Psi = \frac{1}{\sqrt{N!}}\begin{vmatrix}\phi_a(1) & \phi_a(2) & \cdots & \phi_a(N)\\ \phi_b(1) & \phi_b(2) & \cdots & \phi_b(N)\\ \vdots & \vdots & & \vdots\\ \phi_n(1) & \phi_n(2) & \cdots & \phi_n(N)\end{vmatrix}$$ Slater determinant

• for atoms: assumption ~~for~~ that potentials are spherically symmetric

= central-field approximation

⇓ $\vec{r_1} \to r_1$, $\vec{r_2} \to r_2$ } indep. θ, ϕ

$$\psi(r,\theta,\phi) = \frac{P_{nl}(r)}{r} Y_{lm_l}(\theta,\phi)\, \chi_{m_s}$$

where

$$\left[-\frac{\hbar^2}{8m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} - \frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r} + u(r)\right] P_{nl}(r) = E P_{nl}(r)$$

$-\frac{Z_{eff}\, e^2}{4\pi\varepsilon_0 r}$ | extra

* Z_{eff} = effective charge, shielding effects

⇒ $E_n = -13.6\,eV \frac{Z_{eff}^2}{n^2}$

• for Hydrogen energy of orbitals depends only on n, but for other atoms, l also plays role, indep. of m_s, m_l (for ○ sym.)

⇒ motion of e^- in charge distribution

- same n → shell
- same n, l → subshell → each contains max. $2(2l+1)$ e^-
  - → full = filled/closed
  - → partially filled = open

• each l has $2l+1$ states, each spin has $2s+1$ states, $s = 1/2$ for e^- ⇒ ② spin ⇒ $2(2l+1)$

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^{10}\ 5p^6\ 6s^2\ 4f^{14}\ 5d^{10}\ 6p^6 \ldots$

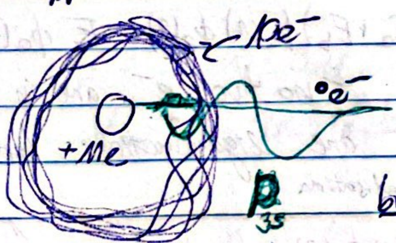
• alkali metal (and alkali earth metals) - very reactive, loosely bound s-electron → low ionisation energy

• halogens - very reactive, missing one electron to be ~~filled~~ closed

• rare/inert gases - unreactive, very high ionisation energies bc closed

☆ Na, $Z = 11$

Suppose we look at what the outter most e^- sees:



sees $+11e - 10e = 1e$ ⇒ charge of $+1$

⇒ $Z_{eff} = +1e$

but actually we see larger binding energies - why?

↳ Part of the wavefunction is "inside" - closer to the nucleus than the shielding e^- ⇒ our investigated electron sees $Z_{eff} = 1$ most of the time but sometimes also $Z_{eff} = 11$ for example ⇒ in total Z_{eff} a bit larger than just 1

• For larger atoms, $Z_{eff} \to 1$ as the probability of being very close is very small

Separable wavefunction

$$\Psi = \frac{1}{\sqrt{2}}\left[\phi_a(1)\phi_b(2) - \phi_a(2)\phi_b(1)\right]$$

but we can also separate spin out: $\phi_a = \phi_c \chi_\alpha$ (spatial, spin) $\quad \phi_b = \phi_d \chi_b$

$$\begin{cases} \Psi = \frac{1}{\sqrt{2}}\left[\phi_c(1)\phi_d(2) - \phi_c(2)\phi_d(1)\right]\chi_\alpha(1)\chi_b(2) \\ \Psi = \frac{1}{\sqrt{2}}\left[\chi_\alpha(1)\chi_b(2) - \chi_\alpha(2)\chi_b(1)\right]\phi_c(1)\phi_d(2) \end{cases} \quad \text{or}$$

we can make either spatial antisymmetric and spin symm.
or spin antisymmetric and spatial symm.

Number of states in a shell

- for each l, we have $(2l+1)$ m_l states
- for each s, we have $2s+1 = 2$ states
  ⇒ each subshell can take $2(2l+1)$ for e^-
- in each n shell: $\sum_{l=0}^{n-1} 2(2l+1) = 2n^2$

$n=1$:	2	$1s^2$
$n=2$:	8	$2s^2 2p^6$
$n=3$:	18	$3s^2 3p^6 3d^{10}$
$n=4$:	32	$4s^2 4p^6 4d^{10} 4f^{14}$

$Z=10$: Ne : $1s^2 2s^2 2p^6$
$Z=18$: Ar : [Ne] $3s^2 3p^6$
$Z=20$: Ca : [Ar] $4s^2$
↳ can easily penetrate cloud of other electrons → gets filled before 3d
$Z=22$: Ti : [Ar] $4s^2 3d^2$
! $Z=24$: Cr : [Ar] $4s\ 3d^5$ → many e^- in partially filled shells ⇒ if align spin then it's actually energetically favorable ($\vec{r}$ small)
$Z=25$: Mn : [Ar] $4s^2 3d^5$

Multiple electrons

$\vec{l}_1 + \vec{l}_2 + \vec{l}_3 + \dots = \vec{L}$ ← capital = total number

small = 1 e^-

$\vec{s}_1 + \vec{s}_2 + \vec{s}_3 + \dots = \vec{S}$

} LS = Russel-Saunders coupling

$\vec{j}_1 + \vec{j}_2 + \vec{j}_3 + \dots \rightarrow \vec{J}$ ← total angular momentum of all e^-

↳ either first add $\vec{l}$'s and $\vec{s}$'s and then $\vec{L} + \vec{S} \rightarrow J$ } each different

or first add l_i and s_i for each electron and then j's to get J

jj-coupling

Ex: "p" "s"

$l_1 = 1$, $l_2 = 0$ ⇒ $L = 1$

$s_1 = \frac{1}{2}$, $s_2 = \frac{1}{2}$ ⇒ $S = 0, 1$

$J = 1$; $J_{max} = 2$, $J_{min} = 0$ } $J = 0, 1, 2$

$j_1 = \frac{1}{2}, \frac{3}{2}$, $j_2 = \frac{1}{2}$ → $J = 1, 2$ → $J = 0, 1$

set of J values is exactly the same $\{0, 1, 1, 2\}$ but in different "groups"

Meaning of Grouping

in C:

E_b ↓

— 1 } singlet ^1P "singlet P"

⇒ LS works well for low Z

— 2, — 1, — 0 } triplet ^3P ← term; "triplet p" ← write ^{2S+1}L (degeneracy of S)

in Pb:

E_b ↓

— 2, — 1

— 1, — 0

⇒ jj works well for high Z

↳ in the middle e.g. Ge

Spin-Orbit Coupling

$A \propto Z^4$ ⇒ very strong spin-orbit coupling for elements with high Z

⇒ interaction of 1 e^- w/ nucleus is important (more than with other e^-) ⇒ jj

for low Z: Coulomb interaction dominates ⇒ L dominates, spin-orbit coupling is weak ⇒ splitting based on LS

⇒ but from now on (unless stated otherwise) use LS coupling

Two electrons
- same n, l → equivalent
- different n, l → non-equivalent

① Equivalent electrons → $S+L$ = even for 2 equivalent electrons
- S: total spin; 0 or 1 for 2 electrons
- L: total orb. ang. momentum
- ↳ write as ^{2S+1}L
  - S = tot. spin number
  - L = total orb. ang. mom. (S, P, D, F, ...)

