SINGLE-e ATOMIC STRUCTURE

486: Hamiltonian

$$\hat{\mathcal{H}}_{\text{BOHR}} = -\frac{\hbar^2 \nabla^2}{2m} - \frac{Ze^2}{4\pi\varepsilon_0 r}$$

Coulomb ≡ electric potential due to nucleus

Gives spectrum $E_{n\,\text{BOHR}} = -\frac{(Z\alpha)^2}{n^2}$ using $\alpha \equiv \frac{e^2}{4\pi\varepsilon_0 (\hbar c)} = \frac{1}{137}$

Add some more detail...

Magnetic dipole moment $\vec{\mu}$ and g-factor

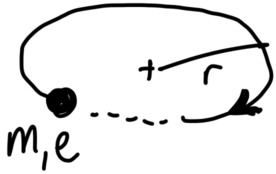
Any charged object that has angular momentum

$J = L$ (orbital) and/OR S (rotational) produces electrical current

and ∴ has magnetic dipole moment $\boxed{\vec{\mu} = \gamma \vec{J}}$

gyromagnetic ratio

classical $\boxed{\gamma = \frac{e}{2m}}$ obtained when a charge e with mass m travels in a circle



$T \equiv$ period

$f =$ frequency $= 1/T = \frac{\omega}{2\pi}$

OR

total charge e
total mass m
with same distributions (then spinning object can be built from current loops with constant ratio e/m)

derivation of γ classical:

$$\frac{\mu}{J} = \frac{\text{current} \cdot \text{area}}{I\omega}$$

J: ang. mom.

$$= \frac{(e/T)\cdot \pi r^2}{(mr^2)\cdot(2\pi/T)} = \frac{e}{2m}$$

Quantum: orbital L $\Leftarrow$ for $\Rightarrow$ Quantum: spin S

p'cle of charge e & mass m

$$\boxed{\vec{\mu}_L = \frac{e}{2m}\vec{L}}$$

$$\boxed{\vec{\mu}_S = g\,\frac{e}{2m}\vec{S}}$$

"g-factor", particle-dependent

e.g. $|\mu_\ell| = \frac{e}{2m}\hbar\sqrt{\ell(\ell+1)}$

$= \left(\frac{e\hbar}{2m}\right)$ (order few, dimensionless)

$\Uparrow$

BOHR MAGNETON
$$\boxed{\mu_B \equiv \frac{e\hbar}{2m_e}}$$

common unit in atomic physics

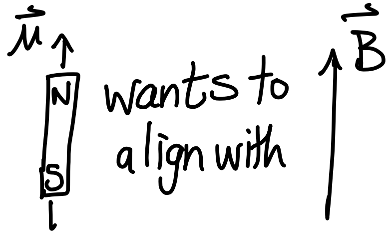
For a "DIRAC PARTICLE" $\equiv$ a point spin-½ particle, e.g. an electron $\boxed{g_e = 2}$

RQM = QFT

$.\underbrace{00023\ldots}_{\text{9 digits known}}$

Zeeman effect: place atom in external $\vec{B}$ field

$$\mathcal{H}'_{Zeeman} = -\vec{\mu} \cdot \vec{B}_{external}$$



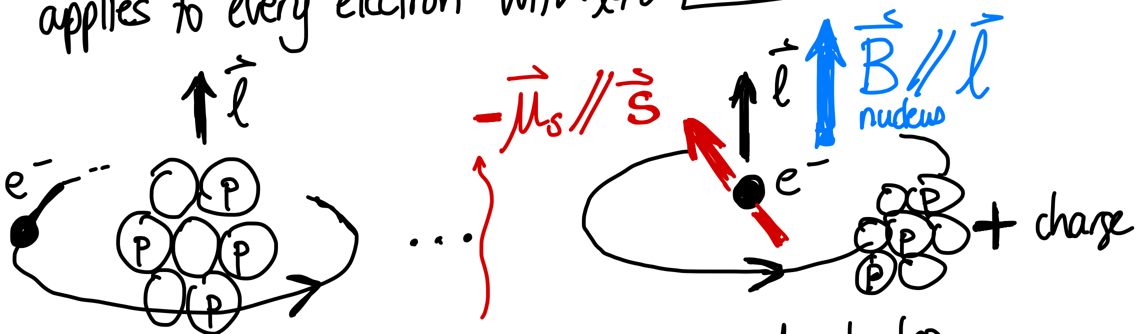
alters En of atomic e's when placed in $\vec{B}$ external

