12: Atoms in a magnetic field:

Zeeman and Paschen-Back effect

Hertel, Schulz:
Atoms, Molecules and optical physics 1

Usual atom with spin-orbit interaction

no external fields

$$\hat{V}_{LS} = a \hat{\vec{L}} \cdot \hat{\vec{S}} \qquad (8.1)$$

↳ spin-orbit coupling parameter

its expectation value is the fine structure splitting (FS)

$$V_{LS} = \langle \hat{V}_{LS} \rangle = \frac{a}{2}\left[J(J+1) - L(L+1) - S(S+1)\right]$$

(8.1) in SI units

$$\hat{V}_{LS} = a \hat{\vec{L}} \cdot \hat{\vec{S}} / \hbar^2$$

L, S, J orbital angular mom., spin, total ang. mom. quantum numbers

M_L, M_S, M_J projections, a.k.a. "magnetic quantum numbers"

now: ext. B field

interaction energy $\hat{V}_B$ depends on magnetic moments $\hat{\mathcal{M}}_L$, $\hat{\mathcal{M}}_S$, $\hat{\mathcal{M}}_J = \hat{\mathcal{M}}_L + \hat{\mathcal{M}}_S$

$\vec{B}$ field defines a direction: z direction

g factors $g_L = 1$ (orbit)

$g_S = 2$ (spin)

Bohr magneton $\mu_B = \frac{e\hbar}{2m_e}$

$$\hat{V}_B = -\hat{\vec{\mathcal{M}}}_J \cdot \vec{B} = -(\hat{\vec{\mathcal{M}}}_L + \hat{\vec{\mathcal{M}}}_S) \cdot \vec{B} =$$

$$\frac{\mu_B}{\hbar}\left(g_L \cdot \hat{L}_z + g_S \cdot \hat{L}_S\right)\cdot B =$$

$$\uparrow \qquad \uparrow$$

$$1 \qquad 2$$

$$= \mu_B \frac{\hat{J}_z + \hat{S}_z}{\hbar} B = -\hat{M}_{J_z} \cdot B$$

assume : we have 0th order solution
for the unperturbed atom

$$\hat{H}_0 |nLM_LSM_S\rangle = W_{nLS}|nLM_LSM_S\rangle$$

$\hat{H}_0$ all electrostatic interactions in the atom
except for spin-orbit interaction

n, L, M_L, S, M_S good quantum numbers

assume only substates of one nLS multiplet
contribute to energy shifts

$$\hat{H} = \hat{H}_0 + \hat{V}_{LS} + \hat{V}_B$$

$$= \underbrace{\hat{H}_0}_{\text{unperturbed}} + \underbrace{a\frac{\hat{J}^2 - \hat{L}^2 - \hat{S}_z^2}{2\hbar^2}}_{\text{spin-orbit interact.}} + \underbrace{\mu_B\frac{\hat{J}_z + \hat{S}_z}{\hbar}\cdot B}_{\text{magnetic int.}}$$

$\left.\begin{matrix} L M_L S M_S \\ L S J M_J \end{matrix}\right\}$ are NOT good quantum numbers any more!

only M_J is a good quantum number

and remaining good quantum numbers
depend on "field high or low?"

B field		perturbation	optimal basis	Name
low	$B \ll \frac{a}{\mu_B}$	$V_B \ll V_{LS}$	$\lvert LSJM_J\rangle$	anomalous Zeeman effect
high	$\gg$	$\gg$	$\lvert LM_LSM_S\rangle$	Paschen-Back effect

