Structure of Matter

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

$$\underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x)}_{\text{kinetic energy}} + \underbrace{V(x)}_{\text{potential energy}}\Psi(x) = E\Psi(x)$$

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

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

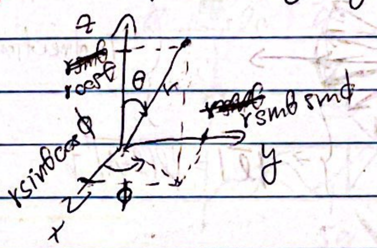
H-like systems : 1 nucleus, 1 electron

$\#$ H, He^+, Ne^{9+}

$V(r) = \frac{-Ze^2}{4\pi\varepsilon_0 r}$ — spherically symmetric $\Rightarrow$ use spherical coord.

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

$[0,2\pi)$ ϕ = azimuthal angle



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

μ ← reduced mass

$$\boxed{\mu = \frac{mM}{m+M}} \approx m \qquad \boxed{\frac{m_{el}}{m_{proton}} = \frac{1}{1836}}$$

m ← mass of electron; M ← mass of nucleus

$\Rightarrow$ M is more than 2000x larger than m

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

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

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

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

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

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

$Y_{lm}(\theta,\varphi) = \Theta_{lm}(\theta)\,\Phi_m(\varphi)$ ↳ $\boxed{\Phi_m = \frac{e^{im\varphi}}{\sqrt{2\pi}}}$

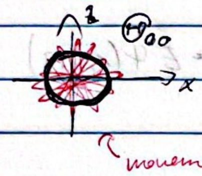
- sign of m says the ~~rotation~~ direction of rotation about $\hat{z}$

Θ_{lm}: probability to find particle at certain angle θ from z-axis

$\boxed{\begin{matrix} -l \leq m \leq l \\ 0 \leq l \leq n-1 \end{matrix}}$

- 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 if rotates along a circle ⇒ not the case

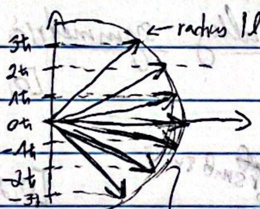
$\hat{l}_z$ = "projection of l onto z-axis"

$l = 3$

$|\vec{l}| = 2\sqrt{3}\hbar$

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

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



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

Energy

$E_{nlm} \approx E_n = -\frac{Rhc\,Z^2}{n^2} \approx \frac{-2.2\cdot 10^{-18}}{n^2} Z^2$

Bohr Model (↑ $\approx$); speed of light (c); Rydberg constant (R); $13.6\,\text{eV} = -2.2\cdot10^{-18}$ (Z^2/n^2)

$R = \frac{1}{1+\frac{m}{M}}$

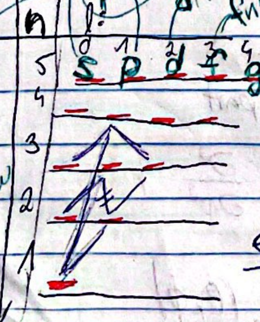
$R \approx 1.1\cdot 10^7\,m^{-1}$

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

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

only one light in transitions ~~and form~~ s-orbitals ⇒ very sharp

sharp, principal, diffuse, fundamental



during (de)excitation l change by 1 ⇒ more excitation levels from s to p because lower binding energy

decay between levels $\Delta l = \pm 1$
↳ -1 >> $+1$ for decay (more likely)

electric dipole/optical transitions
↳ for excitation: $+1$ >> -1 (Δl)

2 ↳ p-type transitions are most common

Radial part of ψ

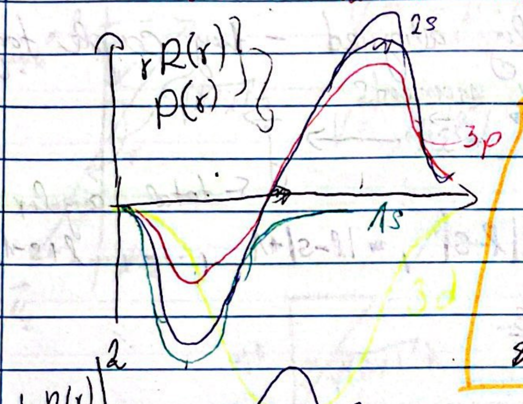
$$\left\{ -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} - \frac{Ze^2}{4\pi\varepsilon_0 r} \right\} P_{nl} = E P_{nl}$$

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

$$d\mathbb{P}(r,\theta,\phi) = |\psi|^2 dV$$
$$= |\psi|^2 r^2 \sin\theta \, dr \, d\theta \, d\phi$$

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

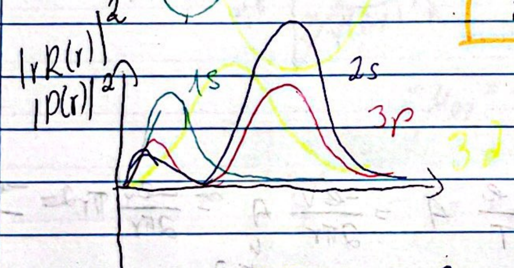
$$d\mathbb{P}(r) = r^2 |R_{nl}|^2 dr = |P_{nl}|^2 dr \Rightarrow \mathbb{P}(r) = |P_{nl}|^2$$

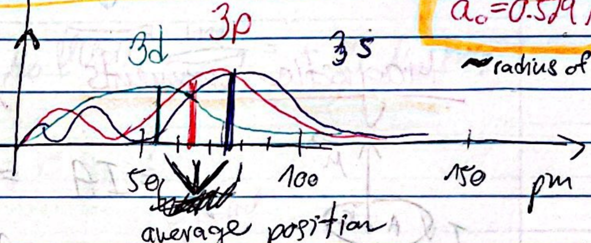


first lobe negative by convention

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

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





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

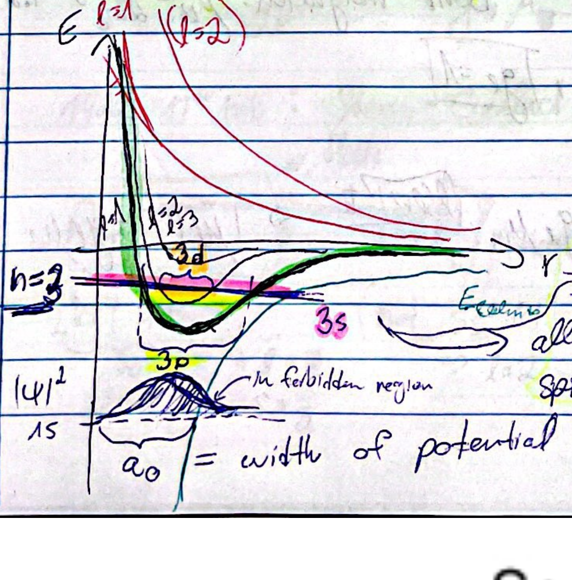
$$\langle f(r) \rangle = \int_0^\infty f(r) \underbrace{|P_{nl}|^2}_{\mathbb{P}(r)} dr$$

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

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

$$\left.\begin{aligned} E_{Coulomb} &= \frac{-Ze^2}{4\pi\varepsilon_0 r} \\ E_{centrifugal} &= \frac{\hbar^2 l(l+1)}{2\mu r^2} \end{aligned}\right\} \text{sum}$$

(μ = mass)



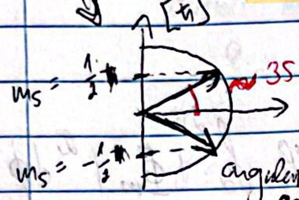
$n=3$ can't have $l=3$ because the well is above $n=3$ energy

all have same binding energy but different spread in options.

a_0 = width of potential well in H (for 1s) ?!

