Zaradi LS popravka se centralna energija pri $n=2$, t.j.

$E_2 = -\frac{13{,}6\,eV}{n^2} \cong -3{,}4\,eV$ razcepi

$\underline{n=2 \;\; l=1 \;\; s=\frac{1}{2}}$ ⋯ $\underline{n=2 \;\; l=1 \;\; s=\frac{1}{2} \;\; j=\frac{3}{2}}$ $\boxed{4x}$

$(2l+1)(2s+1) = 3\cdot 2 = 6$ stanj

$+$

$\underline{}$ $j=\frac{1}{2}$ $\boxed{2x}$

$= 6$ stanj.

Atom vodika v močnem B

$$H = H_0 + H_{ls} \underbrace{- \hat{\mu}_z B_z}_{\text{Zeemanov pojav}} \qquad \text{za } \underset{nlm}{\psi_{100}} \text{ in } \psi_{21(\pm 1, 0)}$$

A) $B=0$, samo $\langle LS \rangle \propto \frac{1}{2}\left(j(j+1) - l(l+1) - s(s+1)\right)$

$\boxed{n=1}$ $\;\; n=1,\ l=0,\ m_l=0$ / $s=\frac{1}{2},\ m_s=\pm\frac{1}{2}$ ..... $n=1 \;\; l=0$ / $s=\frac{1}{2} \;\; j=\frac{1}{2} \;\; m_j=\pm\frac{1}{2}$ ni razcepa.

2x

$\boxed{n=2}$ $\;\; l=0$, isto kot $n=1$, ni razcepa / $l=1,\ m_l=\pm 1, 0,\ s=\frac{1}{2},\ m_s=\pm\frac{1}{2}$

$2+6=8$ stanj

⋯ $l=1 \;\; j=\frac{3}{2}$ 4x

$l=0$ 2x

$l=1 \;\; j=\frac{1}{2}$ 2x

8 stanj

B) Močno magnetno polje: $\mu_B B \gg \Delta E_{ls} \sim 10^{-5}\,eV$.

$$\Delta E_B = -\frac{\mu_B}{\hbar}\left(\overset{-1}{g_l} \langle L_z \rangle + \overset{-2}{g_s} \langle S_z \rangle\right) B = \mu_B (m_l + 2m_s) B.$$

V zelo močnem B lahko zanemarimo LS člene in so dobra kvantna števila spet $n l m_l s m_s$. Poglejmo si razcepe za $n=1$ in $n=2$ ↪

$\boxed{n=1}$

$l=0, \; m_l=0$; $s=\frac{1}{2}, \; m_s=\pm\frac{1}{2}$

$m_s=\frac{1}{2}$: $\Delta E_B = \mu_B B$

$m_s=-\frac{1}{2}$: $-\mu_B B$

Dobimo popoln razcep, ni več degeneracije.

$\boxed{n=2}$

$l=0$ je isto kot pri $n=1$ zgoraj

$l=1, \; m_l=\pm 1, 0; \; m_s=\pm 1/2$ $\quad \Delta E_B = \mu_B B(m_l + \underbrace{2}_{\pm 1} m_s)$

$= \mu_B B \{-2, -1, \underset{2\times}{0}, 1, 2\}$

$l=1, \; m_l=\pm 1, 0$; $s=\frac{1}{2}, \; m_s=\pm\frac{1}{2}$

$(2l+1)(2s+1) = 3\cdot 2 = 6$

$m_l=1, \; m_s=1/2$

$m_l=0, \; m_s=1/2$

$m_l=\pm 1, \; m_s=\pm 1/2$ $\quad \Delta E=0 \; [2\times]$

$m_l=0, \; m_s=-1/2$

$m_l=-1, \; m_s=-1/2$

ATOM VODIKA V MOČNEM B

$$\hat{H} = \hat{H}_0 + \cancel{\hat{H}_{es}} - \hat{\mu}_z B_z \quad , \quad \hat{\mu}_z = \frac{\mu_B}{\hbar}\left(g_e \hat{L}_z + g_s \hat{S}_z\right) B_z$$

zanemarimo

V močnem B, ko $\mu_B B \gg \Delta E_{es} \sim 10^{-5}\,eV$, so dobra kvantna števila l, m_l, s, m_s in obdržimo $\psi_{n l m_l s m_s}$

