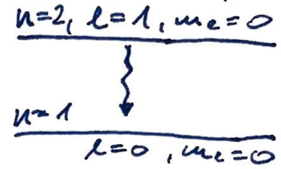
(65) Razpadni čas atoma vodika iz

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

za dipolne sevalne prehode veljajo izbirna pravila



$\Delta l = \pm 1$ in $\Delta m_l = \pm 1, 0$

$\Delta m_s = 0$

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

$$\frac{1}{\tau} = \frac{4\alpha}{3\hbar} E_{12}^3 \left(\frac{r_{12}}{\hbar c}\right)^2 , \quad E_n = -\frac{\alpha^2}{2} m_e c^2 \frac{1}{n^2} = -E_{Ry}\frac{1}{n^2}$$

$$E_{12} = E_2 - E_1 = -E_{Ry}\left(\frac{1}{4}-1\right) = +\frac{3}{4}E_{Ry} = \frac{3\alpha^2 mc^2}{8}$$

$$\psi_{210} = R_{21} Y_{10} = \frac{1}{\sqrt{4\pi}\,(2r_B)^{3/2}}\left(\frac{r}{r_B}\right) e^{-r/2r_B} \cos\theta$$

$$\psi_{100} = R_{10} Y_{00} = \frac{2}{(4\pi r_B^3)^{1/2}} e^{-r/r_B}$$

$\vec r = (x, y, z)$

$$\langle 100 | \vec r | 210 \rangle = \frac{\cancel{2}}{48\sqrt{2}\,\pi r_B^3} \int e^{-\frac{3r}{2r_B}} \frac{r}{r_B} \big(r\sin\theta \cancel{\cos\varphi}^{\,0},\ r\sin\theta \cancel{\sin\varphi}^{\,0},\ r\cos\theta\big)\cos\theta\, d(\cos\varphi)\, d\varphi\, r^2 dr$$

$$\langle 100 | r_z | 210 \rangle = \frac{\cancel{4}\,2\cancel{\pi}}{2\cdot 4\sqrt{2}\,\cancel{\pi}\, r_B^3} \underbrace{\int_0^\infty e^{-t} t^4\, dt}_{} \left(\frac{2r_B}{3}\right)^5 \frac{1}{r_B} \underbrace{\int_{-1}^{1} c_\theta^2\, dc_\theta}_{=\frac{2}{3}}$$

$$= \frac{1\cdot 4!}{\cancel{2}\cancel{\sqrt{2}}\, r_B^4} \frac{2^{\cancel{5}\,4} r_B^5}{3^5} \frac{\sqrt{2}\,2}{3} = \frac{2^7\sqrt{2}}{3^5} r_B = \frac{2^7\sqrt{2}}{3^5}\frac{\hbar c}{mc^2\alpha} = r_{12}$$

$$\frac{1}{\tau} = \frac{4\alpha}{3\hbar}\left(\frac{3\alpha^2 mc^2}{2^3}\right)^3\left(\frac{2^7\sqrt{2}}{3^5 mc^2\alpha}\right)^2$$

$$= \frac{2^2\alpha}{3\hbar}\,\frac{\alpha^4\, mc^2\, 2^6}{3^7} = \frac{\alpha^5\, 2^8}{3^8\,\hbar}\, mc^2$$

$$\tau = \left(\frac{3}{2}\right)^8 \frac{\hbar c}{\alpha^5\, mc^2\, c} = \frac{3^8}{2^8}\,\frac{137^5\ 200\,\cancel{\mathrm{eV}}\,\cancel{\mathrm{nm}}\,\mathrm{ns}}{0{,}500\,\cancel{\mathrm{keV}}\ 3\cdot 10^{28}\,\cancel{\mathrm{m}}}$$

$$= \underline{\underline{1{,}6\ \mathrm{ns}}}$$

b) Razširitev spektralne črte

$$\delta\Gamma = \frac{\hbar}{\tau} = \alpha^5\left(\frac{2}{3}\right)^8 mc^2 = \left(\frac{2}{3}\right)^8 \frac{1}{137^5}\,500\cdot 10^3\,\mathrm{eV}$$

$$= 0{,}4\ \mu\mathrm{eV}.$$

(62) Matrični prehodni elementi za harmonski oscilato

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 x^2 \,, \quad H\psi_n = \underbrace{\hbar\omega\left(n+\tfrac{1}{2}\right)}_{E_n}\psi_n$$

$$\psi_n = \frac{1}{\sqrt{2^n n! \sqrt{\pi}\, a}} H_n(y)\, e^{-y^2/2} \,, \quad y = \frac{x}{a} \,, \quad a = \sqrt{\frac{\hbar}{m\omega}}$$