E: $[cm^{-1}]$ $\left[\frac{1}{\lambda} = \frac{E}{hc}\right] = cm^{-1}$: $1 eV = 8065.54 cm^{-1}$

- splitting due to: electrostatic
  spin-orbit

- Hund's rule
  - lowest LS term has max. S value → largest multiplicity $2S+1$
  - if multiple terms with max. S → max. L is lowest

- ordering of J sub levels
  - min. J lowest if less-than-half filled
  - max. J lowest if more-than-half filled

② Non-equivalent electrons
- different n and/or l

LS coupling

For filled shells: $L=0$, $S=0$ → $J=0$

^{2S+1}L $^{2S+1}L_J$ M_J, $^{2S+1}L_{M_J}$

electronic configuration: $n_1 l_1, n_2 l_2, n_3 l_3, \ldots$
(different names depending on known information)

term ^3P

level - e.g. $^3P_1$ — $2M_J+1$ states

state $^3P_{-1}$

for jj-coupling called multiplets

Filled shells $L=0,\ S=0 \rightarrow J=0 \Rightarrow {}^1S_0$

★ $l=1$ ("p") → $(2)p^6$

m_l / m_s	−1	0	1	M_L
1/2	↓	↓	↓	0
−1/2	↓	↓	↓	0
M_S	0	0	0	0

$M_L = \sum m_l$

6 e⁻ in p-shell, each differs (has different m_s or m_l)

total $M_L = 0$ ↳ no other options for M_L ⇒ ~~there is~~

total $M_S = 0$ → no other options for M_S ⇒ $S=0$ ↳ only 1 option

$0 = M_L + M_S$ ⇒ $L=0$

there is only 1 possible state ⇒ ~~deg~~ deg = 1

deg = $2L+1$ (or $2S+1$ or $2J+1$)

⇒ only partially filled shells need to be considered

★ two "p" electrons, $l_1 = l_2 = 1$ ⇒ $L = 0, 1, 2$

$s_1 = s_2 = 1/2$ ⇒ $S = 0, 1$

⇓

for $n_1 \neq n_2$ (non-equivalent e⁻) $3 \times 2 = 6$ possible terms:

(3 possibilities for L) × (2 possibilities for S)

$^1S_0$ $^1P_{0+1}$ $^1D_{0+2}$

$^3S_1$ $^3P_{0+1+2}$ $^3D_{1+2+3}$

⇒ $2S+1$ states for each level

^1S ^1P ^1D

⇒ $1 + 3 + 5 = 9$

^3S ^3P ^3D

$3 + 3 + 5 + 1 + 3 + 5 + 7 = 27$

$(2l_1+1)(2l_2+1)(2s_1+1)(2s_2+1) = 3 \cdot 3 \cdot 2 \cdot 2 = 36$ states

for $n_1 = n_2$ (equivalent e⁻) ⇒ must differ in at least one q.n. by Pauli exclusion principle

⇒ not all states are allowed

↳ difficult to figure out which

but for two equivalent electrons: $L+S$ = even ~ Pauli exclusion

^1S ~~^1P~~ ^1D

~~^3S~~ ^3P ~~^3D~~

$1+0=1$ $1+2=3$

★ C: $1s^2\ 2s^2\ 2p^2$

↳ possible ~~states~~ states:

^1S, ^3P, ^1D (only $2p^2$ ~~el~~ to consider, rest is filled)

Hund's rules – only apply for grand electronic configuration

① determine all terms of partially filled shells
↳ consider Pauli exclusion principle ($\approx L+S$ = even)

② highest spin terms are strongest bound → preferred → lowest energy, grand state
↳ if we have only are triplet:

*C: $1s^2 2s^2 2p^6$:
from ^1S, ^3P, ^1D
⇒ choose $^3P_0$

③ within highest S (if equal), highest L value is strongest bound

④ grand level: { lowest ↓ if less than 1/2 is filled (or equal) } A>0
{ highest ↓ if more than 1/2 filled } A<0

$$V_{SO} = \frac{A}{2}\left[J(J+1) - L(L+1) - S(S+1)\right]$$

*O: $1s^2 2s^2 2p^4$
⇒ $^3P_2$ ($2p^4$ equivalent to $2p^2$ for allowed states by Pauli)
↳ same counting with holes as electrons
↳ except ⊖
same set of combinations

* Four "p" electrons

m_l / m_s	−1	0	1	Σm_l	
1/2	e⁻	e⁻	e⁻	0	$M_L = 1$
−1/2	□	□	e⁻	1	
Σm_s	1/2	1/2	0		

$M_S = 1$

⇓ two "p" holes

m_l / m_s	−1	0	1	Σm_l	
1/2				0	$M_L = \pm 1$
−1/2	⊕	⊕		−1	
Σm_s	−1/2	−1/2	0		

$M_S = \pm 1$

⇒ opposite numbers because "holes" have opposite charge
↳ positively charge holes

⇄ pointing opposite direction

✱ N : $1s^2 2s^2 2p^3$

$(2p^3)$ $l_1 = l_2 = l_3 = 1$

$l_1 \neq l_2 \rightarrow L_{12} = 0, 1, 2$

$l_3 + L_{12} \rightarrow L$

1	0	→ 1
1	1	→ 0, 1, 2
1	2	→ 1, 2, 3

For spin: $S = \frac{1}{2}, \frac{3}{2}$

↳ $S_{12} = 0, 1$ ↑ $s_3 = \frac{1}{2}$

S \ L	0	1	2	3	
3/2	^4S	^4P	^4D	^4F	- quadruplett
1/2	^2S	^2P	^2D	^2F	- dublett

$m_s = \pm\frac{1}{2}, \frac{3}{2}$; $m_s = \pm\frac{1}{2}$

↳ find which ones are allowed ? ⇒ look at M_L & $M_S \geq 0$

M_S	M_L	terms with these M_S, M_L			
3/2	3	^4F			
↑	2	^4F	^4D		
⁴ quadruplets	1	^4F	^4D	^4P	
	0	^4F	^4D	^4P	^4S
1/2	3	^4F			
↑	2	^4F	^4D		
² duplets and quadruplets	1	^4F	^4D	^4P	
	0	^4F	^4D	^4P	^4S

	2F	
	2F	^2D
	2F	^2D ^2P
	^2F	^2D ^2P ✗

IF one state of a term exists ⇒ all must exist

$M_S = 3/2$

m_{s_1} m_{s_2} m_{s_3} : 1/2 1/2 1/2

$M_S = 1/2$

m_{s_1} m_{s_2} m_{s_3} : 1/2 1/2 −1/2

M_L	m_{l_1} m_{l_2} m_{l_3}	
3	1 1 1	⇒ not allowed by Pauli
2	1 1 0	⇒ 7 of 9 states for ^4F (term)
1	0 0 1	doesn't exist ⇒ the whole term doesn't exist
	−1 1 1	⇒ doesn't exist
0	1 0 −1	✓
	0 0 0	⇒ start from top
3	1 1 1	
2	1 0 1	✓ - same m_l's but differ in m_s so it's allright
1	1 0 0	✓
	−1 1 1	✓
0	1 0 −1	✓ ⇒ only 3 states possible and we have 4 terms ⇒ one cannot exist ⇒ kill ^2S
	1 −1 0	✓
	−1 0 1	✓

$M_S = 3/2$, $3 = M_L$ ⇒ doesn't exist

Elementary Particles

atoms: L, S → fine structure: J; nuclear spin: I → hyperfine structure F

↳ nucleons (neutrons, protons)

↳ elementary particles

fermions { leptons, quarks

bosons - force carriers

gravity → mass, ∞ range

electro-magnetic → γ, $W^{+,-}$, Z^0 → el. charge, 10^{-8}–10^{-13} s

weak (radioactive decay) → leptons/quarks

strong → gluons, 10^{-15} m, range $< 10^{-22}$ s → quarks (colour)

↳ high energy (short distance)

⇒ hardest to be allowed by Heisenberg

↳ massless

QED ← electroweak

QCD ← strong

lifetime of $W^{+,-}$, Z^0: $\sim 10^{-24}$ s, but still interaction time 10^{-8}–10^{-13} s

interaction time [s]

gluons are not only force carriers but also part of the interaction

⇒ have colour

⇒ interact via strong force

⇒ confinement (cannot be alone)

Standard Model

- unites electroweak and strong force

QED + QCD

- 19 or 28 "free" parameters ⇒ their values come from experiments

↳ ? depends on neutrinos (not) having mass (if yes → 28)

Leptons

3 generations / doublets / flavors:

				antimatter		
	e^-	μ^-	τ^-		e^+	μ^+	τ^+
	ν_e	ν_μ	ν_τ		$\bar{\nu}_e$	$\bar{\nu}_\mu$	$\bar{\nu}_\tau$
$[MeV]/c^2$	0.5	105	1800				
lifetime	$>10^{26}$ yrs	2.2 μs	300 fs				

< 0.8 eV/c²

$\mu^- \rightarrow e^- + \bar{\nu}_e + \nu_\mu$

$\tau^- \rightarrow \mu^- + \bar{\nu}_\mu + \nu_\tau$

$\tau^- \rightarrow e^- + \bar{\nu}_e + \nu_\tau$

Neutrino Oscillations

flavours: ν_e, ν_μ, ν_τ ⇒ not eigenstates of mass

masses: m_1, m_2, m_3

when interacting, do so via flavour which are in superposition of m_1, m_2, m_3

ν_e = ○ ○ ○ (m_1 m_2 m_3)