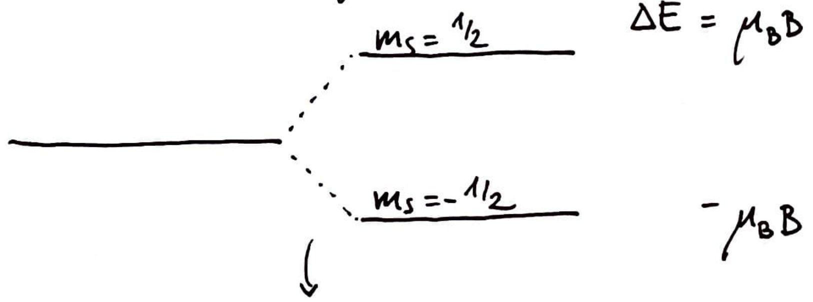
Potem velja: $$\Delta E_B = -\frac{\mu_B}{\hbar}\Big(\underbrace{g_e}_{-1}\langle L_z\rangle + \underbrace{g_s}_{-2}\langle S_z\rangle\Big)B$$

$$= \mu_B\left(m_l + 2 m_s\right)B.$$

Poglejmo si najprej osnovno stanje z $n=1$

$\boxed{n=1}$ $l=0$ $m_l=0$

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



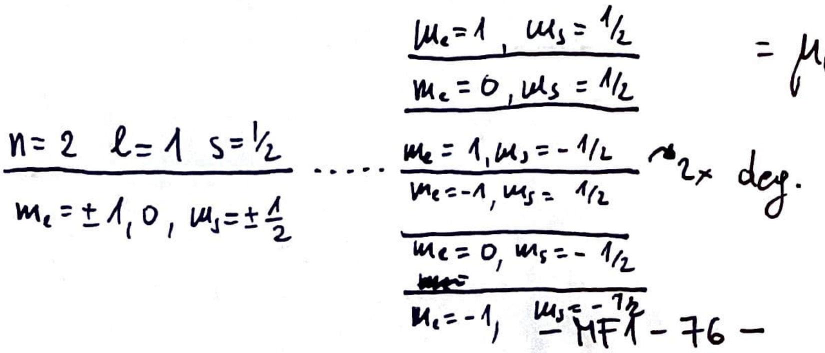
popoln razcep, ni več degeneracije

$\boxed{n=2}$ $l=0$ je popolnoma isto kot zgoraj.

$l=1$, $m_l=\pm 1, 0$, $s=\frac{1}{2}$, $m_s=\pm\frac{1}{2}$.

Dobimo sledeče razcepe: $\Delta E_B = \mu_B B\left((\pm 1, 0) \pm 2\cdot\frac{1}{2}\right)$

$$= \mu_B B\,(-2, -1, \underset{2x}{0}, 1, 2)$$



ŠIBKO MAGNETNO POLJE

V tem primeru obdržimo LS popravek in delamo v $n l s j m_j$ bazi.

$$\Delta E_{\text{šibko } B} = \frac{\mu_B}{\hbar}\left(\langle L_z\rangle + 2\langle S_z\rangle\right) B$$

(glej str. 77, 78 v skripti)

$$\langle L_z\rangle + 2\langle S_z\rangle = \frac{\langle J^2\rangle + \langle SJ\rangle}{\langle J^2\rangle}\langle J_z\rangle = \mu_B\, g_{LSJ}\, m_j\, \hbar$$

Landé-jev faktor — projekcija J na z os

Landéjev faktor dobimo iz skalarnega produkta

$$J = L + S, \quad L = |J - S|^2, \quad L^2 = J^2 + S^2 - 2JS$$

$$\langle JS\rangle = \frac{1}{2}\langle J^2 + S^2 - L^2\rangle = \frac{\hbar^2}{2}\left(j(j+1) + s(s+1) - l(l+1)\right)$$

$$\Rightarrow g_{LSJ} = \frac{j(j+1) + \frac{1}{2}\left(j(j+1) + s(s+1) - l(l+1)\right)}{j(j+1)} = \underbrace{1 + \frac{1}{2}}_{\frac{3}{2}} + \frac{\frac{3}{4} - l(l+1)}{2j(j+1)}$$

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

$$g_{LSJ} = \frac{3}{2} + \frac{\frac{3}{4} - l(l+1)}{2j(j+1)}$$

Poglejmo si te razcepe na primeru atoma H, najprej za osnovno $n=1$, potem za 1. vzbujeno stanje z $n=2$.