- Te funkcije tvorijo ortonormiran set: $\int_{-\infty}^{\infty} \psi_n^* \psi_m \, dx = \delta_{nm}$
- Za Hermitove polinome velja: $H_n(x) = (-1)^n e^{x^2} \frac{d}{dx^n}\left(e^{-x^2}\right)$

↳ velja: $x H_n = \frac{1}{2}\left(H_{n+1} + 2n H_{n-1}\right)$

- Prehodni matrični element je $\langle m | x | n \rangle$

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

$$= \frac{a}{\sqrt{2^{n+m} n! m! \pi}} \int_{-\infty}^{\infty} H_m \frac{1}{2}\left(H_{n+1} + 2n H_{n-1}\right) e^{-y^2} dy$$

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

$$\Rightarrow \langle m|x|n\rangle = a\left(\frac{1}{2} \frac{\sqrt{2}\cdot\sqrt{n+1}}{\sqrt{2^{m+n+1}(n+1)!\, m!\, \pi}} \int_{-\infty}^{\infty} H_m H_{n+1} e^{-y^2} dy \right. +$$

$$\left. \frac{1}{\cancel{2}} \frac{1 \cdot \cancel{2}n}{\sqrt{2n}\, \sqrt{2^{m+n-1}(n-1)!\, m!\, \pi}} \int_{-\infty}^{\infty} H_m H_{n-1} e^{-y^2} dy \right)$$

$$\langle m|x|n\rangle = a\left(\frac{\sqrt{n+1}}{\sqrt{2}}\,\delta_{m\,n+1} + \frac{1}{\sqrt{2}}\sqrt{n}\,\delta_{m\,n-1}\right)$$

$$= \frac{a}{\sqrt{2}}\left(\sqrt{n+1}\,\delta_{m\,n+1} + \sqrt{n}\,\delta_{m\,n-1}\right), \quad a = \sqrt{\frac{\hbar}{m\omega}}$$

- za dipolne prehode $\frac{1}{\tau} \propto \langle m|x|n\rangle^2$, torej velja izbirno pravilo da je $\Delta n = \pm 1$

- z rekurzivno formulo lahko dobimo $\langle x^2\rangle$

$$x H_n = \frac{1}{2}\left(H_{n+1} + 2n H_{n-1}\right)$$

$$= \frac{1}{4}\left(H_{n+2} + 2(n+1)H_n + 2n H_n + 2n\,2(n-1)H_{n-2}\right)$$

$$= \frac{1}{4}H_{n+2} + \frac{1}{2}(2n+1)H_n + n(n-1)H_{n-2}$$

$$\Rightarrow \langle n|x^2|n\rangle = \left(n+\frac{1}{2}\right)a^2 \underbrace{\delta_{nn}}_{=1} = \frac{\hbar}{m\omega}\left(n+\frac{1}{2}\right)$$

$$\langle V\rangle = \frac{1}{2}m\omega^2\langle x^2\rangle = \frac{1}{2}\hbar\omega\left(n+\frac{1}{2}\right)$$

Virialni teorem $2\langle T\rangle = p\langle V\rangle$, $V \propto x^p$, $p=2$

$$\langle T\rangle = \langle V\rangle \quad \text{in} \quad \langle E\rangle = \langle T\rangle + \langle V\rangle = 2\langle V\rangle$$