ν_μ = ○ ○ ○

ν_τ = ○ ○ ○

} oscillating between states - m_i eigenstates: m_1, m_2

$\nu_e \rightarrow \nu_\mu \rightarrow \nu_\tau$

Quarks: 3 generations

			charge
u	c	t	+2/3
d	s	b	-1/3

masses [MeV]			
	1.5–3.1	1.27k	170k
	3.5–6	104	4.2k

HADRONS

MESONS

- 2 quarks ($q\bar{q}$)

charges: • -1, 0, 1

- **pions** (130–140 MeV)

π^+ $u\bar{d}$ $\rightarrow \mu^+ + \nu_\mu$

π^0 $u\bar{u} + d\bar{d}$ — superposition of these two states — lifetime $3 \cdot 10^{-8}$ s

π^- $\bar{u}d$ $\rightarrow \mu^- + \bar{\nu}_\mu$

(own antiparticles; π^- another particle)

$\pi^0 \rightarrow 2\gamma$ — lifetime 8.7×10^{-17} s

significantly heavier than just u/d → mass is stored in the energy of the strong field

- **kaons** (490–500 MeV)

K^+ $u\bar{s}$ $\rightarrow \mu^+ + \nu_\mu$

K^- $s\bar{u}$ $\rightarrow \mu^- + \bar{\nu}_\mu$

no eigenstates of the weak interaction → strong

K^0 $d\bar{s}$

$\bar{K}^0$ $s\bar{d}$

eigenstates of weak interaction:

$K^0_L = \frac{d\bar{s} - s\bar{d}}{\sqrt{2}}$ — 3×10^{-8} s → $\pi^+ + e^- + \bar{\nu}_e$, $\pi^+ + \mu^- + \bar{\nu}_\mu$, $\pi^+ + \pi^- + \pi^0$

$K^0_S = \frac{d\bar{s} + s\bar{d}}{\sqrt{2}}$ — 9×10^{-11} s

BARYONS

- 3 quarks: qqq, $\bar{q}\bar{q}\bar{q}$
- -1, 0, 1, 2 / -2, -1, 0, 1

- ~~par~~ nucleons → 938 MeV
  - p^+ uud — lifetime: $> 10^{31}$ yrs
  - n^0 udd → 940 MeV — 10^3 s ≈ 15 min free

Forces

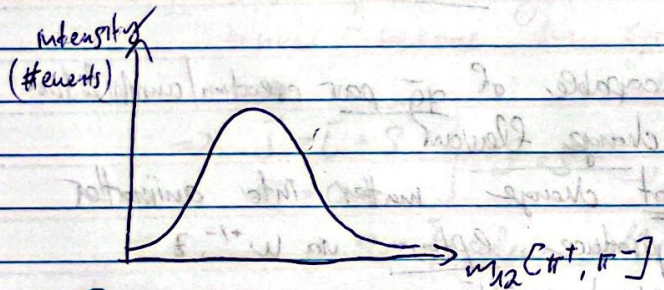
	time	strength	range
weak	10^{-10} s	10^{-6}	10 cm (measurable)
el. magn	10^{-16} s	10^{-2}	0.1 μm
strong	$< 10^{-24}$ s	1	< 1 fm (impossible)

invariant mass

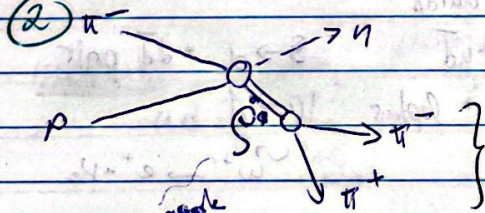
• 2 particles: $$m_{12} = \frac{1}{c^2}\left[(E_1+E_2)^2 - (\vec{p}_1+\vec{p}_2)^2 c^2\right]^{1/2}$$

☆ $\pi^- + p \rightarrow \pi^- + \pi^+ + n$

(1)



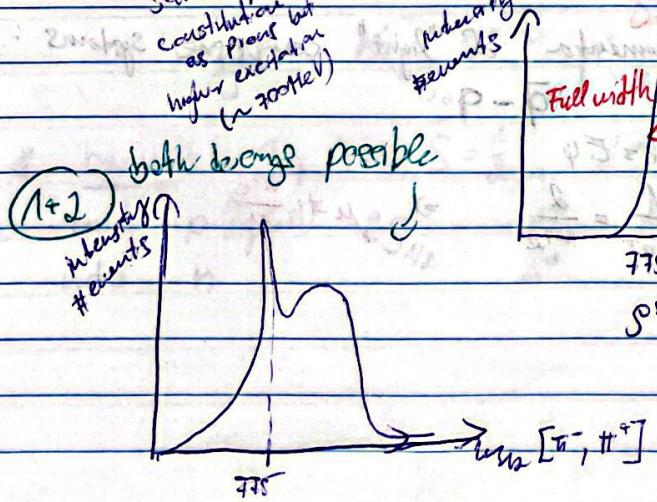
(2)

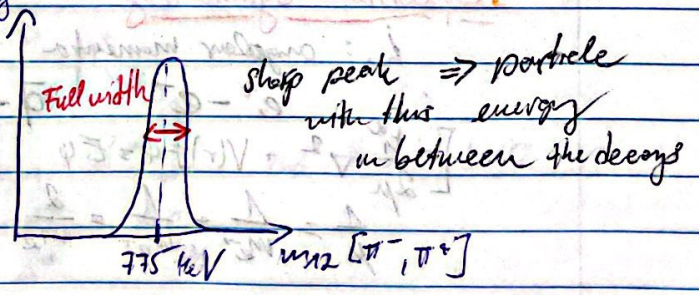


} less freedom in their energies because they have to be able to be S^0

same quark constitution as proton but higher excitation (≈ 300 MeV)

both decays possible





sharp peak ⇒ particle with this energy in between the decays

S^0 short lifetime → large width

$\Delta E \Delta t \geq \frac{\hbar}{2}$

Conservation laws

- energy
- momentum
- charge [in units of e] — additive quantum number
  - can be just added together
  - sign change when matter $\leftrightarrow$ antimatter
- lepton number $L_{e,\mu,\tau}$
- baryon number $B = \frac{1}{3}[N_q - N_{\bar{q}}]$
- strangeness $S = -[N_s - N_{\bar{s}}]$
- charm $C = [N_c - N_{\bar{c}}]$
- beauty $\tilde{B} = -[N_b - N_{\bar{b}}]$
- truth $T = [N_t - N_{\bar{t}}]$

discovery of charmonium $c\bar{c}$
name: J/ψ meson
but roughly same time (slightly known after first)
< Brookhaven (Ting) $c\bar{c} = J$
Stanford (Richter) $c\bar{c} = \psi$
↳ gave: ~~beta~~ J

Strong, Elmag. - $q\bar{q}$ pairs created/annihilated
- flavoured conserved

Weak - also capable of $q\bar{q}$ pair creation/annihilation
- can change flavour
- cannot change matter into antimatter
- can produce leptons via $W^{+/-}, Z$

$\Sigma^+ \to p^+ + \pi^0 = uus \to uud + u\bar{u}d\bar{d}$
$\to n^0 + \pi^+ = udd + u\bar{d}$
$\to \Lambda^0 + e^+ + \nu_e = uds + \text{leptons}$

$s \to d + d\bar{d}$ pair
$u \to d$
$\hookrightarrow W^+ \to e^+ + \nu_e$

Spatial symmetry

L: angular momenta of "light" composite systems:

$e^+ - e^-$, $\bar{q} - q$

$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right]\psi = E\psi$

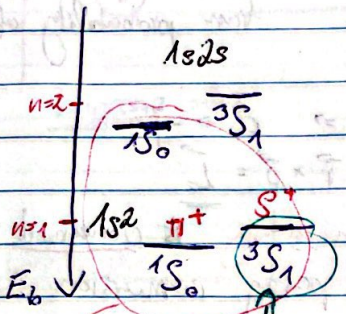
$\frac{1}{\mu} = \frac{1}{m_{e^-}} + \frac{1}{m_{e^+}} = \frac{2}{m_e} \Rightarrow \mu = \frac{m_e}{2}$

hydrogen-like ~~atom~~ nucleus: $n=1$ $L=0$

$n=2$ $L=0,1$

but 2 spins ⇒ closer to He

★ positronium $e^+ - e^-$



→ energies very close together → hard to distinguish

- not as H w He because equivalent electrons can't have same m_s

e^+e^- can have aligned spins as they are not equivalent since they are different particles

lowest 3 levels are all S & all have $L=0$ (same for all)