<u>OSNOVNO STANJE</u> : $n=1,\ l=0,\ s=\frac{1}{2},\ j=\frac{1}{2},\ m_j=\pm\frac{1}{2}$

$$g_{LSJ} = \frac{3}{2} + \frac{\frac{3}{4}-l(l+1)}{2j(j+1)} = \frac{3}{2} + \frac{\frac{3}{4}-0}{\cancel{2\cdot\frac{1}{2}}\frac{1}{2}+1} = \frac{3}{2}+\frac{1}{2} = 2.$$

$$\Delta E = \mu_B B g_{LSJ} m_j = \mu_B B \cdot 2 \cdot \left(\pm\frac{1}{2}\right) = \pm\mu_B B$$

$m_s = \pm\frac{1}{2}$ .... $m_j = \frac{1}{2}$ $\Delta E = \mu_B B$

.... $m_j = -\frac{1}{2}$ $-\mu_B B$

SPEKTROSKOPSKE OZNAKE

$n l_j$

$\Downarrow$

$1s_{1/2}$

<u>1. VZBUJENO STANJE</u> $n=2,\ l=0,1,\ s=\frac{1}{2},$

- za $l=0$ je popolnoma enako kot zgoraj
- za $l=1$ najprej določimo možne vrednosti za

$$j \in [j^{max}, j^{min}] = [1-\frac{1}{2}, 1+\frac{1}{2}) = [\frac{1}{2}, \frac{3}{2}]$$

Potem izračunamo Landéjev faktor:

$$g_{LSJ}\left(j=\frac{3}{2}\right) = \frac{3}{2} + \frac{\frac{3}{4}-2}{2\cdot\frac{3}{2}\cdot\frac{5}{2}} = \frac{3}{2} + \frac{\frac{3-8}{\cancel{4}}}{\frac{2\cdot3\cdot5}{\cancel{4}}} = \frac{3}{2} - \frac{\cancel{5}\,1}{2\cdot3\cdot\cancel{5}} = \frac{9-1}{2\cdot3} = \frac{4}{3},$$

$$g_{LSJ}\left(j=\frac{1}{2}\right) = \frac{3}{2} + \frac{\frac{3}{4}-2}{2\cdot\frac{1}{2}\frac{3}{2}} = \frac{3}{2} - \frac{\frac{5}{\cancel{4}}}{\frac{2\cdot3}{\cancel{4}}} = \frac{9-5}{2\cdot3} = \frac{2}{3}.$$

$$\Delta E = \mu_B B \cdot \begin{cases} \frac{4}{3}\left(\pm\frac{3}{2}, \pm\frac{1}{2}\right) \\ \frac{2}{3}\left(\pm\frac{1}{2}\right) \end{cases} = \mu_B B\left(-2, -\frac{2}{3}, -\frac{1}{3}, \frac{1}{3}, \frac{2}{3}, 2\right)$$

$j=3/2$ $\quad m_j=3/2$ $\quad 2\ [\mu_B]$

Še skica razcepa stanj

$n=2\quad l=1\quad s=\frac{1}{2}$

$m_l=\pm 1,0\ ,\quad m_s=\pm\frac{1}{2}$

$(2l+1)(2s+1)=3\cdot 2=6$ stanj

$j=3/2\quad m_j=1/2\quad 2/3$

$j=1/2\quad m_j=1/2\quad 1/3$

- - - - - - - - - - - -

$j=1/2\quad m_j=-1/2\quad -1/3$

$j=3/2\quad m_j=-1/2\quad -2/3$

$j=3/2\quad m_j=-3/2\quad -2$

6 stanj

Spektroskopska oznaka

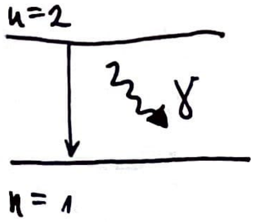
$n=2,\ l=1,\ j=\frac{3}{2}$

$\boxed{2p_{3/2}}$

- Še o poimenovanju, oz. spektroskopskih oznakah:

l	0	1	2	3	4 ...
OZNAKA	s	p	d	f	g ...
IME	sharp	principle	diffuse	fundamental / fine	