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

$$\Rightarrow \Psi_{n l m_l m_s} = R_{nl} Y_{l m_l} \mathcal{X}_{m_s}$$



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

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

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

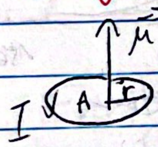
$$\vec{l} + \vec{s} \longrightarrow \vec{j} \leftarrow \text{total angular momentum}$$

$3p$: $l = 1$ $\quad j = |l-s|, |l-s|+1, \dots, l+s-1, l+s$

$s = \frac{1}{2}$

↳ $j = \frac{1}{2}, \frac{3}{2}$

Magnetic moments μ



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

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

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

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

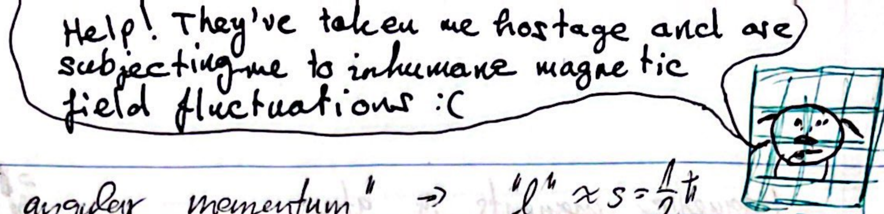
↳ always perpendicular $\quad$ in opposite direction

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

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

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

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

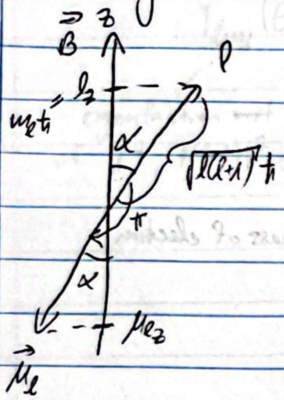


"spin is angular momentum" $\Rightarrow$ "l" $\approx s = \frac{1}{2}\hbar$

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

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

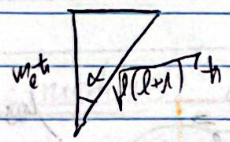
· magnetic moment in external magnetic field



$\boxed{V = -\vec{\mu}\cdot\vec{B}}$ $\quad \mu = \mu_l$ or μ_s

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

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



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

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

$\Rightarrow \boxed{V_l = -g_l \mu_B m_l B}$!

↳ discrete potential energies

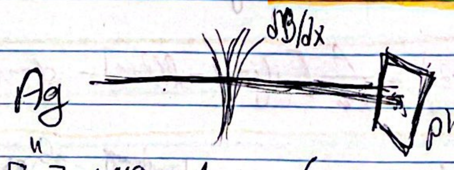
m_l states $= 2l+1$

for spin:

$\boxed{V_s = -g_s \mu_B m_s B}$

$F = -\frac{\partial V}{\partial x} = +g_{l/s} \mu_B m_{l/s} \frac{\partial B}{\partial x}$

1922 17th Feb: Stern - Gerlach



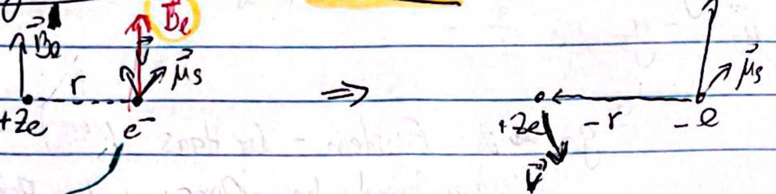
no $\vec{B}$:
w/ $\vec{B}$ field:

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

$\underbrace{[Kr]\ 4d^{10}}_{L=0,\ S=0}\ 5s^1$ $\quad l = 0$, $s = \frac{1}{2}$

(not $5s^2\,4d^9$ as would be expected
↳ $l = 2 \rightarrow m_l = \pm 2, \pm 1, 0$)

Magnetic moments in atom



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

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

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

back transformation to coordinate system with nucleus at origin

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

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

$\mu_B = \frac{e\hbar}{2m}$

$\mu_0\varepsilon_0 = \frac{1}{c^2}$

mass of electron

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

Fine structure

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

λ of photon with energy 1eV

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

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

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

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

$$\Rightarrow \boxed{V_{SO} = \frac{A}{2\hbar^2}\left(\vec{j}^2 - \vec{l}^2 - \vec{s}^2\right) = \frac{A}{2}[j(j+1) - l(l+1) - s(s+1)]}$$

$2l+1 = 3$
$2s+1 = 2$
↳ $2 \cdot 3 = 6$
6 states in 3p

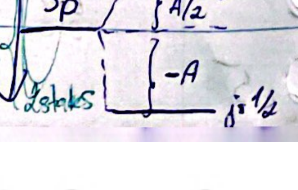
#m_j's is $2j+1$

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

$$\boxed{\begin{aligned} V_{SO}(j = \tfrac{1}{2}) &= -A \\ V_{SO}(j = \tfrac{3}{2}) &= +\tfrac{A}{2} \end{aligned}}$$

energy wrt 3p energy without coupling effects

binding energy



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Addition of Angular Momenta

- two angular momenta j_1, m_1 ; j_2, m_2

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

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

$$\underbrace{Y_{lm_l}(\theta,\phi)\,\chi_{m_s}}_{\text{get definite values for } j, m}$$

Y_{lm_l}: eigenfunction of $\hat{l}^2$, $l(l+1)\hbar^2$ eval

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

$\Rightarrow$ coupled states $|(l\tfrac{1}{2})jm\rangle$

$\hookrightarrow$ eigenfunctions wrt. $\hat{j}^2$ and $\hat{j}_z$ ~~eval~~ $j(j+1)\hbar^2$, with ~~and~~ $\hat{l}^2$ and $\hat{s}^2$ eval

$l(l+1)\hbar^2$; $\frac{3}{4}\hbar^2$

Fine structure

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

$$\boxed{\xi = \frac{1}{2m^2c^2}\,\frac{1}{4\pi\varepsilon_0}\,Ze^2\left\langle\frac{1}{r^3}\right\rangle}$$
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 $\Rightarrow$ $h_{so} = \frac{\xi}{2}(\hat{j}^2 - \hat{s}^2 - \hat{l}^2)$

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

fine structure const.

$$\xi = \frac{\alpha^2}{2}Z^4\left(\frac{1}{4\pi\varepsilon_0}\frac{e^2}{a_0}\right)\left\langle\left(\frac{a_0}{Zr}\right)^3\right\rangle \qquad \boxed{\alpha = \frac{1}{137}}$$

$$\boxed{\xi \propto Z^4}$$

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

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

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

$g_j = ?$

• for weak $\vec{B}$: $\vec{l}$ and $\vec{s}$ precess rapidly about $\vec{j}$

while $\vec{j}$ precesses slowly about $\vec{B}$

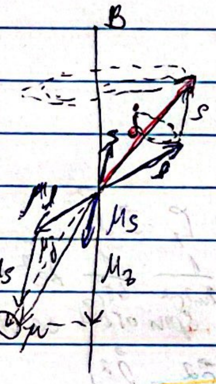
⇒ components of $\vec{l}$ and $\vec{s}$ ⊥ $\vec{j}$ cancel out over ~~per~~ time = many revolutions

⇒ replace $\vec{l}$ and $\vec{s}$ with their projection along $\vec{j}$

→ $(\vec{l}\cdot\hat{j})\hat{j}$ → in dir. of $\vec{B}$: $(\vec{l}\cdot\hat{j})\hat{j}_z$

⇒ avg l_z for coupled states w/ definite j and m:

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



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

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

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

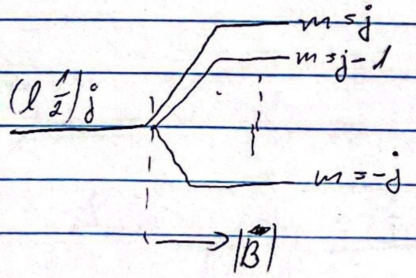
$$\boxed{V_{mag} = \frac{e}{2m}B(l_z + g_s s_z) = \frac{e}{2m}B\, g_j\, j_z} \quad \text{where}$$

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

• coupled states = eigenfunctions of j_z corresponding to $m\hbar$

→ splitting of V (m-levels):

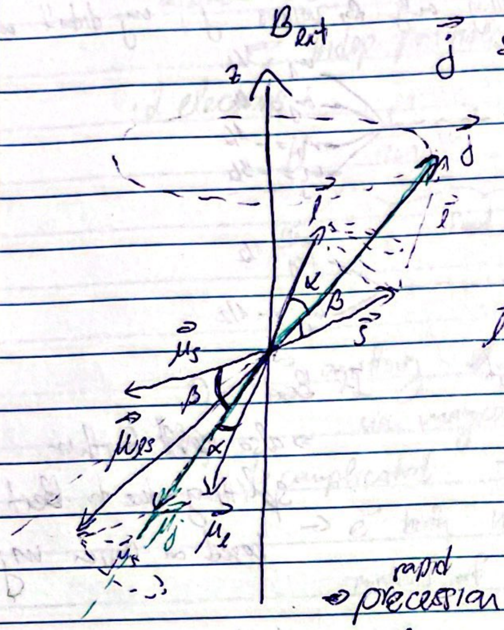
$$\Delta E = \frac{e}{2m}\hbar B m g_j = g_j \mu_B B m$$