↳ when considering light elementary particles, we take $L=0$

↳ nice because then symmetric spatial Ψ is symmetric given by $(-1)^L$

$\Rightarrow \bar{J} = \bar{L} + \bar{S}$, $L=0$ $\Big\}$ $\bar{J} = \bar{S}$ → true for light particles

$\Rightarrow \bar{J}$ often called spin of el. part. or hadron spin

★ mesons

$u\bar{d}$: π^+ ($^1S_0$) ground — excitation → S^+ ($^3S_1$) 1st excitation

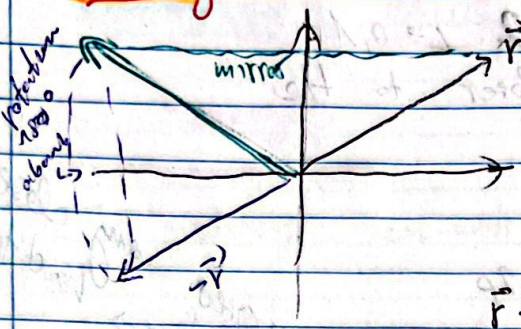
$u\bar{s}$: K^+ ($^1S_0$) → ρ^+ ($^3S_1$)

★ baryons $3q$: $S = \frac{1}{2}$, $S = \frac{3}{2}$ and lowest: $L=0$

uud p (lightest) $^2S_{1/2}$ Δ^+ $^4S_{3/2}$

udd n Δ^0

Parity $\vec{r} \to -\vec{r}$



- all laws of nature are invariant under rotation
- (?) mirroring
  - ↳ if it is, we can see that from probability of event

$\vec{r} \to -\vec{r}$

$\vec{v} \to -\vec{v} \Rightarrow \vec{p} \to -\vec{p}$

$\vec{L} = -\vec{r} \times -\vec{p} = \vec{r} \times \vec{p} = \vec{L}$

⇒ angular momentum is conserved under parity conversion

⇒ same goes for spin

Parity operator

$\hat{P}\,\psi(r,t) = P_a\,\psi(-r,t) = P_a(-1)^L\,\psi(r,t)$

- ↳ wavefunction of a single particle A (~~fermion~~/quark)
- ↳ intrinsic eigenvalue of particle A

$\hat{P}^2\,\psi(r,t) = \psi(r,t) = P_a^2\,\psi(r,t)\,(-1)^{2L}$, $(-1)^{2L} = 1$

$\Rightarrow P_a^2 = 1$

$\Rightarrow P_a = \pm 1$

by convention? $P_{e^-} = P_{\mu^-} = P_{\tau^-} = P_q = 1$

$P_{e^+} = P_{\mu^+} = P_{\tau^+} = P_{\bar{q}} = -1$

mesons $P_{meson} = (-1)^L P_q P_{\bar{q}} = (-1)^L \cdot 1 \cdot (-1) = (-1)^{L+1}$

for lightest mesons: $L = 0$

$\Rightarrow P_{meson} = -1$

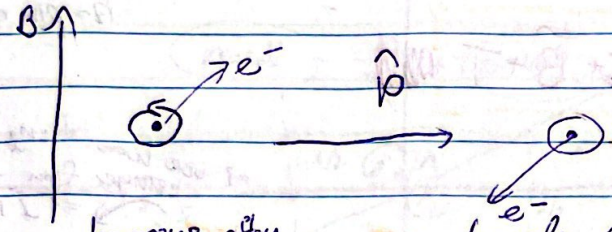
baryons $P_{baryon} = P_{q_1} P_{q_2} P_{q_3} (-1)^{L_{total}} = (-1)^{L_{total}}$

for baryons (& antibaryons)

$= 1$ for lightest baryons

✡ Madame Wu experiment

$^{60}Co \xrightarrow{\beta^-} {}^{60}Ni + e^- + \bar{\nu}_e$



measure electron emission in upper/lower hemisphere

happens often — barely occurs ⇒ parity violation

⇒ event happens more in one direction than the opposite

Charge Conjugation (C parity)

particle ↔ anti-particle

- without changing spatial characteristic

$\hat{C}\,\pi^+ = \hat{C}\,(u\bar{d}) = \bar{u}d = \pi^-$

not the same thing!

⇒ $\pi^{+/-}$ are not eigenstates of the $\hat{C}$ operator

⇒ we need neutral particles which are their own antiparticles (not all neutral antiparticles) to be the eigenstates of $\hat{C}$

↳ ✡ $\pi^0 = u\bar{u} + d\bar{d}$ → $L=0, S=0$ because lowest (singlet) spin

✡ e^+e^- positronium ⇒ $C_{\pi^0} = 1$

✡ ρ^0 ⇒ $L=0, S=1$ ⇒ $C_{\rho^0} = -1$

$\hat{C}^2 \psi_a = C_a^2 \psi_a \Rightarrow C_a = \pm 1$

$\hat{C}$

✡ $e^+ \ldots e^- \xrightarrow{\hat{C}} e^- \ldots e^+$

spatially the same as $r \to -r$

⇒ Symmetry of spatial part: $(-1)^L$

but spin unaffected

$S=1$ { $M_S=1$ $\uparrow\uparrow$; $M_S=0$ $\uparrow\downarrow + \downarrow\uparrow$; $M_S=-1$ $\downarrow\downarrow$ } symmetric ⇒ symmetry for spin $(-1)^{S+1}$

$S=0$, $M_S=0$ $\uparrow\downarrow - \downarrow\uparrow$ antisymmetric

$(-1)^L (-1)^{S+1} = (-1)^{L+S+1}$ doesn't quite work ⇒ extra (-1) from fermion ↔ antifermion (Ref. QM) ⇒ $(-1)^{L+S} = C$

Isospin: hypercharge Y, azimuthal isospin I_3

↳ ~ projection of isospin on symmetry axis

$$Y = B + S + C + \tilde{B} + T$$

$$I_3 = Q - \frac{Y}{2}$$

as we wanted I_3 to range from $-I$ to $+I$ ⇒ I range from $-I_3$ to I_3

for quarks:

	B	S/C/B̃/T	Y	Q	I_3	I
d	1/3	0	1/3	-1/3	-1/2	1/2
u	1/3	0	1/3	2/3	1/2	1/2
s	1/3	-1	-2/3	-1/3	0	0
c	1/3	1	4/3	2/3	0	0
b	1/3	-1	-2/3	-1/3	0	0
t	1/3	1	4/3	2/3	0	0

I perpendicular to z-axis or $I_3 \neq 0$

⇒ u/d : isospin 1/2 (multiplet) duplet (more conservedly)

hadronic spin $P = (-1)^L$

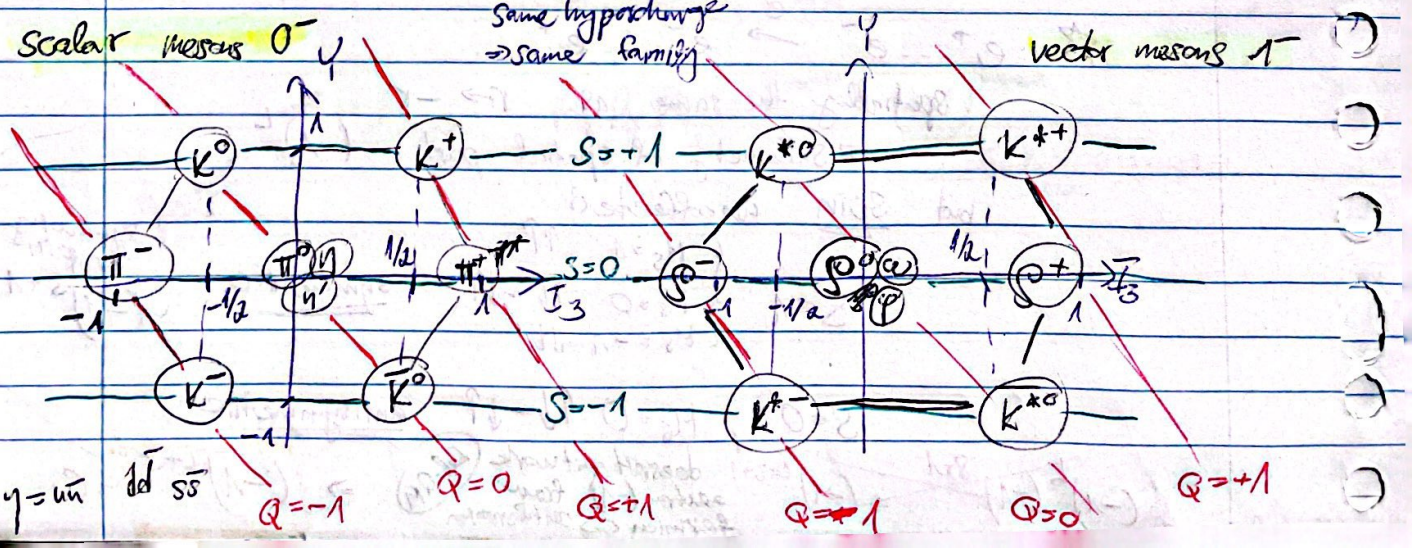
☆ L=0					
S=0	π pions	J=0	-1	0^-	scalar mesons
S=1	ρ rhos	J=1	-1	1^-	vector

using u,d,s ⇒ octet

	0^-	1^-		Y	I_3	I
$u\bar{d}$	π^+	ρ^+	B=0 S=0 C=0 B̃=0 T=0	0	1	1
$u\bar{u}/d\bar{d}$	π^0	ρ^0		0	0	=1
$\bar{u}d$	π^-	ρ^-		0	-1	1