$$= \hbar\omega\left(n+\frac{1}{2}\right) \checkmark$$

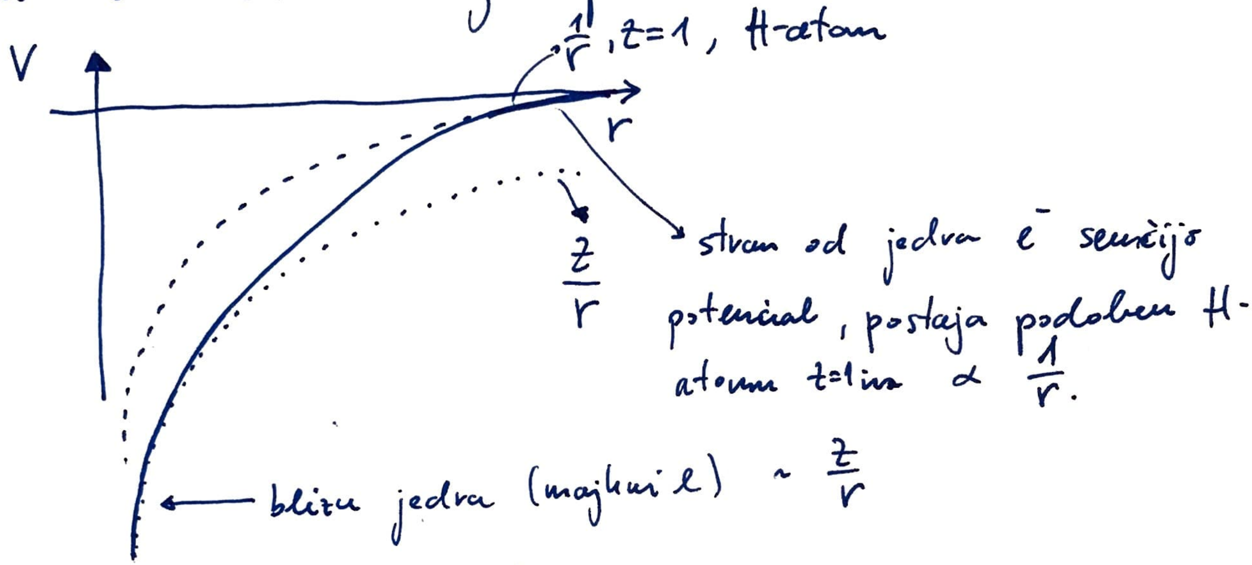
Večelektronska stanja

$$\hat{H} = \sum_i \frac{p_i^2}{2m} - Z \sum_i \frac{\alpha \hbar c}{r_i} + \sum_{j<i} \frac{\alpha \hbar c}{|r_j - r_i|}$$

naboj jedra

med-elektronska interakcija

Heuristično razumevanje potenciala



* manjši l : $E_n \sim -\frac{Z^2}{n^2} E_0 \Rightarrow$ bolj vezana stanja

* večji l : $E_n \sim -\frac{1}{n^2} E_0$ šibkeje vezana stanja

Spektroskopske oznake : s, p, d, f ... za $l = 0, 1, 2, 3$ ...

l \ n	1	2	3	4
0	1s [2x]	2s [2x]	3s [2x]	4s [2x]
1		2p [6x]	3p [6x]	4p [6x]
2			3d [10x]	

E ↓

H, He [n=1]
Li, Be [n=2]
B, C, N, O, F, Ne
Na, Mg [n=3]
Al, Si, P, S, Cl, Ar

Pri razporeditvi elektronskih energijskih nivojih veljajo Hundova pravila.

i) Regularni spekter z manj kot $1/2$ zasedenih e^-

max S, max L, min J

S... celotni spin, vsota po vseh e^-, podobno za L in J

ii) Invertirani spekter več kot pol zasedenih stanj

max S, max L, max J
(1) (2) (3)

Hundova pravila so dobra za določevanje osnovnih stanj in včasih za vzbujena stanja.

(1) $S = \max.$: večji spin $\Rightarrow$ bolj simetričen spinski del $\Rightarrow$ anti-simetrični prostorski del, ki zmanjša Coulombsko interakcijo.

(2) $L = \max$: podobno kot zgoraj, e^- gredo stran od izhodišča za velik L $\Rightarrow$ manjši Coulombski odboj $\Rightarrow$ bolj vezano

(3) a) e^- zasedeni nad polovico $\max J = L+S$

b) e^- pod $\min J = |L-S|$

III. 1 Atomska stanja

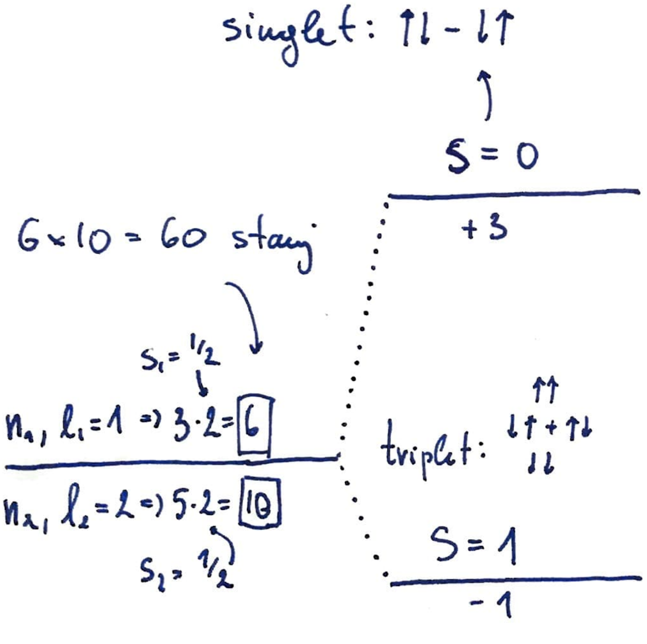
$\boxed{{}^{2S+1}L_J}$ spektroskopske oznake

$n_1, l_1 = 1$, $s_1 = \frac{1}{2}$ in n_2; $l_2 = 1$, $s_2 = \frac{1}{2}$

$L = l_1 + l_2$, $S = s_1 + s_2$, velja LS sklopitev / režim

LS režim: $\Delta E_{ls} = \frac{1}{2(mc)^2} \frac{1}{r} \frac{dV}{dr} \langle LS \rangle$