Stark effect = similar effect with $\vec{E}_{external}$

SPIN-ORBIT INTERACTIONⁿ:

$$\boxed{\mathcal{H}'_{s\text{-}o} \sim \vec{s} \cdot \vec{\ell}}$$

applies to every electron with $\ell \neq 0$



FRAME of nucleus

FRAME of electron

due to neg. charge of spinning electron

∴ new potential energy to add to $\mathcal{H}$:

$$\mathcal{H}'_{s\text{-}o} \sim -\vec{\mu}_s \cdot \vec{B}_\ell \sim -\vec{\mu}_s \cdot \vec{\ell}$$

$$\sim -\left(-\frac{e}{2m} \cdot g_e \cdot \vec{S}\right) \cdot \vec{\ell} \sim +\vec{S} \cdot \vec{\ell}$$

SPIN is NOT rotational angular momentum!

$\equiv$ orbital $(\vec{r} \times \vec{p})$ ang. mom. around an object's CM

- $g_{SPIN} = 2$ & $g_L = 1$ for e^-
- We found from $\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}}$ that $\ell = 0, 1, 2, \ldots$ = INTEGERS ONLY

We found from $[L_x, L_y] = i\hbar L_z$

$\xrightarrow{\text{copied to}} [S_x, S_y] = i\hbar S_z$

$\xrightarrow{\text{copied to}} [J_x, J_y] = i\hbar J_z$ for ANY ang. mom

$\xrightarrow{\text{leads to}}$ restriction $j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$ = INTEGERS & HALF-INTEGERS

.... spin uses both integers & half-integers!

$\therefore$ spin is not a form of $\vec{r} \times \vec{p}$

g-factor for NUCLEONS $\neq 2$ $\because$ p & n are not point particles → have structure!

$g_p = 5.59$

$g_n = -3.83$

(↑ for p, n SPIN, implied!)

"anomalous magnetic moments" of p, n

$\mu_p = 2.79\,\mu_N$

$\mu_n = -1.91\,\mu_N$

where

$$\boxed{\text{NUCLEAR MAGNETON} \quad \mu_N \equiv \frac{e\hbar}{2m_N}}$$

Good quantum numbers $\equiv$ those associated with e-values of observables that are CONSERVED

for atomic e^- when spin-orbit interaction is present

recall $\frac{d\langle\hat{Q}\rangle}{dt} = \frac{i}{\hbar}\langle[\hat{\mathcal{H}},\hat{Q}]\rangle + \cancel{\left\langle\frac{\partial\hat{Q}}{\partial t}\right\rangle} \to 0$ almost always

when $\uparrow$ is ZERO, we say $\hat{Q}$ is CONSERVED

$\Rightarrow$ If you place system in an e-state of a conserved $\hat{Q}$ (with e-value q), then it will REMAIN in that e-state (w e-value q)

[t-dep evolution produced by the $\hat{\mathcal{H}}$ via the Schr. Equ, $i\hbar\frac{\partial\psi}{\partial t} = \hat{\mathcal{H}}\psi$]

Complete set of good q. nos. for an e^- in a hydrogenic atom:

- $\hat{\mathcal{H}}_{BOHR}$: $|\underbrace{n\,l\,m_l}_{\text{space}} \times \underbrace{(s)\,m_s}_{\text{spin}}\rangle$

- $\hat{\mathcal{H}}_{s\text{-}o} \sim \vec{l}\cdot\vec{S}$: $|n\,l\,(s)\,\underbrace{j\,m_j}_{\text{q. nos of}}\rangle$ $\quad \underset{\text{TOTAL}}{\vec{j}} = \vec{l} + \vec{S}$

[DISC 3]

FINE STRUCTURE $\equiv$ corrections to atomic energy levels due to

§6.3.2 $\longrightarrow$ spin-orbit interaction

§6.3.1 $\longrightarrow$ + relativistic correction (approx)

$$\boxed{\hat{H}'_{s-o} = \frac{1}{2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)\frac{\hat{\vec{S}}\cdot\hat{\vec{l}}}{m^2c^2r^3}}$$ full spin-orbit formula

relativistic correction "Thomas precession" $\because$ calculation of $\vec{B}$ done in accelerating frame of orbiting e^-

Atomic notation

1 Electronic configuration of an atom

$\boxed{n\mathcal{L}^{\#}\ldots}$ e.g. H ground state: $1s^1$

$|n=1,\ l=0\rangle$ one electron

He ground state: $1s^2$

C ground state: $1s^2 2s^2 2p^2$

l	letter "$\mathcal{L}$"
$\emptyset$	s
1	p
2	d
3	f
4	g
$\vdots$	$\vdots$

2 Term Symbols a.k.a. Spectral Term $\boxed{(n)\,^{2S+1}\mathcal{L}_J}$

e.g. ground state of H:

one e^- in $|n=1, l=0\rangle$ ... and $s=\frac{1}{2}$ $\therefore j \equiv l+s = \frac{1}{2}$