B fields : 1-2 Tesla

30 Tesla   sc magnets

$\mu_B = 5.788 \cdot 10^{-5}\ eV/T$

"wave numbers" $\hat{=}$ energy

$\langle V_B \rangle \approx 2 \cdot 10^{-3}\ eV \hat{=} 14\ cm^{-1}$

This is ~ 10^{-3} of usual electronic excitation

FS splitting P state of H: $0.37\ cm^{-1}$

Li $0.36\ cm^{-1}$

He, Be $\sim 1\ cm^{-1}$

Zeeman effect in low field

0th order $\quad H_0 = \hat{H}_0 + \hat{V}_{LS}$

$\rightarrow$ eigenstates $|J M_J\rangle = |L S J M_J\rangle$

$2S+1$ substates, each with

$2J+1$ degenerate magnetic substates

$\hat{V}_B$: 1st order perturbation

$$V_B = \langle \hat{V}_B \rangle = \frac{\mu_B}{\hbar} \langle J M_J | \hat{J}_z + \hat{S}_z | J M_J \rangle B$$

$$= \frac{\mu_B}{\hbar} \Big[\underbrace{\langle J M_J | \hat{J}_z | J M_J \rangle}_{M_J \cdot \hbar} + \langle J M_J | \hat{S}_z | J M_J \rangle \Big] B$$

$$V_B = \left[1 + \frac{\langle J M_J | \hat{S}_z | J M_J \rangle}{\hbar M_J} \right] \mu_B M_J B$$

$\vdots$

$$V_B = \underbrace{\left[1 + \frac{\langle J M_J | \hat{\vec{S}} \cdot \hat{\vec{J}} | J M_J \rangle}{J(J+1)\hbar^2} \right]} \mu_B M_J B$$

= Landé g factor $\quad g_J = \dfrac{3J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$

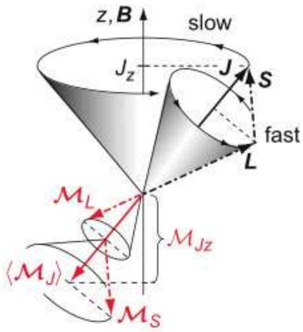
$$V_B = g_J \mu_B M_J \cdot B = -\mathcal{M}_{J_z} \cdot B$$

for low B fields each J level splits into $2J+1$ equally spaced levels

Vector model

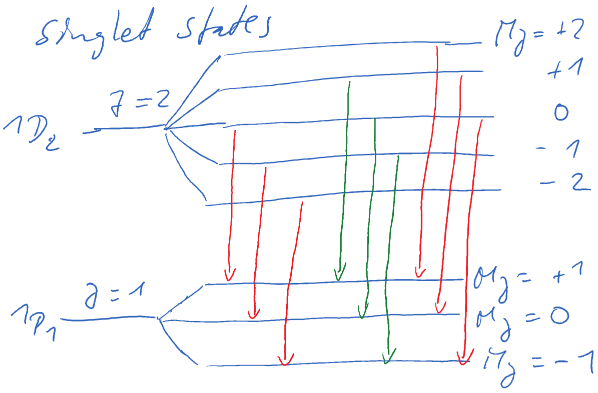
$\vec{J} = \vec{L} + \vec{S}$

LS coupling stronger than magn. interaction (low B)



- Examples:

- Singlet states



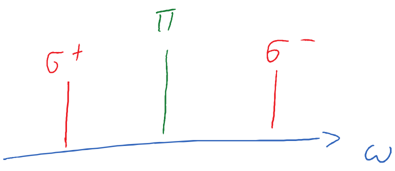
equal splitting

transitions $\Delta M_J =$ +1 0 -1

σ_+ π σ_- light

circular polarized light lin polarized light

the 9 transitions appear at 3 different frequencies



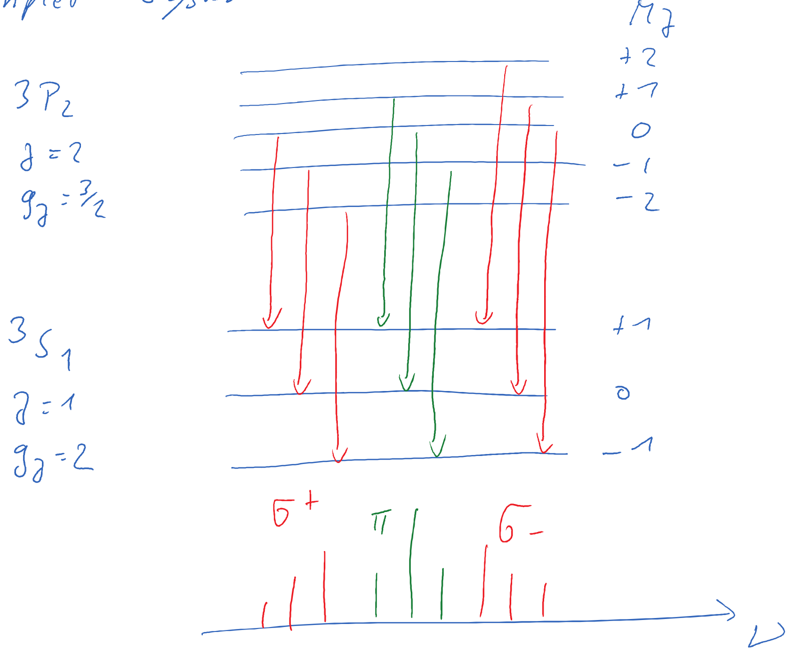
this can not be observed along $\hat{z}$

this can <u>not</u> be observed along $\hat{z}$

"normal Zeeman effect"

He singlet states

- triplet system



all 9 lines separated

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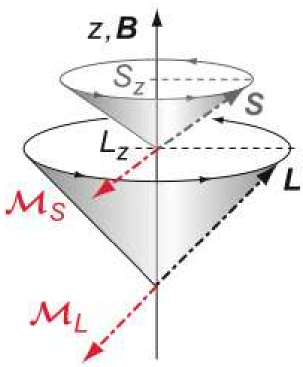
large B field : Paschen Back

easy for H, He, Li, ...

also for highly excited states of all other atoms : $FS \propto \frac{1}{n^3}$



neglect LS-coupling

$$H_{PB} = \hat{H}_0 + \hat{V}_B =$$

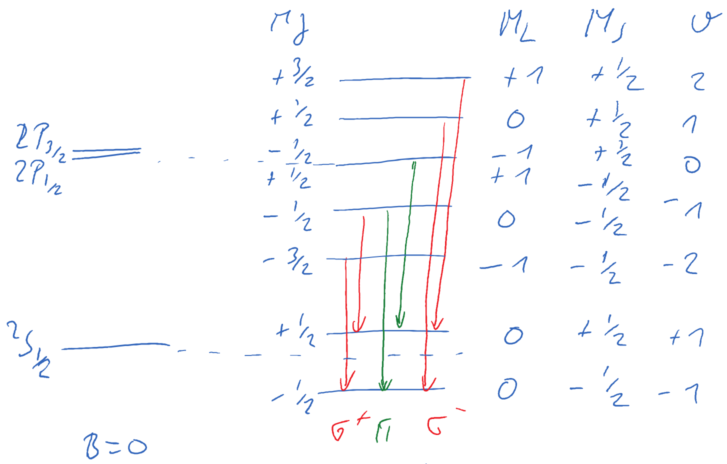
$$= \hat{H}_0 + \frac{\mu_B}{\hbar}\left(\hat{L}_z + 2\hat{S}_z\right)B$$

g factors

$$\hat{V}|M_L M_S\rangle = \frac{\mu_B}{\hbar} B(\hat{L}_z + 2\hat{S}_z)|M_L M_S\rangle$$

$$= \mu_B B (M_L + 2M_S)|M_L M_S\rangle$$

$\Rightarrow$ splitting is $\quad V_B = \mu_B \cdot B \cdot (M_L + 2M_S)$



6 transitions at 3 frequencies

ν = proj. of magn. moment onto z axis ($\vec{B}$)

$\nu = M_L + 2M_S$

selection rules for E1 transition in high B fields

$\Delta M_L = 0, \pm 1$

$\Delta M_S = 0 \quad \longleftarrow \quad$ E1 dipole operator acts on

$\Delta L = \pm 1 \qquad\qquad\qquad$ L, but not on spin!