- za lažje atome velja LS režim, za težje pa J-J sklopitev (naslednja naloga)



singlet je bližje skupaj

$\Delta E = \frac{e^2}{|r_1 - r_2|^2} > 0$ singlet je manj vezan

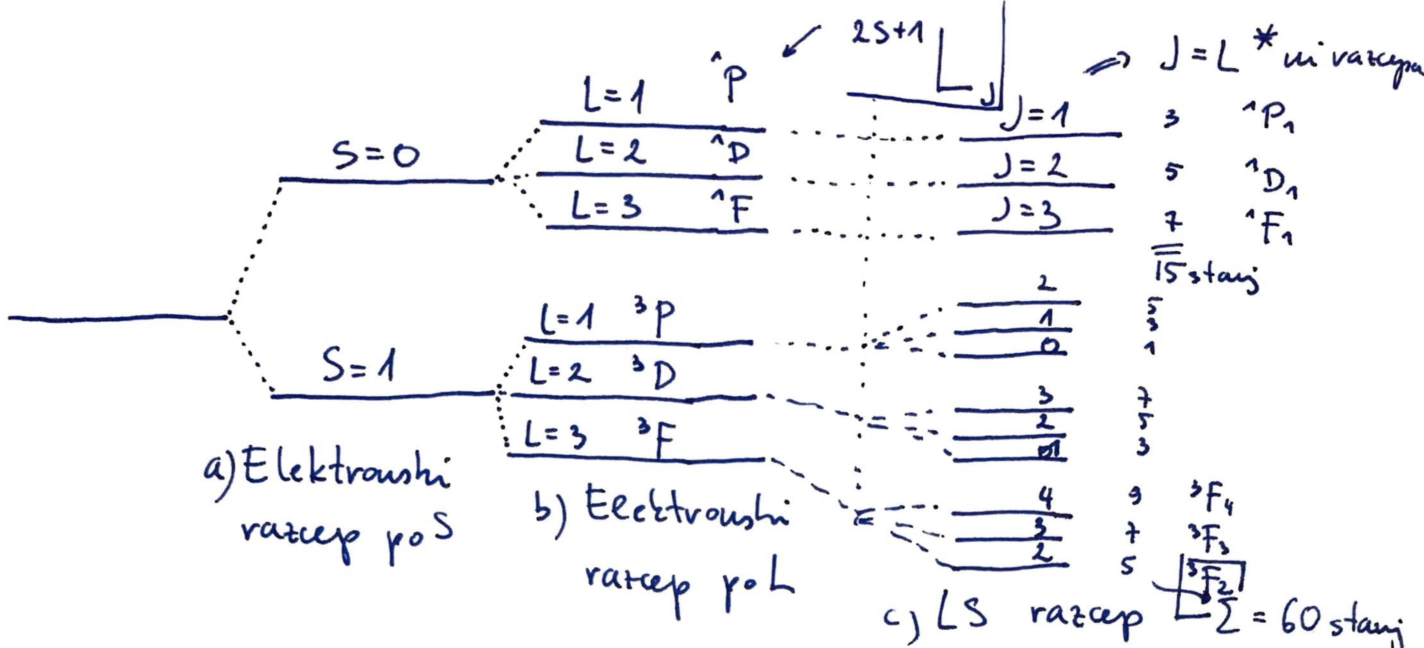
$s_1 + s_2 = 1 = S^{max}$

$|s_1 - s_2| = 0 = S^{min}$

a) spinski razcep: $\hat{H}_s = -\mu\, \hat{\vec{s}}_1 \cdot \hat{\vec{s}}_2$
$= -\frac{\mu}{2}(S^2 - s_1^2 - s_2^2)$

$\langle E_{S=0} \rangle = -\frac{\mu}{2}\left(0 - 2 \cdot \frac{3}{4}\right) = +\frac{\mu}{4} \cdot 3$

$S=1$: $\langle E_{S=1} \rangle = -\frac{\mu}{2}\left(1 \cdot 2 - \frac{3}{2}\right) = -\frac{\mu}{4}$



b) Večji kot je L, bolj so e^- narazen $\frac{e^2}{|r_i - r_j|}$ je manjši.

c) $\Delta E_{LS} \propto \frac{\hbar^2}{2}\left(J(J+1) - L(L+1) - S(S+1)\right)$

* za $S=0$: $J=L$ in $\Delta E_{LS} = 0$ ni razcepa

$\Rightarrow$ Stanje z najnižjo energijo je $^3F_2$ z $S=1$, $L=3$ in $J=2$.