(64) Dipolni sevalni prehodi v potencialni jami



$$a = 0{,}3\,\mathrm{nm} \qquad n=2 \to n=1 \qquad \delta E\,? \quad \delta E\,\delta t = \hbar$$

$$\tau^{-1} = \frac{4}{3\hbar}\,\alpha\,E_{12}^3\left(\frac{x_{12}}{\hbar c}\right)^2$$

$$E_{12} = E_2 - E_1\,, \qquad x_{12} = \int_0^a \psi_2^*\, x\, \psi_1\, dx$$

↑ dipolni prehodni matrični element

Za jamo velja: $E_n = \frac{1}{2m}\left(\frac{\hbar n\pi}{a}\right)^2 \Rightarrow E_{12} = \frac{\hbar^2\pi^2}{2ma^2}(4-1) = \frac{3\pi^2(\hbar c)^2}{2mc^2a^2}$.

Dipolni matrični element dobimo z direktno integracijo

$$x_{12} = \frac{2}{a}\int_0^a \sin\left(\frac{2\pi x}{a}\right)\sin\Big(\underbrace{\frac{\pi x}{a}}_{=t}\Big)\, x\, dx\,, \quad \text{ker } \psi_n = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$$

DVA INTEGRALA

$$= \frac{2}{a}\left(\frac{a}{\pi}\right)^2\int_0^\pi \sin 2t\,\sin t\, dt = \frac{4a}{\pi^2}\int_0^\pi (1-\cos^2 t)\cos t\; t\, dt$$

Potrebno je 2x izračunati per-partes:

$$\int_0^\pi \underbrace{t}_{u}\,\underbrace{\cos t\, dt}_{dv} = t\sin t\Big|_0^\pi - \int_0^\pi \sin t\, dt = \cos t\Big|_0^\pi = -1-1 = -2$$

$du = dt$, $\sin t = v$

$$\int_0^\pi t\cos^3 t\, dt = t\left(\sin t - \frac{1}{3}\sin^3 t\right)\Big|_0^\pi - \int_0^\pi\left(\sin t - \frac{\sin^3 t}{3}\right)dt = *$$

$$du = dt\,, \quad v = \int 1-\sin^2 t\; d(\sin t) = \sin t - \frac{1}{3}\sin^3 t$$

$$* = \cos t\Big|_0^\pi + \frac{1}{3}\int_{-1}^{1}(1-\cos^2 t)\, d(\cos t) = -2 + \frac{1}{3}\left(2-\frac{2}{3}\right) = \frac{-18+4}{9} = -\frac{14}{9}$$

$$\Rightarrow \quad x_{12} = \frac{4a}{\pi^2}\left(-2+\frac{14}{9}\right) = -\frac{16a}{9\pi^2}.$$

Nedoločenost:

$$\hbar\tau^{-1} = \frac{4}{3}\alpha\left(\frac{3\pi^2}{2}\frac{(\hbar c)^2}{mc^2a^2}\right)^3\left(-\frac{2^4 a}{9\pi^2\hbar c}\right)^2$$

$$= \frac{4}{3}\alpha\frac{\cancel{3^3}\pi^6(\hbar c)^{\cancel{6}4}}{\cancel{2^3}(mc^2)^3a^{\cancel{6}4}}\frac{2^{\cancel{8}5}\cancel{a^2}}{\cancel{3^4}\pi^4\cancel{(\hbar c)^2}} = \underbrace{\frac{2^7}{3^2}}_{0{,}5}\pi^2\alpha\underbrace{\left(\frac{\hbar c}{mc^2a}\right)^4}_{\left(\frac{0{,}2\,\mu m\,keV}{0{,}3\,\mu m\,511\,keV}\right)^4}mc^2$$

$$= 10^{-6}\,eV = \underline{\underline{\mu eV}}.$$

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(65) Razpadni čas atoma vodika $n=2, l=1, m_l=0$

IZBIRNA PRAVILA: $\Delta l = \pm 1,\ \Delta m_l = \pm 1, 0,\ \Delta m_s = 0,$

$\Delta j = \pm 1, 0,\ \Delta m_j = \pm 1, 0,\ j=0 \not\to j=0.$

$n=2\ l=1\ m_l=0$

$n=1\ l=0\ m_l=0$

$$\tau^{-1} = \frac{4\alpha}{3\hbar}E_{12}^3\left(\frac{r_{12}}{\hbar c}\right)^2$$

$$E_n = -E_{Ry}\frac{1}{n^2},\quad E_{12} = E_2 - E_1 = -E_{Ry}\left(\frac{1}{4}-1\right)$$