Kaons

same hypercharge ⇒ same family

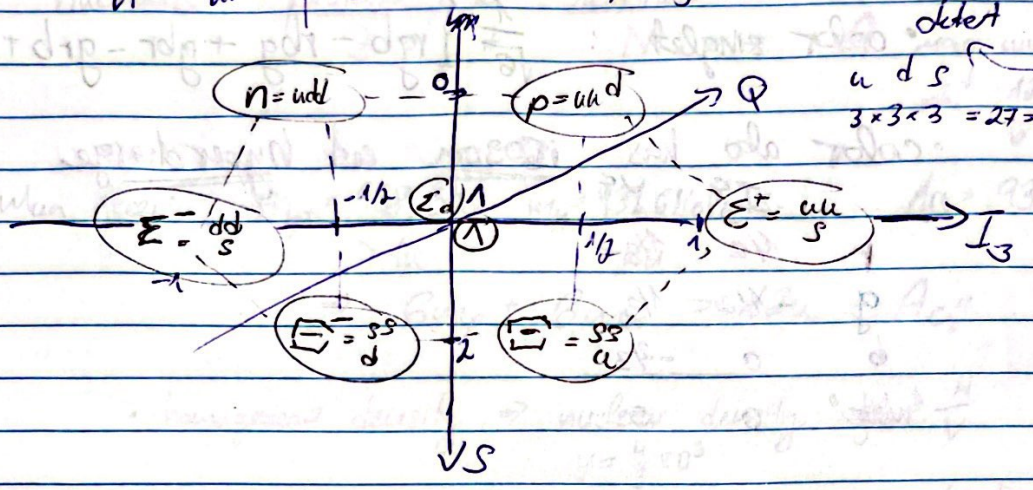


	Q	Y	I_3	I
p uud	1	1	1/2	1/2
n udd	0	1	−1/2	1/2

$\Rightarrow S = \frac{1}{2}, \frac{3}{2}$ ↓ octet, ↓ decuplet

u d s

$3 \times 3 \times 3 = 27 = 10 + 8 + 8 + 1$



↳ u d s

spins: $\frac{1}{2} + \frac{1}{2} \rightarrow 0, 1$

$+\frac{1}{2} \rightarrow 1/2$

$+\frac{1}{2} \rightarrow 1/2, 3/2$

2x in 1/2 octet → 1x in 3/2 decuplet

↳ uud, uus, ssd, ssu, ddu, dds

6 x in 1/2 octet — 6 x in 3/2 decuplet

- first couple spin of same flavour q

S = 0 spin system anti-symmetric under exchange

S = 1 — " — symmetric — " —

+ 1/2

↳ ~~S = 0 → 1/2~~ doesn't exist (not in experiment)

S = 1 → 1/2, 3/2 ⇒ spin symmetric

↳ uuu, ddd, sss — 0x in 1/2 octet — 3x in 3/2 decuplet

— " — $S = \frac{3}{2}$, $m_S = \frac{1}{2}$ for all q's

↳ spin system is symmetric

Symmetric? but we have fermions - Pauli? !!

these are lightest baryons ⇒ L = 0 ⇒ also symmetric spatial

⇒ problem ⇒ introduce new quantum number → to make antisymmetric

1965 Greenberg

Color r g b

- color singlet : $\frac{1}{\sqrt{6}}\{rgb - rbg + gbr - grb + brg - bgr\}$

- color also has isospin and hypercharge

	I_3^c	Y^c
r	1/2	1/3
g	-1/2	1/3
b	0	-2/3
"white"	0	0

Nucleus

nucleons: protons Z & neutrons N $= A$ mass number

ref. $^{12}_{6}C$: $A = 12.0000\ldots u$

$1u = 931.5\ MeV$

when free: $m_p = 938.3 MeV$ $m_n = 939.6 MeV$ vs.

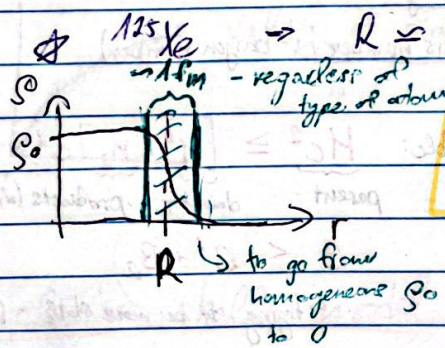
$> 1u$ $> 1u$

$\Rightarrow 6m_p + 6m_n > 12u = A_{C^{12}_6}$

- homogeneous density $\Rightarrow$ nuclear density $\rho_0 = \frac{A}{V}$

$V = \frac{4}{3}\pi R^3$

$\Rightarrow R \simeq 1.2\, A^{1/3}\ [fm]$



$\sim 1 fm$ - regardless of type of atom

$$\rho(r) = \frac{\rho_0}{1 + e^{-(R-r)/a}}$$

Binding energy

mass of atomic isotope

$$B(N,Z) = [N m_n + Z m_H - M]c^2$$

$m_p + m_e$

liquid drop model parametrization of B

$Z = N$ even-even -11.2

odd-even / odd-odd 0 / 11.2

$$B = aA - bA^{2/3} - d\frac{Z^2}{A^{1/3}} - s\frac{(N-Z)^2}{A} - \frac{\delta}{A^{1/2}}$$

MeV: 15.4 18.3 0.7 23.2

cohesive energy of liquid drop $\propto V \propto R^3 \propto A$

other terms: corrections to behaving like a droplet

surface correction $A^{2/3} \propto R^2$

~ surface tension

bc strong force only over short distance

$\Rightarrow$ surface nucleons have less neighbors

$\Rightarrow$ less strong force affecting them

$\Rightarrow$ lower binding energy

$\frac{Z^2}{A^{1/3}} \propto \frac{Z^2}{R}$ Coulomb repulsion between protons

$\Rightarrow$ protons repelling each other

$\Rightarrow$ lower binding energy

reducing imbalance between number of protons and neutrons $\Rightarrow$ try for $N \approx Z$

$\hookrightarrow$ binding is stronger for $p-n$ than for $n-n$ and $p-p$

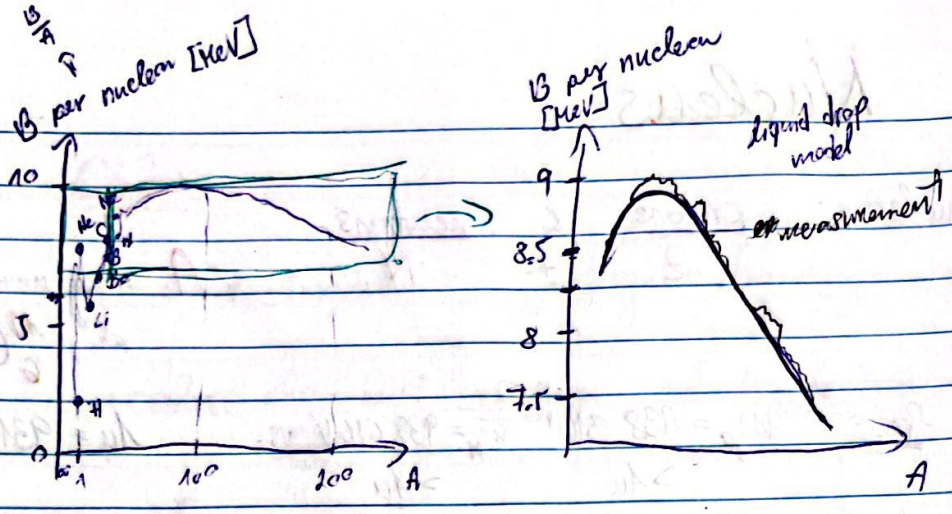
(Pauli exclusion - equivalent p/n's cannot be as close)

acting against each other: { trying to min. $\#p^+$ / trying to $\#p \approx \#n$ }

odd	odd		
15	13	13	13
n	p	n	p
14	14	14	12
even	even	even	even

preferred state

why? eh



Decay: α, β, γ

- conserves: energy, momentum, charge, mass number (= baryon number)