→ spin-orbit coupling

Zeeman effect $B_{ext} < B_{int}$ ⇒ 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 processing ~~about~~ around $\vec{B}_{ext}$

$\vec{l}, \vec{s}$ 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 it

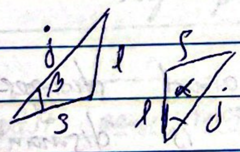
(ratios of $|\vec{\mu}_l|, |\vec{\mu}_s|$ are different than of $|\vec{l}|, |\vec{s}|$ although same angles) ↳ $g_s \neq g_l$

⇒ rapid precession ⇒ averaging out over a whale cycle → component $\perp \vec{j}$ cancels out and so 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 $|\vec{s}|^2 = |\vec{j}|^2 + |\vec{l}|^2 - 2|\vec{j}||\vec{l}|\cos\alpha$

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



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

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

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

$g_l = 1$, $g_s = 2$ ↘ $= \frac{\mu_B}{2|\vec{j}|\hbar}\left[3|\vec{j}|^2 - |\vec{l}|^2 + |\vec{s}|^2\right] \frac{|\vec{j}|}{|\vec{j}|} = \frac{\mu_B |\vec{j}|}{\hbar}\left[\frac{|\vec{j}|^2 + 2|\vec{j}|^2 - |\vec{l}|^2 - |\vec{s}|^2}{2|\vec{j}|^2}\right] =$

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

Now for energy:

precession about z-axis $= B_{ext}$ → over time $\perp z$ cancels out

$V = -\vec{\mu}_{ls} \cdot \vec{B}_{ext} = -\vec{\mu}_j \cdot \vec{B}_{ext} = -\mu_{jz} \cdot B_{ext}$

$|\mu_{jz}| = -\frac{\mu_B}{\hbar} g_j m_j \hbar = -\mu_B g_j m_j$

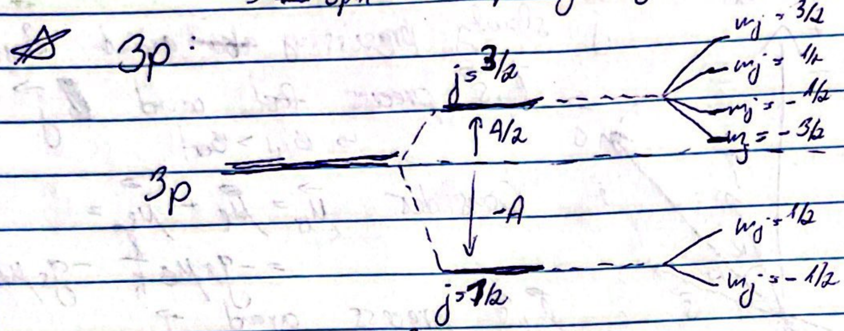
⇒ $\boxed{V_{mag} = \mu_B g_j m_j B_{ext}}$

= Zeeman effect

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

$\Rightarrow$ energy splitting based on various m_j, due to B_{ext}

$\hookrightarrow$ ~~...~~ spin-orbit splitting only for various j, m_j didn't matter



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

If $B_{ext} \neq 0$

$\Rightarrow$ also ~~...~~ further splitting due to B_{ext} based on various m_j

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

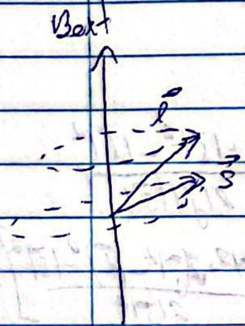
What if $B_{ext} \gg B_{int}$?

$\Rightarrow$ the system will precess around strongest $\vec{B}$

$\Rightarrow$ spin-orbit coupling is "dismantled" (negligible)

and $\vec{l}, \vec{s}$ process around B_{ext} independently

= Pashen-Bach effect



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

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

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

Many electron atoms

- assume electrons move independently in avg field of nucleus & e^-'s
  $\Rightarrow$ indep. particle model ~ good approx.
- 2 electrons:

$$H = \underbrace{-\frac{\hbar^2}{2m}\nabla_1^2}_{KE_1} \underbrace{- \frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r_1}}_{\text{first } e^-} \underbrace{- \frac{\hbar^2}{2m}\nabla_2^2}_{KE_2} \underbrace{- \frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r_2}}_{\text{second } e^-} + \underbrace{\frac{1}{4\pi\varepsilon_0}\frac{e^2}{r_{12}}}_{\text{mutual influence (Coulomb)}}$$

r_1: distance from nucleus; r_{12}: distance between e^-

↳ omitting ~~/~~ 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 i-th electron

but electrons = fermions $\Rightarrow \psi$ need odd

⇒ simplest wave function description: product: $\Phi = \phi_a(1)\,\phi_b(2)$ — quantum numbers

If $h_0(i)\,\phi_{a/b}(i) = \varepsilon_{a/b}\,\phi_{a/b}(i)$ (eigenfunctions) $\Rightarrow H\Phi = E_0\Phi$, $E_0 = \varepsilon_a + \varepsilon_b$

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

two sols with same energy

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

Pauli exclusion principle = no two e^- are in the same state
- product wavefunctions are eigenfunctions but don't satisfy

⇒ instead take:

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

($\frac{1}{\sqrt{2}}$: normalisation)

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

a, b = state ~~constant~~ characterised 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 efunctions ⇒ their lin. comb. also efun 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 that ~~for~~ 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

$$\left[-\frac{\hbar^2}{8m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} \underbrace{- \frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r} + u(r)}_{-\frac{Z_{eff}\, e^2}{4\pi\epsilon_0 r} \,|\, \text{extra}}\right] P_{nl}(r) = E P_{nl}(r)$$

* Z_{eff} = effective charge, shielding effects

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

• for Hydrogen energy of orbitals depends only on n
but for other atoms, l also plays role, indep. of m_s, m_l
⇒ motion of e^- in charge distribution

- same n → shell
- same n, l → subshell → each contains max. $\boxed{2(2l+1)}$ 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 → $\boxed{2(2l+1)}$

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

• 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: $\phi_a = \underbrace{\phi_c}_{\text{spatial}} \underbrace{\chi_a}_{\text{spin}}$

$\phi_b = \phi_d \chi_b$

$$\Psi = \frac{1}{\sqrt{2}}\left[\phi_c(1)\phi_d(2) - \phi_c(2)\phi_d(1)\right]\chi_a(1)\chi_b(2)$$

or

$$\Psi = \frac{1}{\sqrt{2}}\left[\chi_a(1)\chi_b(2) - \chi_a(2)\chi_b(1)\right]\phi_c(1)\phi_d(2)$$

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

$\Rightarrow$ each subshell can take $2(2l+1)$ for e^-

- in each n shell: $\boxed{\sum_{l=0}^{n-1} 2(2l+1) = 2n^2}$

$n=1$: 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
$Z=25$: Mn : $[Ar]\ 4s^2 3d^5$

$\vec{l}\cdot\vec{s}$ small

Multiple electrons

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

small = 1 e^-

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

$\Downarrow$ total angular momentum of all e^-

$\vec{j}_1 + \vec{j}_2 + j_3 + \dots \rightarrow J$

} LS = Russel-Sanders coupling

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

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

jj-coupling

Ex. "p" "s"

$l_1 = 1$ $l_2 = 0$ $\Rightarrow L = 1$

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

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

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

$\boxed{J = 1, 2}$

$\boxed{J = 0, 1}$

set of J values is exactly the same $\{0, 1, 1, 2\}$

but in different "groups"

Meaning of Grouping

in C:

1 } singlet ^1P "singlet P"

$\Rightarrow$ LS works well for low Z

2, 1, 0 } triplet ^3P ← term "triplet P" ← write ^{2S+1}L

degeneracy of S

E_b

in Pb:

2, 1

1, 0

E_b

$\Rightarrow$ jj works well for high Z

↳ in the middle e.g. Ge

Spin-Orbit Coupling

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

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

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

$\Rightarrow$ 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 = total spin number; L ↳ total orb. ang. mom. $(S, P, D, F, \ldots)$

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: $L=0$, $S=0$ → $J=0$

what we know: $n_1 l_1, n_2 l_2, n_3 l_3, \ldots$ — ^{2S+1}L — $^{2S+1}L_J$ — M_J, $^{2S+1}L_{M_J}$