$\therefore$ ground state's term symbol: $1\,^2S_{1/2}$

"doublet-S-half"

- $(2s+1)$ = # of possible m_s values $= -s, \dots +s$ in STEPS of 1

  $(2l+1)$ = # ... m_l values $= -l, \dots +l$ STEPS of 1

- Term symbol q'ties $S, \mathcal{L}, J$: TOTAL (Σ all e^-)

  Electron configuration : electron-by-electron

Contributions to atomic E levels: Table in Gr §5.2

	source	order of mag.
E_n	Bohr H	$\alpha^2 (m_e c^2)$
ΔE	Fine structure: s-o ~ $\vec{l}\cdot\vec{s}$ & relativ.	$\alpha^4 (m_e c^2)$
ΔE	Lamb shift: Q.E.D.	$\alpha^5 (m_e c^2)$
ΔE	Hyperfine structure: $\vec{S}\cdot\vec{S}_{\text{NUCLEUS}}$	$\alpha^4 (m_e c^2)\cdot\left(\frac{m_e}{m_p}\right)$ ← $\frac{1}{2000}$

NOTE: $H'_{relativ} = T_{relativ} - T_{classical}$ §Gr 6.3

$$= \left[\sqrt{(pc)^2 + (mc^2)^2} - mc^2\right] - \frac{p^2}{2m} \approx -\frac{p^4}{8m^3c^2} \sim \alpha^4 (mc^2)$$

H energy levels: diagram for $n = 1, 2$

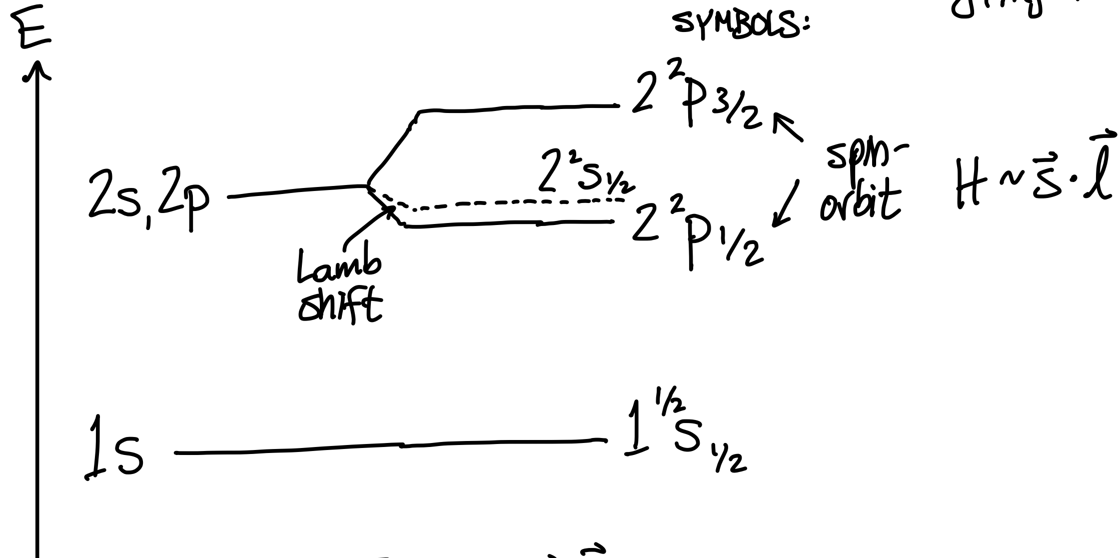
$$|\underbrace{n\,\ell\,m_\ell}_{\psi(r,\theta,\phi)\ \text{spatial}}\ \underbrace{(s)\,m_s}_{\chi_{m_s}\ \text{spin}}\rangle$$

n	> ℓ	$\xrightarrow{\times s = 1/2}$ j	m_j
1	0	$1/2$	$+1/2, -1/2$
2	0	$1/2$	$+1/2, -1/2$
	1	$1/2$	$+1/2, -1/2$
		$3/2$	$+3/2, +1/2, -1/2, -3/2$

⋮

m_ℓ, m_s not good q. nos in presence of spin-orbit → j, m_j ARE

TERM SYMBOLS:



E_n Bohr $+ E_{fine\ struct} \sim \vec{s} \cdot \vec{\ell} +$ relativ