$$= \frac{3}{4}E_{Ry} = \frac{3}{8}\alpha^2 mc^2.$$

Sedaj potrebujemo še matrični dipolni element

$$\vec{r}_{12} = \int \psi_{100}^* \vec{r}\,\psi_{210}\,dV,\quad \psi_{210} = R_{21}Y_{10} = \frac{1}{\sqrt{4\pi(2r_B)^3}}\frac{r}{r_B}e^{-\frac{r}{2r_B}}\cos\theta,$$

$$\psi_{100} = R_{10}Y_{00} = \frac{2}{\sqrt{4\pi r_B^3}}e^{-\frac{r}{r_B}}$$

$$\vec{r}_{12} = \frac{2}{4\pi 2^{3/2}r_B^3}\int_0^\infty\int_{-1}^1\int_0^{2\pi}\frac{r}{r_B}e^{-\frac{3r}{2r_B}}\cos\theta\, r\left(\sin\theta\overset{0}{\cancel{\cos\varphi}}, \sin\theta\overset{0}{\cancel{\sin\varphi}}, \cos\theta\right)$$

$$\times r^2dr\,d(\cos\theta)\,d\varphi \quad \neq 0 \text{ samo v } z\text{-smeri!}$$

Dipolni element v z smeri

$$r_{12z} = \frac{2\pi}{2\, 4\pi\sqrt{2}\, r_B^3} \underbrace{\int_0^\infty \left(\frac{3r}{2r_B}\right)^4 e^{-\overbrace{\frac{3r}{2r_B}}^{=t}} dt}_{} \overbrace{\int_{-1}^{1} d(\cos\theta)\cos^2\theta}^{\frac{2}{3}} \left(\frac{2r_B}{3}\right)^5 \frac{1}{r_B}$$

$$= \frac{2^5 r_B}{3\sqrt{2}\, 3^5} 4! = \frac{2^7\sqrt{2}}{3^5} \frac{\hbar c}{\alpha mc^2}.$$

$$\tau^{-1} = \frac{4}{3}\frac{\alpha}{\hbar} E_{12}^3 \left(\frac{r_{12}}{\hbar c}\right)^2, \; E_{12} = \frac{3}{8}\alpha^2 mc^2, \; r_{12} = \frac{2^7\sqrt{2}}{3^5}\frac{\hbar c}{\alpha mc^2}$$

$$\Rightarrow \tau^{-1} = \frac{2^2 \alpha c}{3\hbar c} \frac{\cancel{3^3}\alpha^{\cancel{6}\,4}\cancel{(mc^2)^3}}{\cancel{2^9}} \frac{2^{\cancel{15}\,6}}{3^{\cancel{10}\,7}\cancel{\alpha^2}\cancel{(mc^2)^2}} = \left(\frac{2}{3}\right)^8 \alpha^5 \frac{mc^2}{\hbar c}\cdot c$$

Sedaj lahko določimo razpadni čas in razširitev:

a) $\tau = \left(\frac{3}{2}\right)^8 \frac{\hbar c}{\alpha^5 mc^2}\cdot c = 1{,}6\ \text{ns},$

b) $\Gamma = \frac{\hbar}{\tau} = \left(\frac{2}{3}\right)^8 \alpha^5 mc^2 = 0{,}4\ \mu\text{eV}.$

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(62) Matrični prehodni elementi za HO, $V = \frac{1}{2}m\omega^2 x^2$

velja: $x H_n = \frac{1}{2} H_{n+1} + n H_{n-1}$

oz.: $\int \psi_m x \psi_n = \frac{a}{\sqrt{2}}\left(\sqrt{n+1}\,\delta_{m\,n+1} + \sqrt{n}\,\delta_{m\,n-1}\right), \; a = \sqrt{\frac{\hbar}{m\omega}}$

$$\psi_n = \frac{1}{\sqrt{2^n n! \sqrt{\pi} a}} e^{-y^2/2} H_n(y), \; y = \frac{x}{a} \quad \text{in} \quad \int_{-\infty}^{\infty} \psi_m \psi_n dx = \delta_{mn}$$

$$\delta_{mn} = \frac{1}{\sqrt{2^{n+m} m! n! \sqrt{\pi}\cancel{a}}} \int_{-\infty}^{\infty} e^{-y^2} H_m(y) H_n(y)\, \cancel{a}\, dy$$