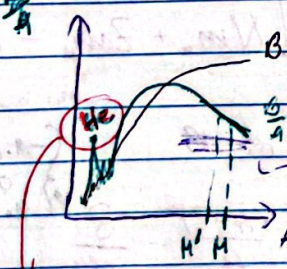
- for decay to be possible: $Mc^2 \geq [M' + M_2]c^2$

  parent — daughter — products (α, β, γ)

$$B < B' + B_2$$

↳ trying to be more stable – bound more closely

↳ ~ minimization of energy (binding energy = negative energy



although binding energy per nucleon decreases, the total binding energy increases

→ we need B_2 to tip the inequality

↳ otherwise unstable $B' < B$

high binding energy → sufficient to compensate for the loss in binding energy due to decrease in atomic number → for high A

α

$$^{A}_{Z}X \rightarrow {}^{A-4}_{Z-2}X' + {}^{4}_{2}He$$

β

$\beta^- \rightarrow e^-$, $\beta^+ \rightarrow e^+$

β^- : $n \rightarrow p + e^- + \bar{\nu}_e$

$$^{A}_{Z}X \rightarrow \left({}^{A}_{Z+1}X'\right)^{+} + e^- + \bar{\nu}_e$$

$Q_{\beta^-} = [m_X - m_{X'}]c^2$

β^+ requires more energy → $m_{X'} + 2m_e$

$Q_{\beta^+} = [m_X - m_{X'} - 2m_e]c^2$

β^+ : $p \rightarrow n + e^+ + \nu_e$

$$^{A}_{Z}X \rightarrow {}^{A}_{Z-1}X' + e^- + e^+ + \nu_e$$

β^- doesn't require extra energy $\Rightarrow$

$$\Rightarrow Mc^2 = [Nm_n + Zm_H]c^2 - B = [Nm_n + Zm_H]c^2 - aA + bA^{2/3} + d\frac{Z^2}{A^{1/3}} + s\frac{(N-Z)^2}{A} + \frac{\delta}{A^{3/4}}$$

$N = A - Z$; $s\frac{(A-2Z)^2}{A}$

$$Mc^2 = \underbrace{Am_n c^2 - aA + bA^{2/3} + sA + \frac{\delta}{A^{1/2}}}_{\alpha} + Z\underbrace{[-(m_n - m_H)c^2 + 4s]}_{\beta} + Z^2\underbrace{\left[\frac{d}{A^{1/3}} + \frac{4s}{A}\right]}_{\gamma}$$

$$Mc^2 = \alpha - \beta Z + \gamma Z^2$$

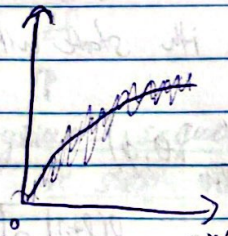
$$\frac{\partial Mc^2}{\partial Z} = -\beta + 2\gamma Z = 0 \Rightarrow Z = \frac{\beta}{2\gamma} = \frac{(m_n - m_H)c^2 + 4s}{\frac{2d}{A^{1/3}} + \frac{8s}{A}} = \frac{A}{2}\left[\frac{4s + (m_n - m_H)c^2}{4s + dA^{2/3}}\right]$$

$(m_n - m_H)c^2 = 0.8\,MeV$; $dA^{2/3} \approx 0.7A^{2/3}\,MeV$

optimal number of protons to be stable

for $A \geq 2$: $dA^{2/3} > (m_n - m_H)c^2$

$\Rightarrow Z \leq \frac{A}{2}$



$N = A - Z$

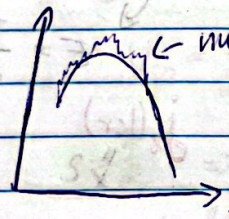
$A - N \leq \frac{A}{2}$

$A - \frac{A}{2} \leq N$

$N \geq \frac{A}{2}$

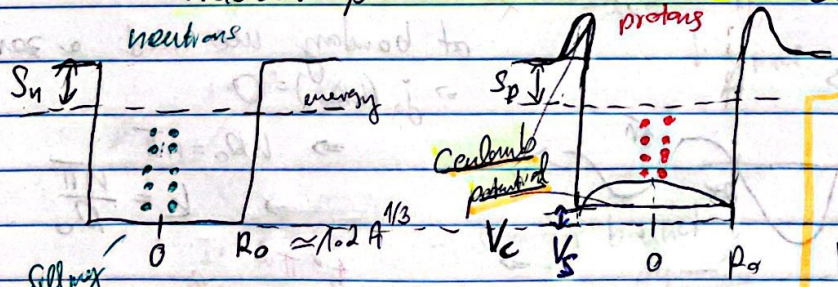
$\Rightarrow N \geq \frac{A}{2}$

Nuclear shell model



$\Rightarrow$ "magic numbers"

Nuclear potential wells = Wood-Saxon potential



$$V_c = \frac{(Z-1)e^2}{4\pi\varepsilon_0 r}, \quad r > R_0$$

$$V_c = \frac{(Z-1)e^2}{4\pi\varepsilon_0 R_0}\left(\frac{3}{2} - \frac{r^2}{2R_0^2}\right), \quad r \leq R_0$$

filling n, p in pairs with $S=0, L=0$ per pair

$\Downarrow$

energetically favorable

Statistical "shift" between neutrons and protons because there's more neutrons than protons – n-n and p-p same strong but there's more n's $\Rightarrow$ deeper neutron well

$S_{n,p}$ = separation energy = = needed to remove one n/p from nucleus ~ransfer energy

Similar for n, p because β^+: $p^+ \to n + e^+ + \nu$ requires extra E, β^- doesn't $\to$ symmetry around until equal $\Rightarrow S_n \simeq S_p$

• similarly as for atom, the nuclear potential is spherically symmetric ⇒ indep. of θ, ϕ

⇒ spherical harmonics $Y_{lm}(\theta, \phi)$

⇒ $l = 0, 1, 2, 3, 4, \ldots$ = s, p, d, f, g, ...

$-l \leq m_l \leq l$

but there's not a series of integer principal quantum numbers "n"

- first s → 1s
- first p → 1p
- first d → 1d

⇐ number at front indicates ith state with certain l

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi \quad \Rightarrow \psi = R\, Y_{lm}(\theta, \phi)$$

For radial: $$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)R - \frac{l(l+1)}{r^2}R\right] = ER$$

$$-\frac{\partial^2 R}{\partial r^2} - \frac{2}{r}\frac{\partial R}{\partial r} + \frac{l(l+1)}{r^2}R = \frac{2m}{\hbar^2}ER = k^2 R$$

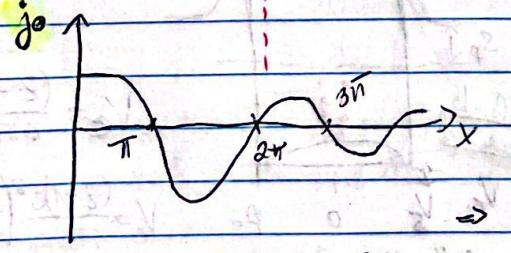
↳ Solution: spher. Bessel functions $j_l(kr)$

↳ $E = \frac{\hbar^2 k^2}{2m}$

x

$l = 0$ $\quad j_0(x) = \frac{\sin x}{x}$

$l = 1$ $\quad j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}$



1 2 3 ...

at boundary we need a zero.