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general treatment

$$\hat{H} = \hat{H}_0 + \hat{H}_{BLS} =$$

$$= \hat{H}_0 + \overbrace{\frac{a}{\hbar^2}\hat{\vec{L}}\cdot\hat{\vec{S}} + \frac{\mu_B}{\hbar}(L_z + 2S_z)B}$$

assume: $\hat{H}_0 |n L M_L S M_S\rangle = W_{nLS} |n L M_L S M_S\rangle$ solved

only one $\underline{n}$

ansatz

$$|L S \nu M_J\rangle = \sum_{M_L M_S} c_{M_L} c_{M_S} |L M_L S M_S\rangle$$

eigenvalues of $\hat{H}_{BLS}$ are splittings of energy levels in B field

$$\upsilon = M_L + 2M_S = M_J + M_S$$

write $\hat{H}_{BLS}$ in matrix form

$$\langle L M_L' S M_S' | \hat{H}_{BLS} | L M_L S M_S \rangle =$$

$$= \mu_B (M_L + 2M_S) B \times \delta_{M_L' M_L} \delta_{M_S' M_S} +$$

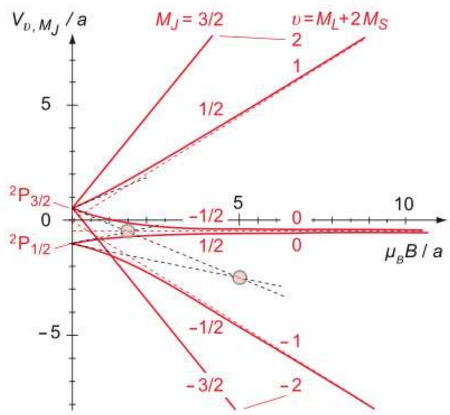
$$+ \frac{a}{\hbar^2} \langle L M_L' S M_S' | \hat{L} \cdot \hat{S} | L M_L S M_S \rangle$$

Table 8.2 Matrix elements of $\widehat{H}_{BLS}$ for a ^{2}P state in the uncoupled $|LM_L SM_S\rangle$ basis

$M_L M_S$		$\|1\frac{1}{2}\rangle$	$\|0\frac{1}{2}\rangle$	$\|1-\frac{1}{2}\rangle$	$\|-1\frac{1}{2}\rangle$	$\|0-\frac{1}{2}\rangle$	$\|-1-\frac{1}{2}\rangle$
	υ	2	1	0	0	-1	-2
	M_J	3/2	1/2	1/2	$-1/2$	$-1/2$	$-3/2$
$\langle 1\frac{1}{2}\|$		$2\mu_B B + a/2$	0	0	0	0	0
$\langle 0\frac{1}{2}\|$		0	$\mu_B B$	$a/\sqrt{2}$	0	0	0
$\langle 1-\frac{1}{2}\|$		0	$a/\sqrt{2}$	$-a/2$	0	0	0
$\langle -1\frac{1}{2}\|$		0	0	0	$-a/2$	$a/\sqrt{2}$	0
$\langle 0-\frac{1}{2}\|$		0	0	0	$a/\sqrt{2}$	$-\mu_B B$	0
$\langle -1-\frac{1}{2}\|$		0	0	0	0	0	$-2\mu_B B + a/2$