- electronic configuration
- term ^3P
- level $^3P_1$ – contains $2M_J+1$ states
- state, e.g. $^3P_{-1}$

different names depending on known information

for jj-coupling called multiplets

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

☆ $l=1$ ("p^n") → (?)p^6

m_s \ m_l	-1	0	1	M_L
$1/2$	✓	✓	✓	0
$-1/2$	✓	✓	✓	0
M_s	0	0	0	$0 = M_L + M_S$

$M_L = \sum m_l$

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

total $M_L = 0$

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

$\sum m_s$: total $M_S = 0$ → no other options for M_S ⇒ $S=0$

↳ only $\underline{1}$ option

there IS only $\underline{1}$ possible state ⇒ deg = 1

⇒ only partially filled shells need to be considered

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

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

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

⇓

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

(3 possibilities for L, 2 possibilities for S)

$S=0$: ${}^1S_0 \quad {}^1P_1 \quad {}^1D_2$

$S=1$: ${}^3S_1 \quad {}^3P_{0/1/2} \quad {}^3D_{1/2/3}$

⇒ $2J+1$ states for each level

⇒ $\overset{1S}{1} + \overset{1P}{3} + \overset{1D}{5} = 9$

$\overset{3S}{3} + \overset{3P}{3+5+1} + \overset{3D}{3+5+7} = 27$

$$\underbrace{(2l_1+1)}_{3}\underbrace{(2l_2+1)}_{3}\underbrace{(2s_1+1)}_{2}\underbrace{(2s_2+1)}_{2} = \underline{\underline{36 \text{ states}}}$$

(9 + 27)

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

$1S \quad \cancel{{}^1P}\ (0+1=1) \quad {}^1D$

$\cancel{3S}\ (1+0=1) \quad 3P \quad \cancel{3D}\ (1+2=3)$

⇒ not all states are allowed

↳ difficult to figure out which

but for two equivalent electrons: $\boxed{L+S = \text{even}}$ ~ Pauli exclusion

☆ C: $1s^2\ 2s^2\ 2p^2$

↳ possible ~~config~~ states:

${}^1S,\ {}^3P,\ {}^1D$ (only $2p^2$ ~~elec~~ to consider, the rest is filled)

Hund's rules – only apply for ground 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, ground state
↳ if we have only one triplet :

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

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

④ ground level:
- lowest J if less than (or equal) 1/2 is filled — $A>0$
- highest J 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 : $1s^2 2s^2 2p^4$
> ⇒ $^3P_2$
> equivalent to $2p^2$ for allowed states by Pauli
> ↳ same counting with holes as electrons
> ↳ except ⊖

☆ Four "p" electrons

m_s \ m_l	−1	0	1	Σm_L
1/2	e^-	e^-	e^-	0
−1/2	□	□	e^-	1
Σm_s	1/2	1/2	0	

$M_s = 1$, $M_L = 1$

⇕ two "p" holes

same set of combinations

m_s \ m_l	−1	0	1	Σm_L
1/2				0
−1/2	⊞	⊞		−1
Σm_s	−1/2	−1/2	0	

$M_s = -1$, $M_L = -1$

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

$\vec{L}$ pointing opposite direction

N : $1s^2\,2s^2\,2p^3$

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

$l_1 + l_2 \rightarrow L_{12} = 0, 1, 2$ — For spin: $S = \frac{1}{2}, \frac{3}{2}$

$l_3 + L_{12} \rightarrow L$ — $\hookrightarrow S_{12} = 0, 1 \quad s_3 = \frac{1}{2}$

l_3	L_{12}	L
1	0	→ 1
1	1	→ 0, 1, 2
1	2	→ 1, 2, 3

$m_s = \pm\frac{1}{2}, \frac{3}{2}$ ← ^3G

$m_s = \pm\frac{1}{2}$ ← ^2S

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

↳ 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~~						
↗ for quadruplets	~~2~~	~~^4F~~	~~^4D~~					
	~~1~~	~~^4F~~	~~^4D~~	~~^4P~~				
	0	^4F	^4D	^4P	^4S			
~~1/2~~	~~3~~	~~^4F~~				~~^2F~~		
↗ for duplets and quadruplets	2	^4F	^4D			^2F	^2D	
	1	^4F	^4D	^4P		^2F	^2D	^2P
	0	^4F	^4D	^4P	^4S	^2F	^2D	^2P ~~^2S~~

If one state of a level/term exists ⇒ all must exist

$M_S = 3/2$

m_{s_1}	m_{s_2}	m_{s_3}	M_L	m_{l_1}	m_{l_2}	m_{l_3}	
1/2	1/2	1/2	3	1	1	1	⇒ not allowed by Pauli
			2	1	1	0	⇒ if one of five states for ^4F (term) doesn't exist ⇒ the whole term doesn't
			1	0	0	1	
				-1	1	1	⇒ doesn't exist
			0	1	0	-1	✓
				0	0	0	⇒ start from top

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

~~if one possi~~

$M_S = 1/2$

m_{s_1}	m_{s_2}	m_{s_3}	M_L	m_{l_1}	m_{l_2}	m_{l_3}	
1/2	1/2	-1/2	3	1	1	1	
			2	1	0	1	✓ - same m_l's but differ in m_s so it's alright
			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	✓

Test 1

Elementary Particles

atoms: L, S } fine structure: J } hyperfine structure F
nuclear spin: I
↳ nucleons (neutrons, protons)
↳ elementary particles

fermions { leptons, quarks

bosons – force carriers

- gravity → mass, ∞ range
- electro-magnetic 10^{-16}–10^{-20} γ → el. charge, ∞ range
- weak (radioactive decay) $W^{+/-}, Z^0$ 10^{-8}–10^{-13} → leptons/quarks
- strong 10^{-15} m range, gluons $<10^{-22}$ → quarks (colour)

interaction time [s]

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

QED ← electroweak (Nobel prize: Glashow, Salam, Weinberg)

QCD ← strong (Nobel prize: Gross, Politzer, Wilczek)

↓ high energy (short distance) ⇒ shortest to be allowed by Heisenberg ↳ massless

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:

	e^-	μ^-	τ^-
	ν_e	ν_μ	ν_τ
[MeV/c²]	0.511	105	1800
lifetime	$>10^{26}$ yrs	2.2 µs	300 fs

ν_e: <0.8 eV/c²

antimatter: e^+ μ^+ τ^+; $\bar\nu_e$ $\bar\nu_\mu$ $\bar\nu_\tau$

μ^- → $e^- + \bar\nu_e + \nu_\mu$

τ^- → $\mu^- + \bar\nu_\mu + \nu_\tau$, $e^- + \bar\nu_e + \nu_\tau$

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

	m_1	m_2	m_3
ν_e =	O	o	∘
ν_μ =	∘	O	O
ν_τ =	∘	o	O

} oscillating between states – m_n eigenstates: m_1, m_2

$\nu_e \to \nu_\mu \to \nu_\tau$

Quarks: 3 generations

				charge
	u	c	t	+2/3
	d	s	b	−1/3
masses [MeV]	1.5–3.1	1.27k	178k	
	3.5–6	104	4.2k	

HADRONS

MESONS

- 2 quarks ($q\bar{q}$)
- charges: −1, 0, 1
- **pions** (130–140 MeV)

anti particles

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

π^0 $u\bar{u} + d\bar{d}$ – superposition of these two states

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

anti particles

lifetime $3 \cdot 10^{-8}$ s

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

significantly heavier than just u/d
⇒ mass instead in the energy of the strong field

BARYONS

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

- **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

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

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

• ~~p~~ **nucleons**

p^+ uud → 938 MeV lifetime: $> 10^{31}$ yrs

n^0 udd → 940 MeV 10^3 s ≈ 15 min free

Forces

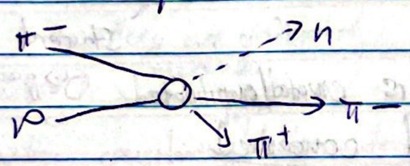
	time	strength	range
weak	10^{-10} s	10^{-6}	10 cm (0.96c) measurable
el. magn	10^{-18} s	10^{-2}	0.1 µm
strong	$< 10^{-24}$ s	1	< 1 fm impossible