$\Rightarrow j_0(kR_0) = 0$

$\Rightarrow kR_0 = n\pi$

$\Rightarrow k = \frac{n\pi}{R_0}$

$\Rightarrow E = \frac{\hbar^2 \pi^2}{2mR_0^2} n^2$

l		x_l			
0	s	π	2π	3π	...
1	p	4.49	7.73	10.9	
2	d	5.76	9.1	--	
3	f	6.99	10.42	--	
4	g	8.18	--	--	
5	h	9.36	--	--	

order: π 4.49 5.76 2π 6.99 7.73 8.18

⇒ 1s 1p 1d 2s 1f 2p 1g

9.1 9.36 3π 10.42 10.9

2d 1h 3s 2f 3p ---

X_e	"name"	# states	total
$\hbar\omega$	1s	2	2
4.49	1p	6	8
5.76	1d	10	18
$2\hbar\omega$	2s	2	20
6.99	1f	14	34
7.73	2p	6	40
8.18	1g	18	58
9.1	2d	10	68
9.36	1h	22	90
$3\hbar\omega$	3s	2	92
10.42	2f	14	106

$\Rightarrow$ Magic numbers
2, 8, 20, 28, 50, 82, 126
✓ ✓ ✓
in list

↑ generic sequence of shell filling

Spin - Orbit interaction – very very strong effect in nucleus

$\vec{j} = \vec{l} + \vec{s}$

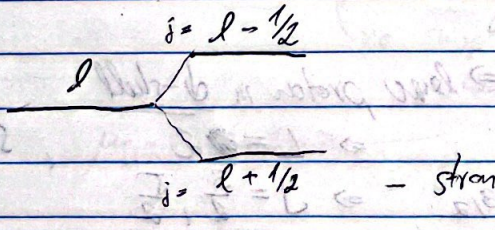
$V_{so} \sim$ MeV

$$V_{so} = \frac{1}{2} A^{nucl} \cdot [j(j+1) - l(l+1) - s(s+1)]$$

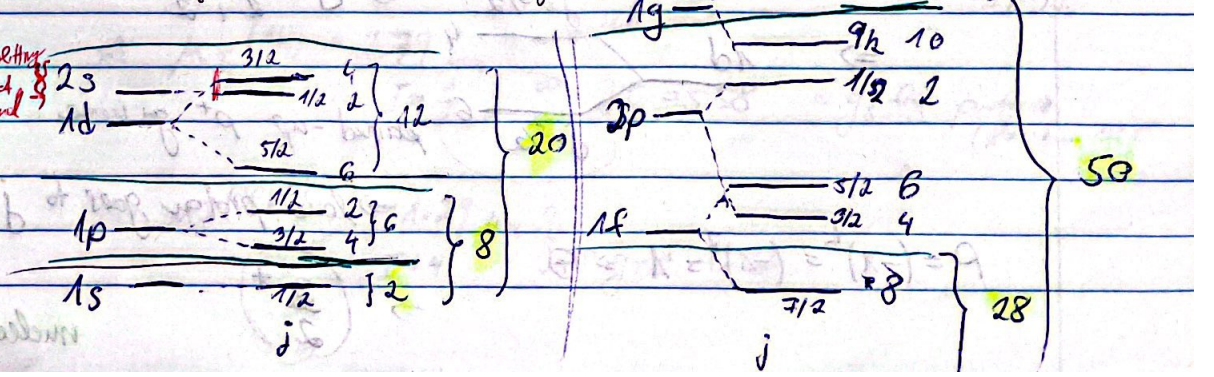
$s = \frac{1}{2} \Rightarrow j = l - \frac{1}{2}, l + \frac{1}{2}$

- $j = l + \frac{1}{2} \Rightarrow V_{so} = \frac{1}{2} A^{nucl} \, l$
- $j = l - \frac{1}{2} \Rightarrow V_{so} = \frac{1}{2} A^{nucl} (l-1)$

$\downarrow$ $A^{nucl} < 0$



– stronger bound



Total angular momenta L, S, J

- nucleons form pairs of $L=0, S=0 \Rightarrow J=0$
  = **homonucleonic pairs**
  - either 2 neutrons or 2 protons
- in **even-even** nuclei, all nucleons can pair up $\rightarrow$ for all $L=0, S=0 \Rightarrow J=0$
  $\Rightarrow$ also for whole nucleus $L=0, S=0, J=0$
  $\hookrightarrow$ parity $P = (-1)^0 = 1$
  $\Rightarrow$ 0^+

- in **even-odd** nuclei, only odd proton/neutron relevant
  $\hookrightarrow$ all but one can pair up to $L=0, S=0$
  $\Rightarrow$ only 1 left $\hookrightarrow$ which determines L, S, J
  $S = \frac{1}{2}$, $L = l$, $J = L \pm \frac{1}{2}$
  (see nuclear shells)

J = nuclear spin
$\Rightarrow$ how the nucleus shows itself to the outside world

- in **odd-odd** nuclei, no simple rule to find total L, S, J
  uncommon in nature
  only stable odd-odd: ☆ ${}^{2}_{1}D$, ${}^{6}_{3}Li$, ${}^{10}_{5}B$, ${}^{14}_{7}N$

For $J = L \pm \frac{1}{2}$: strong spin-orbit interactions
$\Rightarrow J = L + \frac{1}{2}$ strongest bond

☆ ${}^{31}_{15}P$: 15 p, 16 n
$\hookrightarrow$ even $\Rightarrow L = S = 0$, $J = 0$

1s : 2
1p : 6
1d : 10
$\rightsquigarrow 1s^2\, 1p^6\, 1d^7$ $\Rightarrow$ lone proton in d-shell
$\Rightarrow L = 2$, $S = 1/2$
$\Rightarrow J = \frac{3}{2}, \frac{5}{2}$

7 pairs of $L = S = J = 0$
1 lone proton

$\Rightarrow$ 1d: $j = 3/2$ (4), $j = 5/2$ (6)
paired-up p^+ go here
$\Rightarrow$ lone proton goes to $j = 3/2$
$\Rightarrow J = 3/2$

$P = (-1)^L = (-1)^2 = 1 \Rightarrow \oplus$

$\Rightarrow \left(\frac{3}{2}^+\right)$

nuclear spin

$^{31}_{13}Al$: 13p⁺, 18n°

$1s^2$ ↓ → L=0, S=0, J=0

$1p^6$ 12 protons in pairs, L=0, S=0, J=0

$1d^5$ 1 lone proton in 1d, L=2

fitting into $j = 5/2$ ⇒ $\frac{5}{2}^+$ nucleus

$P = (-1)^2 = 1$

Hyperfine Structure (F, M_F)

- nuclear spin couples/aligns to the total angular momentum of the electrons

total ang. momentum $\vec{J}$ ⇒ $\vec{J} + \vec{J} = \vec{F}$ ⇒ $\boxed{\vec{J} + \vec{I} = \vec{F}}$

use $\vec{I}$ to distinguish it from total ang. mom. of e^- in atomic orbit

- $\vec{I}$ couples to $\vec{J}$ via its nuclear mag. moment

$\vec{\mu}_{nucl} = \frac{\mu_N}{\hbar} \sum_{i=1}^{A} (g_l \vec{l}_i + g_s \vec{s}_i)$ (sets scale, similar to μ_B)

for protons 1, for neutrons 0 (electrons 1)

5.58 protons, −3.83 neutrons (2 electrons)

$\vec{\mu}_N = \frac{e\hbar}{2m_p} = \frac{m_e}{m_p}\frac{e\hbar}{2m_e} = \frac{m_e}{m_p}\mu_B$ ($\mu_B = \frac{e\hbar}{2m_e}$)

⇒ $\vec{\mu}_N = \frac{m_e}{m_p}\mu_B \approx \frac{1}{1836}\mu_B$

$\vec{\mu}_I = \vec{\mu}_{nucl} = g_I \mu_N \frac{\vec{I}}{\hbar}$

vs. fine structure: no minus sign; no simple generic expression for g_I ⇒ tabulated in units of μ_N

$\mu_{I,z} = g_I \mu_N m_I$ and for $m_I = I$ (largest m_I value) $-I, \dots, I$

$\mu_I(^1H) = 2.79\,\mu_N$, $I = \frac{1}{2}$ } tabulated ⇒ $g_I = 5.58$ = g_s for protons ($l = 0$ for 1H)