off-diagonal elements nonzero only for $M_J' = M_J$

$$M_J' = M_L' + M_S'$$
$$M_J = M_L + M_S$$

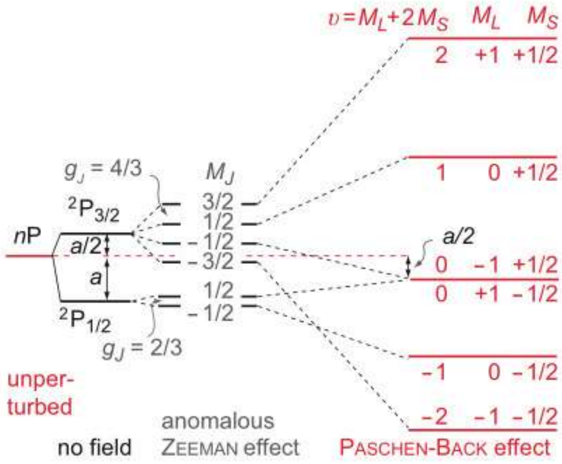


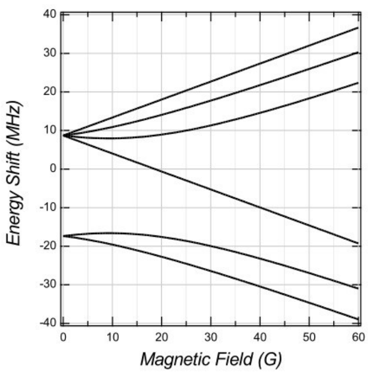
Breit-Rabi diagram for $^2P_{3/2}$ and $^2P_{1/2}$

Fig. 8.9 Transition from a low to a high magnetic field B for the example of a ^{2}P$_{3/2,1/2}$ system. Plotted as *full red lines* are the splittings $V_{\upsilon M_J}$ of the levels as a function of the field strength B. The parameters $M_J = M_L + M_S$ and $\upsilon = M_L + 2M_S$ characterize the 6 states (see text). *Dashed black (red) lines* show the extrapolation in the case of a *low (high) field*. Two avoided crossings are marked by pink circles. The energy splitting $V_{\upsilon M_J}$ is given in units of the fine structure parameters a, the field strength B in units of a/μ_B

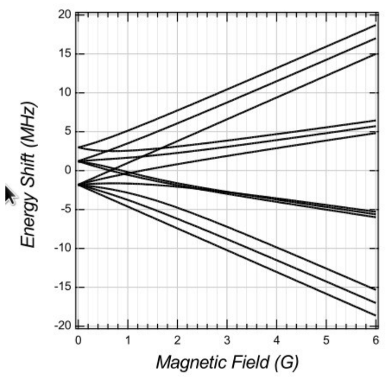
no level crossings are allowed for states with equal $M_J = M_L + M_S$

repulsion of states with same M_J

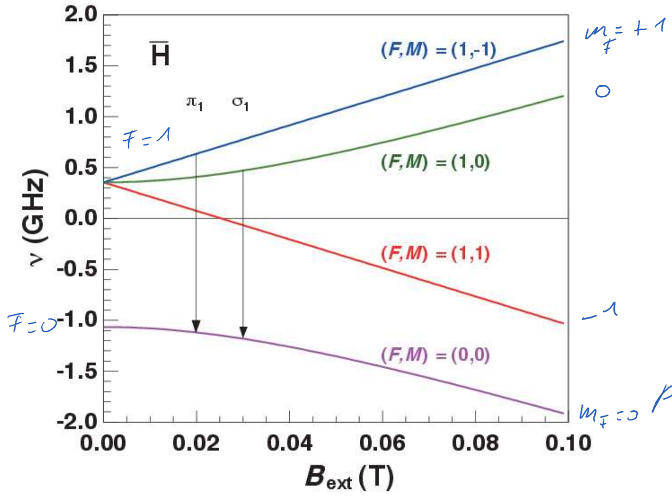




^6Li: $2P_{1/2}$ shift



$2P_{3/2}$ state of ^6Li



Hydrogen 1S ground state

$L = 0$

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

p nuclear spin $I = \frac{1}{2}$

$F = J + I = 0, 1$ for H

$m_F = -F \ldots\ldots F$

Breit-Rabi diagram for (Anti) hydrogen