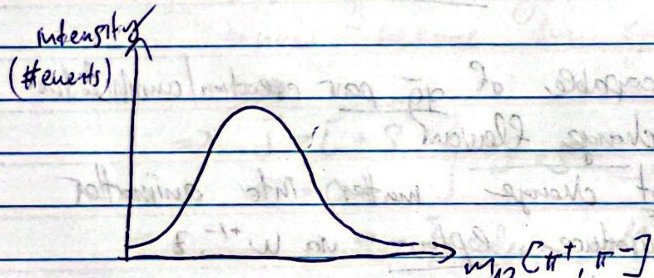
invariant mass

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

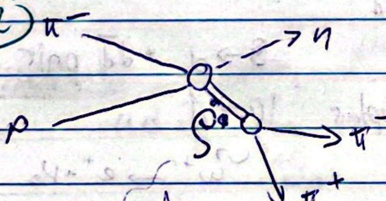
☆ $\pi^- + p \rightarrow \pi^- + \pi^+ + n$

(1)



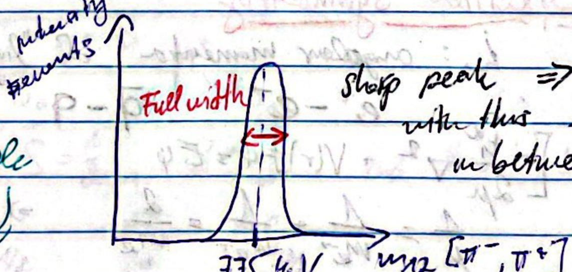


(2)



} less freedom in their energies because they had to be able to be ρ^0

same quark constitution as pions but higher excitation (~ 700 MeV)

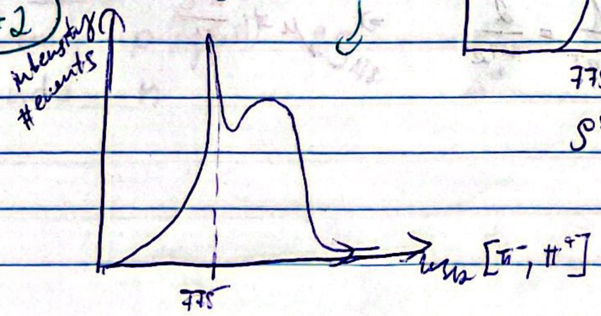


sharp peak ⇒ particle with this energy in between the decays

ρ^0 short lifetime ⇒ large width

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

(1+2) both decays possible



Conservation laws

- energy
- momentum
- charge [in units of e] – additive quantum number
  - can be just added together
  - sign change when matter ⟷ 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 (nobody knows who first)
Brookhaven (Ting) $c\bar{c} = J$
Stanford (Richter) $c\bar{c} = \psi$
↳ greek: ~~Tsta~~

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

$\Sigma^+_{uus} \to p^+ + \pi^0$ = uud + uūdd̄
$\to n^0 + \pi^+$ = udd + uđ   s→d + dd̄ pair
$\to \Lambda^0 + e^+ + \nu_e$ = uds + leptons   u→d
↳ $W^+ \to e^+ + \nu_e$

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 ~~gst~~ wavefunction : $n=1$ $L=0$
$n=2$ $L=0,1$

but 2 spins $\Rightarrow$ closer to He

☆ positronium $e^+ - e^-$

1s2s   1s2p

$n=2$ — $^1S_0$ $^3S_1$ $^3P_0$ $^3P_1$ $^3P_2$ $^1P_1$ $\Rightarrow$ energies very close together $\Rightarrow$ hard to distinguish

$n=1$ — 1s2 π^+ $^1S_0$ ρ^+ $^3S_1$ — not in H or 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

same for all { lowest 3 lvls are all S, all have $L=0$

↳ when considering light elementary particles, we take $L=0$
↳ nice because then symmetric spatial Ψ
↳ symmetry given by $(-1)^L$

$\Rightarrow$ $\left.\begin{matrix} \bar{J} = \bar{L} + \bar{S} \\ L = 0 \end{matrix}\right\}$ $\bar{J} = \bar{S}$ → true for light particles

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

☆ **mesons**

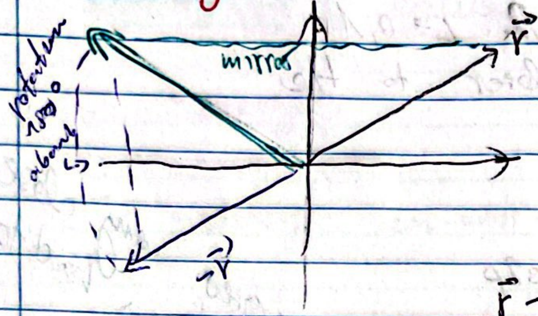
$u\bar{d}$: ground π^+ ($^1S_0$) $\xrightarrow{\text{excitation}}$ 1st excitation ρ^+ ($^3S_1$)

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

☆ 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
- ② 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 (~~for~~ lepton/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 lighest mesons: $L=0$

$$\Rightarrow P_{meson} = -1$$

baryons

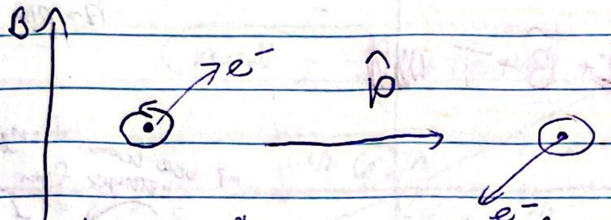
$$P_{baryon} = P_{q_1} P_{q_2} P_{q_3} (-1)^{L_{total}} = (-1)^{L_{total}} = 1$$

for baryons (& antibaryons)

for lightest baryons

☆ Madame Wu experiment

$$^{60}Co \xrightarrow{n \to p} {}^{60}Ni + e^- + \bar{\nu}_e$$



measure electron emission in upper/lower hemisphere

happens often — barely occurs $\Rightarrow$ parity violation

$\Rightarrow$ event happens more in one direction than the opposite

Charge Conjugation (C parity)

particle $\leftrightarrow$ anti-particle

- without changing spatial characteristic

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

not the same thing!

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

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

↳ ☆ $\pi^0 = u\bar{u} + d\bar{d}$ $\Rightarrow L=0, S=0$ because lowest (singlet) spin $\Rightarrow \boxed{C_{\pi^0} = 1}$

☆ e^+e^- positronium

☆ $\rho^0 \Rightarrow L=0, S=1 \Rightarrow \boxed{C_{\rho^0} = -1}$ ~~ν~~ $\bar{\nu}$ K^0

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

☆ $e^+ \text{---} e^- \xrightarrow{\hat{C}} e^- \text{---} e^+$

spatially the same as $r \to -r$

$\Rightarrow$ symmetry of spatial part: $(-1)^L$

but spin unaffected

$$S=1 \begin{cases} M_S = 1 & \uparrow\uparrow \\ M_S = 0 & \uparrow\downarrow + \downarrow\uparrow \\ M_S = -1 & \downarrow\downarrow \end{cases} \quad \text{symmetric}$$

$$S=0,\ M_S = 0 \quad \uparrow\downarrow - \downarrow\uparrow \quad \text{antisymmetric}$$

symmetry for spin $(-1)^{S+1}$

$\cancel{(-1)^L (-1)^{S+1} = (-1)^{L+S+1}}$ doesn't quite work (Rel. QM) $\Rightarrow$ extra (-1) from fermion $\leftrightarrow$ antifermion

$$\Rightarrow \boxed{(-1)^{L+S}} = C$$

Isospin: hyperchange ~~[illegible]~~ Y, azimuthal isospin I_3

↳ ~ projection of isospin on symmetry axis

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

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

as we would like to range from $-l$ to $+l$ ⇒ I range from $-I_3$ to I_3

for quarks:

	B	S+C+B+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 $I = 0$

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

☆ L = 0 — hadronic spin — $P = (-1)^L$

s=0	π	pions	J = 0	-1	0^-	scalar mesons
s=1	ρ	rhos	J = 1	-1	1^-	vector

using u, d, s ⇒ 9 scalar vector ⇒ nonet

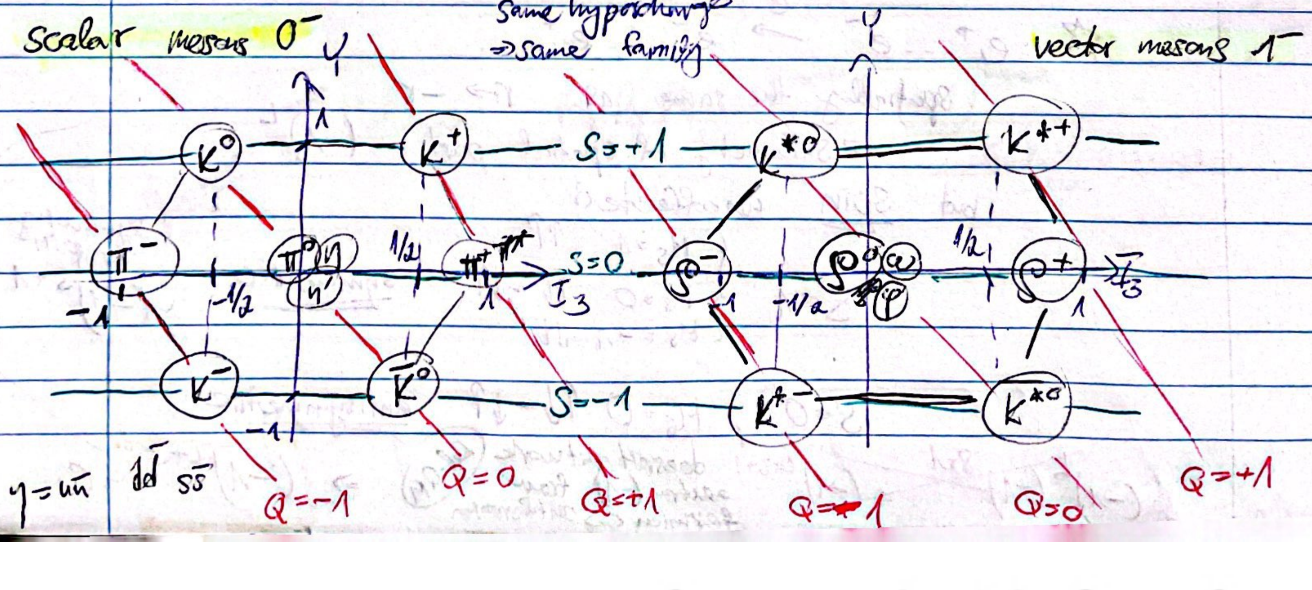
Kaons

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

I_3 goes from $-I$ to $+I$

⇓ same hyperchange ⇒ same family

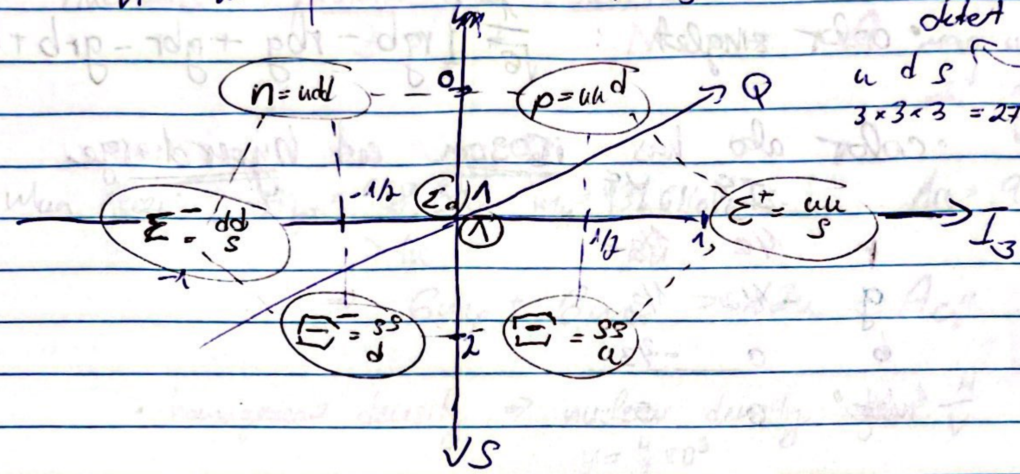
scalar mesons 0^- — vector mesons 1^-



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

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

u d s
$3 \times 3 \times 3 = 27 = 10 + 8 + 8 + 1$



↳ uds
spin: $\frac{1}{2} + \frac{1}{2} \to 0, 1$
$+\frac{1}{2} \to \frac{1}{2}$
$+\frac{1}{2} \to \frac{1}{2}, \frac{3}{2}$

$\boxed{2x \text{ in } 1/2 \text{ oktet}}$ $\boxed{1x \text{ in } 3/2 \text{ decuplet}}$

↳ uud, uus, ssd, ssu, ddu, dds
$\boxed{6 \times \text{ in } 1/2 \text{ oktet}}$ $\boxed{6 \times \text{ in } 3/2 \text{ decuplet}}$

- 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 $\boxed{0x \text{ in } 1/2 \text{ oktet}}$ $\boxed{3x \text{ in } 3/2 \text{ decuplet}}$

— " — $S = \frac{3}{2}$, $m_s = \frac{1}{2}$ 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
↖ 1964 Greenberg

Color r g b

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

- color also has isospin and hyperdharge

	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 & neutrons

$Z + N = A$ mass number

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

when free: $m_p = 938.3\,MeV$ $m_n = 939.6\,MeV$ vs. $1u = 931.5\,MeV$

$> 1u$ $> 1u$

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

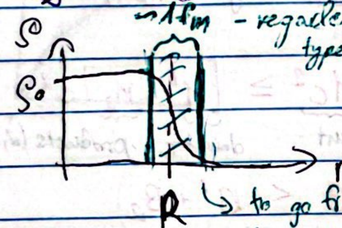
• homogeneous density $\Rightarrow$ nuclear density $\rho_0 = \frac{A}{V}$

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

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

$^{125}Xe \rightarrow R \simeq 6\,fm$

~1fm - regardless of type of atom



$\hookrightarrow$ to go from homogeneous ρ_0 to 0

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

Binding energy

mass of atomic isotope

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

m_H: $m_p + m_e$

liquid drop model parametrization of B

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

MeV: $a = 15.4$, $b = 18.3$, $d = 0.7$, $s = 23.2$

δ: Z − N: -11.2 even-even; 0 odd-even; 11.2 odd-odd

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

other terms: corrections to behaving like a droplet

b: surface correction $A^{2/3} \propto R^2$
~ surface tension
strong force only over short distance
$\Rightarrow$ surface nucleons have less neighbors
$\Rightarrow$ less strong force affecting them
$\Rightarrow$ lower binding energy

d: coulomb repulsion $\frac{Z^2}{A^{1/3}} \propto \frac{Z^2}{R}$ between protons
$\Rightarrow$ protons repelling each other
$\Rightarrow$ lower binding energy

s: 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)

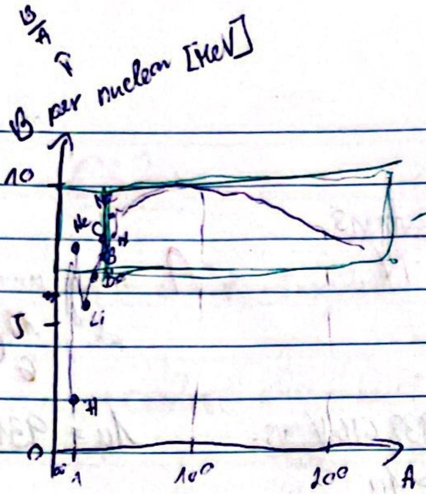
δ: odd odd

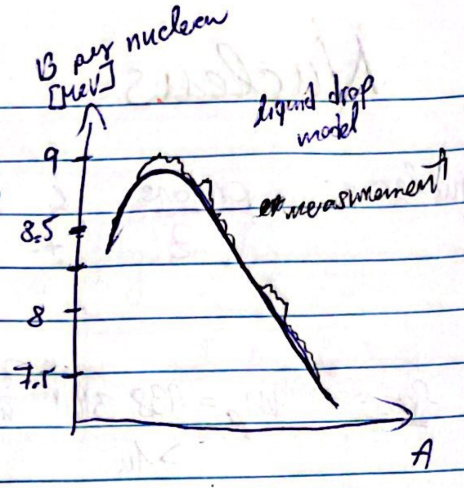
15 13 n − p 14 14 even even

13 13 n p 14 12 even even preferred state

why? eh

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





Decay: α, β, γ

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

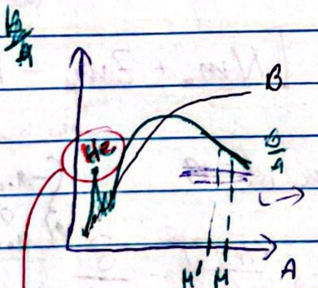
- for decay to be possible: $Mc^2 \geq [M' + M_2]c^2$

  M: parent, M': daughter, M_2: 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 wouldn't work $B' < B$