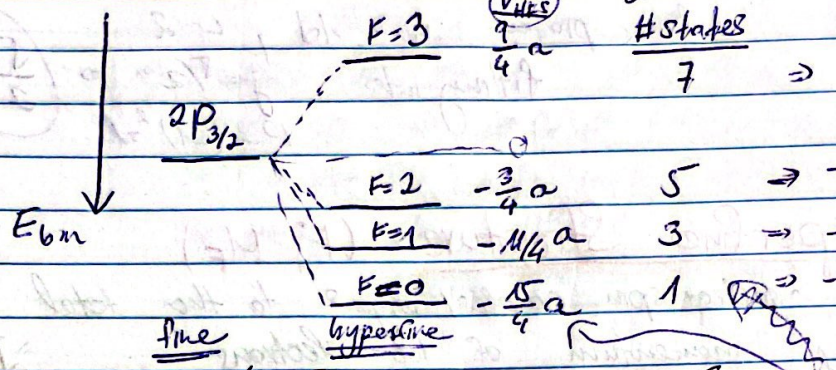
$\mu_I(^{40}K) = -1.29\,\mu_N$, $I = 4$ } ⇒ $g_I = -0.32$

$\vec{F} = \vec{J} + \vec{I}$

fine structure level → split into 4 hyperfine structure

★ $Na(3p) \rightarrow {}^2P_{3/2} \Rightarrow J = \frac{3}{2}$ { $F = 0, 1, 2, 3$

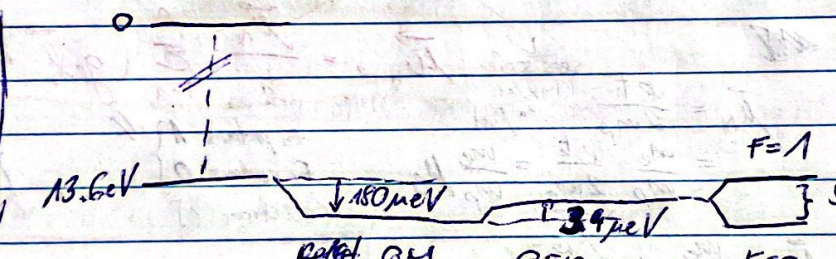
tab: $I = \frac{3}{2}$



fine structure: $V_{SO} = \frac{1}{2} A[J(J+1) - L(L+1) - S(S+1)]$

hyperfine structure: $V_{HFS} = \frac{1}{2} a[F(F+1) - J(J+1) - I(I+1)]$

★ $H(1s)$ config. $1s$ term ^2S level $^2S_{1/2}$, $I = \frac{1}{2} \Rightarrow F = 0, 1$



but heavily forbidden

⇝ occurs only $2.6 \times 10^{-15}\ s^{-1}$

↳ very weak but there's so much hydrogen that it's actually common

$\Delta E = 5.8\mu eV = hf$

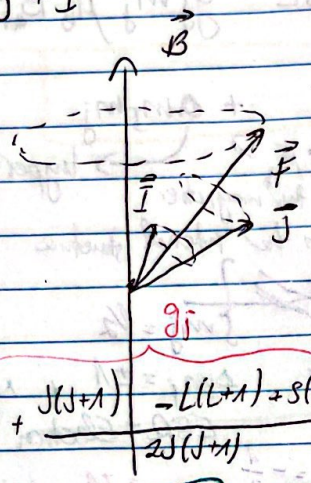
$\Rightarrow f = \frac{\Delta E}{h} = 1.42\ GHz$ H clock

$= 0.047\ cm^{-1}$

$\Rightarrow \frac{1}{0.047}\ cm = 21\ cm$ line

Hyperfine structure in a magnetic field

$\vec{F} = \vec{J} + \vec{I}$



Zeeman effect

$\Delta E_{HFS} = g_F m_F \mu_B B$

$g_F = g_J \frac{F(F+1) - I(I+1) + J(J+1)}{2F(F+1)} - g_I \frac{\mu_N}{\mu_B} \frac{F(F+1) - J(J+1) + I(I+1)}{2F(F+1)}$

$g_J = 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}$

$\frac{\mu_N}{\mu_B} \approx \frac{1}{2000}$ can be neglected usually (~2000x smaller)

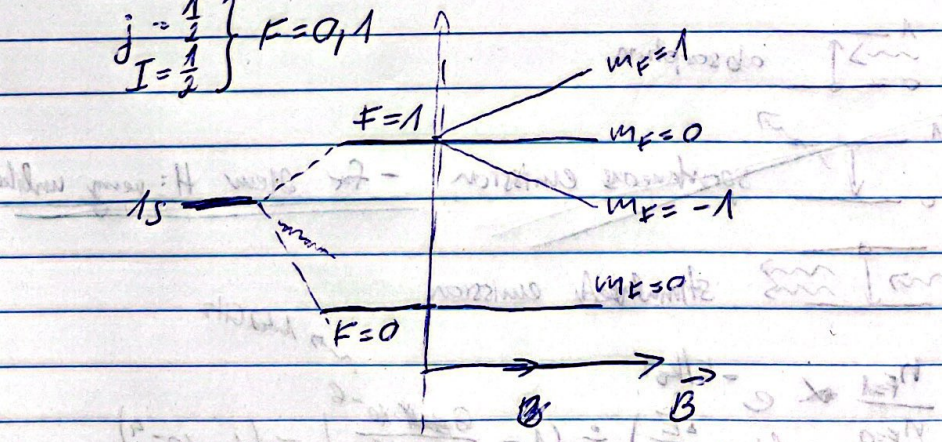
$\mu_B g_F = \mu_B g_J \frac{F(F+1) - I(I+1) + J(J+1)}{2F(F+1)} - \mu_N g_I \frac{F(F+1) - J(J+1) + I(I+1)}{2F(F+1)}$

$\Rightarrow$ $g_F = g_J \frac{F(F+1) - I(I+1) + J(J+1)}{2F(F+1)}$

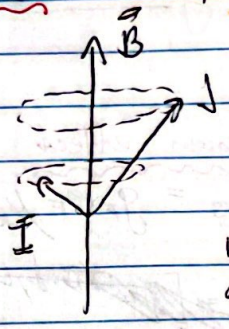
☆ $H(1s)$

$L = 0, \; S = \frac{1}{2}$

$j = \frac{1}{2}$, $I = \frac{1}{2}$ $\Rightarrow F = 0, 1$



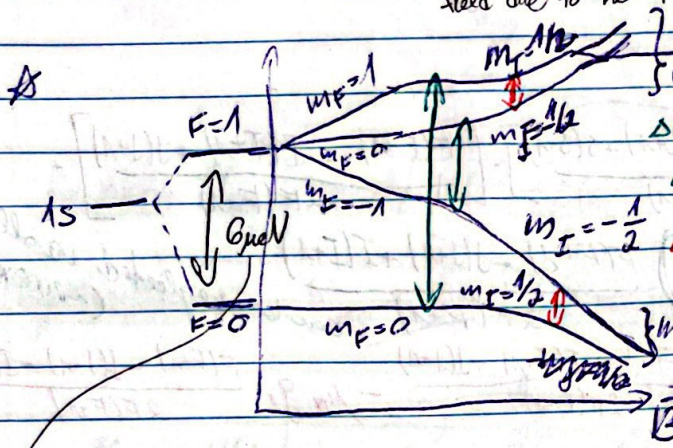
at higher B : I, J coupling breaks (~Paschen-Bach)



$$\Delta E = g_j m_j \mu_B B_{ext} - g_I m_I \mu_N B_{ext} + a m_I m_j$$

neglected in drawing below ~2000x weaker

nuclear mag. μ experiencing the magnetic field due to the internal structure → hyperfine structure constant



$\Delta m_j = \pm 1$, $\Delta m_I = 0$

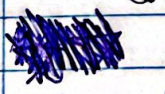
ESR = Electron Spin Resonance

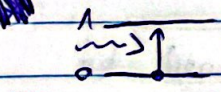
$\Delta m_I = \pm 1$, $\Delta m_j = 0$

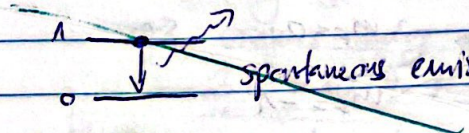
NMR = Nuclear Magnetic Resonance

= MRI = Mag. Resonance Imaging

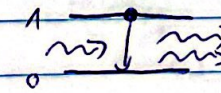
- oscillating magnetic fields allow for transitions
  - ↳ condition: $\Delta m = \pm 1$
    - ↳ either m_I = const. and $\Delta m_j = \pm 1$
    - or $\Delta m_I = \pm 1$ and Δm_j = const







– for 21cm H: very unlikely



$$\frac{n_{F=1}}{n_{F=0}} \propto e^{-E/k_B T}$$

$$\approx \left(1 - \frac{\Delta E}{k_B T}\right) \doteq \left(1 - \frac{6 \cdot 10^{-6}}{2.5 \cdot 10^{-2}}\right) \approx (1 - 10^{-4})$$

1.42 GHz