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

α

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

β $\beta^- \Rightarrow e^-$, $\beta^+ \Rightarrow e^+$

β^-: $n \to p + e^- + \bar{\nu}_e$

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

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

β^+: $p \to n + e^+ + \nu_e$

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

β^+ requires more energy: $m_{X'}^{\prime\prime} + m_e$

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

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

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

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

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

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

$$\frac{\partial Mc^2}{\partial Z} = -\beta + 2\gamma Z = 0 \Rightarrow Z = \frac{\beta}{2\gamma} = \frac{(m_n - m_H)c^2 + 4s}{\frac{2d}{A^{1/3}} + \frac{8s}{A}} = \frac{A}{2}\left[\frac{4s + \overbrace{(m_n - m_H)c^2}^{=0.8\,MeV}}{4s + \underbrace{dA^{2/3}}_{0.7A^{2/3}\,MeV}}\right]$$

optimal number of protons to be stable

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

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

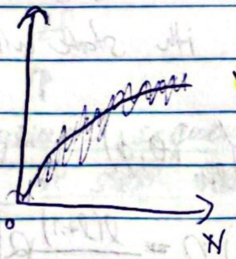
$N = A - Z$

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

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

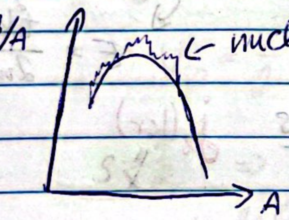
$N \geq \frac{A}{2}$

$\Rightarrow N \geq \frac{A}{2}$ (?)



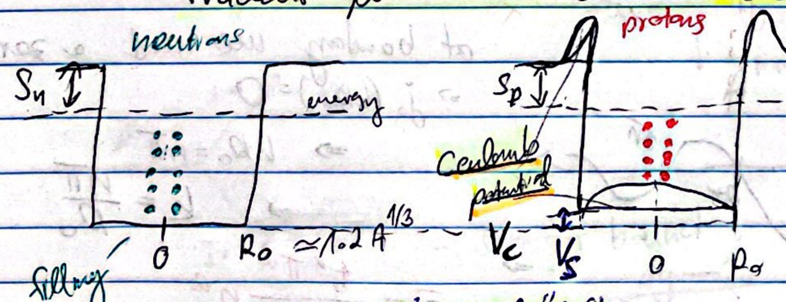
Valley of stability

Nuclear shell model



$\leftarrow$ nuclear shell closing $\Rightarrow$ "magic numbers"

Nuclear potential wells = Wood-Saxon potential



$R_0 \simeq 1.2A^{1/3}$

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

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

filling

1 n° in pairs with $S=0, L=0$ per pair

$\Downarrow$

energetically favourable

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 ~ ionisation energy

$\hookrightarrow$ similar for n, p because

β^+: $p^+ \to n + e^+ + \nu_e$ requires extra E,

β^- doesn't $\to$ switching around until equal

$\Rightarrow S_n \simeq S_p$

- similarly as for atom, the nuclear potential is spherically symmetric $\Rightarrow$ indep. of θ, ϕ

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

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

$-l \leq m_l \leq l$

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

- first $s \rightarrow 1s$
- first $p \rightarrow 1p$
- first $d \rightarrow 1d$

$\Leftarrow$ number at front indicates ith state with certain l

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

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

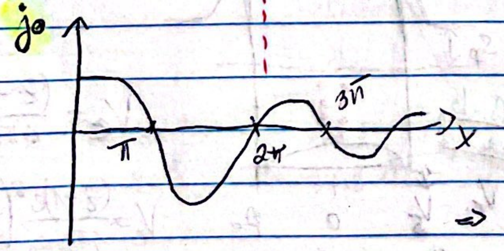
$$-\frac{\partial^2 R}{\partial r^2} - \frac{2}{r}\frac{\partial R}{\partial r} + \frac{l(l+1)}{r^2}R = \frac{2m}{\hbar^2}ER = k^2 R$$

$E = \frac{\hbar^2 k^2}{2m}$

solution: spher. Bessel functions $j_l(\underbrace{kr}_{x})$

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

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



at boundary we need a zero.

$\Rightarrow j_0(kR_0) = 0$

$\Rightarrow kR_0 = n\pi$

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

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

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

$\underbrace{\quad}_{x_l}$

order: π 4.49 5.76 2π 6.99 7.73 8.18 9.1 9.36 3π 10.42 10.9

$\Rightarrow$ 1s 1p 1d 2s 1f 2p 1g 2d 1h 3s 2f 3p ——

x_ℓ "$k R_0$"	"name"	# states	total
π	1s	2	2
4.49	1p	6	8
5.76	1d	10	18
2π	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
3π	3s	2	92
10.42	2f	14	106

↑ generic sequence of shell filling

⇒ **Magic numbers**
2, 8, 20, 28, 50, 82, 126
✓ ✓ ✓
in list

Spin-Orbit interaction – very very strong effect in nucleus

$\bar{j} = \bar{\ell} + \bar{s}$

$V_{so} \sim \text{MeV}$

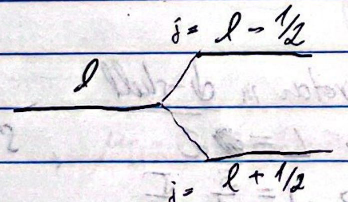
$$\boxed{V_{so} = \frac{1}{2} A^{\text{nucl.}} \left[j(j+1) - \ell(\ell+1) - s(s+1) \right]}$$

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

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

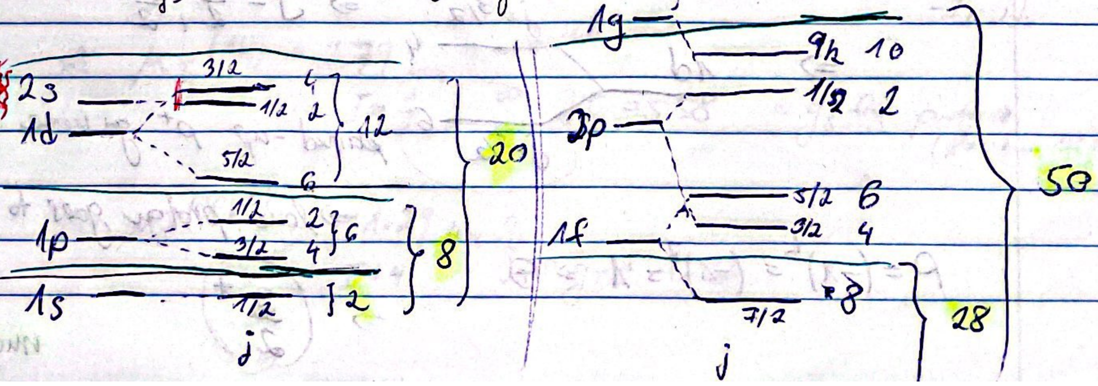
$\downarrow$

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



– stronger bound

notice: SO splitting has larger effect than the actual ordering!



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 $L=0, S=0, J=0$
  $\Rightarrow$ parity $P = (-1)^0 = 1$
  $\Rightarrow$ 0^+

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

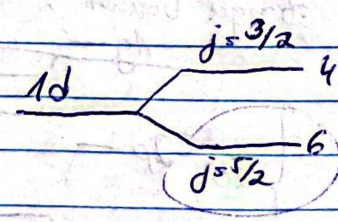
J = nuclear spin
$\Rightarrow$ how the nucleus shows itself to the outside world

- 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 bound

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

$1s : 2$ — 7 pairs of $L=S=J=0$
$1p : 6$ — 1 lone proton
$1d : 10$
$\Rightarrow 1s^2\ 1p^6\ 1d^7$ $\Rightarrow$ lone proton in d-shell
$\Rightarrow L = 2$, $S = 1/2$
$\Rightarrow J = \frac{3}{2}, \frac{5}{2}$

$\Rightarrow$ 

paired-up p^+ go here

$\Rightarrow$ lone proton goes to $j = 3/2$
$\Rightarrow J = 3/2$ nuclear spin

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

$\Rightarrow \frac{3}{2}^+$

☆ $^{31}_{13}Al$: $13p^+$, $18n^0$ $\Rightarrow L=0, S=0, J=0$

$1s^2$
$1p^6$ — 12 protons in pairs, $L=0, S=0, J=0$
$1d^5$ — 1 lone proton in 1d, $L=2$

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

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

Hyperfine Structure (F, M_F)

• nuclear spin couples/aligns to the total angular momentum of the electrons $\vec{J}$

total ang. momentum J ↓ use I to distinguish it from total ang. mom. of e^- in atomic world

$\Rightarrow$ ~~$\vec{J} + \vec{J} = \vec{F}$~~

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

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

$$\boxed{\vec{\mu}_{nucl} = \frac{\vec{\mu}_N}{\hbar} \sum_{i=1}^{A} \left(g_l \vec{l}_i + g_s \vec{s}_i \right)}$$

sets scale (similar to μ_B)

g_l: for protons 1, for neutrons 0 (electrons 1)

g_s: 5.58 protons, −3.83 neutrons (2 electrons)

$$\vec{\mu}_N = \frac{e\hbar}{2m_p} = \frac{m_e}{m_p} \underbrace{\frac{e\hbar}{2m_e}}_{\mu_B} = \frac{m_e}{m_p} \mu_B$$

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

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

vs. fine structure: no minus sign

no simple generic expression for g_I $\Rightarrow$ tabulated in units of μ_N

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

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

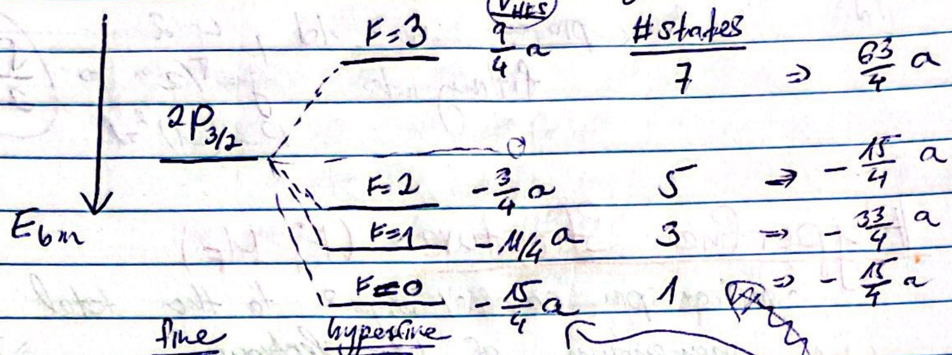
$\mu_I(^{40}K) = -1.29 \mu_N$, $I = 4$ } $\Rightarrow g_I = -0.32$

Scanned with CamScanner

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

fine structure level — split into 4 hyperfine structure

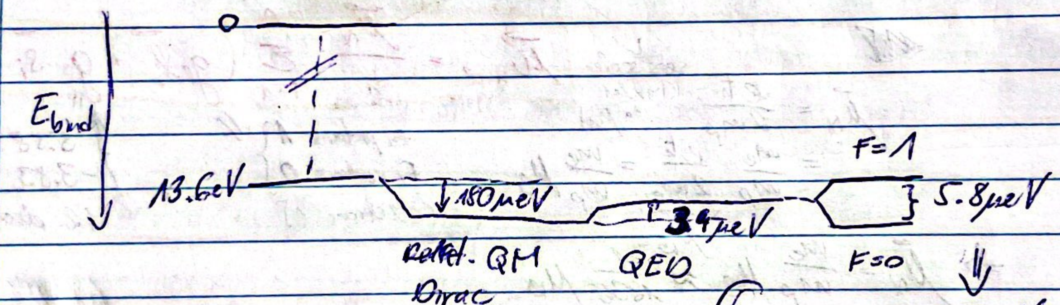
☆ Na(3p) → $^2P_{3/2}$ → $J = \frac{3}{2}$
tab: $I = \frac{3}{2}$ } $F = 0, 1, 2, 3$



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

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

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



$\Downarrow$

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

but heavily forbidden $\Rightarrow f = \frac{\Delta E}{h} = 1.42\,GHz$

⇝ occurs only ~~...~~ H clock

$2.6 \cdot 10^{-15}\,s^{-1}$ $= 0.047\,cm^{-1}$

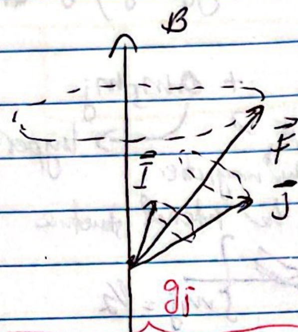
↳ very weak but $\Rightarrow \frac{1}{0.047}\,cm = 21\,cm$ line

there's so much hydrogen

that it's actually common

Hyperfine structure in a magnetic field

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



Zeeman effect

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

$$g_F = \underbrace{\left[1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}\right]}_{g_J} \cdot \left[\frac{F(F+1) - I(I+1) + J(J+1)}{2F(F+1)}\right] +$$

$$- g_I \underbrace{\frac{\mu_N}{\mu_B}}_{\approx \frac{1}{2000}} \frac{F(F+1) - J(J+1) + I(I+1)}{2F(F+1)}$$

can be neglected usually (~2000x weaker)

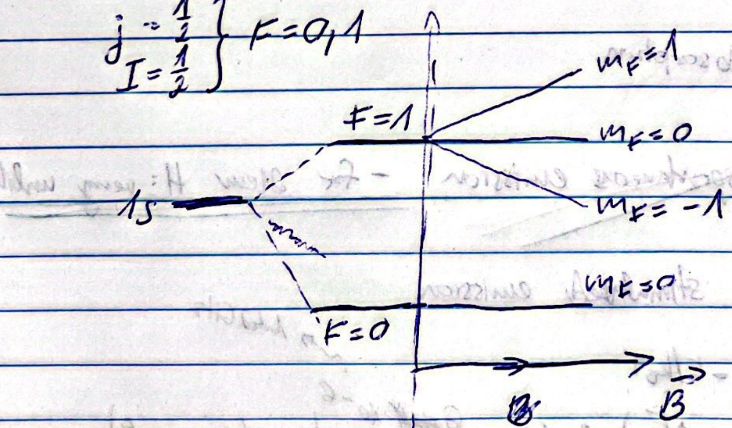
$$\mu_B g_F = \mu_B g_J \frac{F(F+1) - I(I+1) + J(J+1)}{2F(F+1)} - \mu_N g_I \frac{F(F+1) - J(J+1) + I(I+1)}{2F(F+1)}$$

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

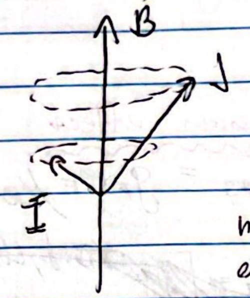
H(1s)

$l = 0,\ s = \frac{1}{2}$

$\left.\begin{array}{l} j = \frac{1}{2} \\ I = \frac{1}{2} \end{array}\right\} F = 0, 1$



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

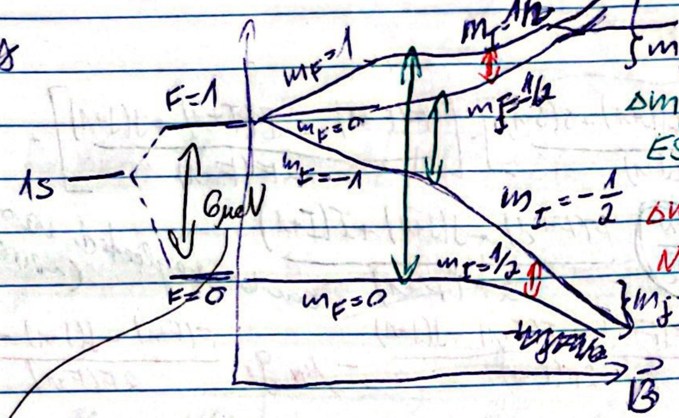


$$\boxed{\Delta E = g_J m_J \mu_B B_{ext} - g_I m_I \mu_N B_{ext}} + a m_I m_J$$

neglected in drawing below ~2000x weaker

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

hyperfine structure constant



$m_j = 1/2$

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

ESR = Electron Spin Resonance

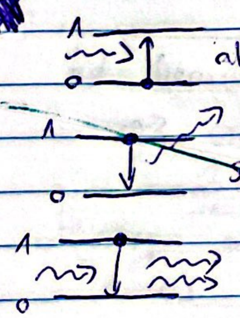
$\Delta m_I = \pm 1$, $\Delta m_j = 0$

NMR = Nuclear Magnetic Resonance

$m_j = -1/2$

= 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



~~spontaneous emission~~ – for 21cm H: very unlikely

$$\frac{n_{F=1}}{n_{F=0}} \propto e^{-E/k_BT} \approx \left(1 - \frac{\Delta E}{k_BT}\right) \doteq \left(1 - \frac{6 \cdot 10^{-6}}{2.5 \cdot 10^{-2}}\right) \approx \left(1 - 10^{-4}\right)$$

1.42 GHz