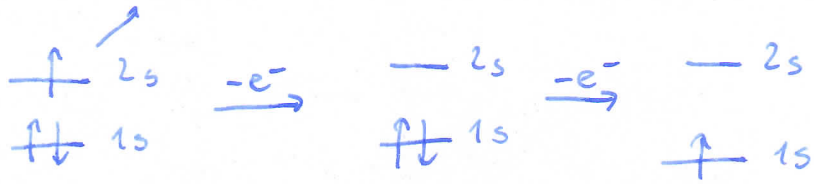
Prva ion. en. je 520,2 kJ/mol za Li, druga je 7298,1 kJ/mol. Kolikšna je skupna el. energija za litij?

$$Li \xrightarrow{-e^-} Li^+$$
$$Li^+ \xrightarrow{-e^-} Li^{2+}$$
$$Li^{2+} \xrightarrow{-e^-} Li^{3+}$$



$E_{vz} = -E_{i1}$ $E_{vz\,1s} = -E_2$ $E_{vz\,1s} = \frac{-13{,}6\,eV\,Z^2}{n^2} = -122{,}4\,eV$

$$\frac{520{,}2\ kJ/\cancel{mol}}{6{,}02\cdot10^{23}\ \cancel{mol}^{-1}} = 8{,}6369\cdot10^{-19}\,J : 1{,}6\cdot10^{-19}\,J/eV =$$
$$= 5{,}39\,eV = E_{i1}$$

$$E_{i2} = 75{,}73\,eV$$

$$E_{sk} = E_{vez} = -E_{i1} - E_{i2} + E_{vz\,1s} =$$
$$= -5{,}39\,eV - 75{,}73\,eV - 122{,}4\,eV =$$
$$= -203{,}5\,eV$$

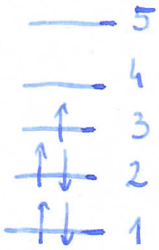
Neskončna pot. jama širine 5 Å. V jami se nahaja 5e⁻. El. konf. teh e⁻? Najnižja E, ki jo sistem absorbira, da preide v vzbujeno stanje v približku neinteragirajočih stanj?

$a = 5\,Å$

$5e^-$

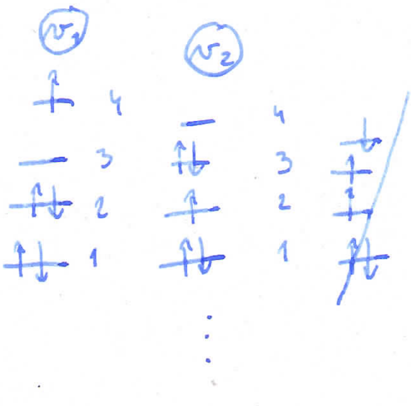
$$E_n = \frac{n^2 h^2}{8ma^2}$$

$n \in \mathbb{N}$



$1^2 2^2 3^1$

možnosti:



prehod ni možen - iz sodega na sodo

$E_0 = 2E_1 + 2E_2 + E_3$ } elektroni ne vplivajo eden na drugega

$E_{v1} = 2E_1 + 2E_2 + E_4$

$E_{v2} = 2E_1 + E_2 + 2E_3$

$\Delta E_1 = E_{v_1} - E_0 = E_4 - E_3 = \dfrac{7h^2}{8ma^2}$ prehod 1. možnosti

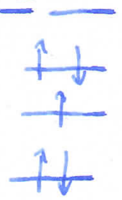
$\Delta E_2 = E_{v_2} - E_0 = -E_2 + E_3 = \underline{\underline{\dfrac{5h^2}{8ma^2}}}$ prehod 2. možnosti

$E_2 = \dfrac{4h^2}{8ma^2}$

$E_3 = \dfrac{9h^2}{8ma^2}$

$E_4 = \dfrac{16h^2}{8ma^2}$

Najnižja energija $\Delta E_2 \Rightarrow$ prvo vzbujeno stanje



Imamo dvonivojski sistem, v katerem deluje $\hat{H}$ v obliki
$\hat{H}_0 = \delta \hat{S}_z$; tu imamo še motnjo $\hat{H}' = \delta\Omega \hat{S}_x$.

Kakšen imamo energijski sistem (brez motenj)? In kakšnega z motnjo?

$$[\hat{H}_0, \hat{S}_z] = [\delta \hat{S}_z, \hat{S}_z] = \delta [\hat{S}_z, \hat{S}_z] = 0$$

$$\hat{S}_z \alpha = \tfrac{1}{2}\hbar \alpha \qquad \hat{H}_0 \alpha = \delta \hat{S}_z \alpha = \delta \tfrac{1}{2}\hbar \alpha = \tfrac{1}{2}\hbar \delta \alpha$$

$$\hat{S}_z \beta = -\tfrac{1}{2}\hbar \beta \qquad \hat{H}_0 \beta = \delta \hat{S}_z \beta = \delta \cdot -\tfrac{1}{2}\hbar \beta = -\tfrac{1}{2}\hbar \delta \beta$$

stanji	energiji		
β	$-\frac{1}{2}\hbar\delta$	- osnovno stanje	brez motenj
α	$\frac{1}{2}\hbar\delta$	- vzbujeno stanje	

Popravek 1. reda :

I os. stanje : $E_1 = \langle \beta | \hat{H}' | \beta \rangle$

spina: spin $\uparrow$, spin $\downarrow$

$\alpha = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ $\langle \alpha | \alpha \rangle = 1$

$\beta = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ $\langle \beta | \beta \rangle = 1$

$\langle \alpha | \beta \rangle = 0$

$$\hat{S}_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\hat{S}_z \beta = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} 0 \\ 1 \end{bmatrix} = \frac{\hbar}{2}\begin{bmatrix} 0 \\ -1 \end{bmatrix} = -\frac{\hbar}{2}\begin{bmatrix} 0 \\ 1 \end{bmatrix} = \underline{\underline{-\frac{\hbar}{2}\beta}}$$

$$\hat{S}^2 = \frac{3\hbar^2}{4}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad \hat{S}^2 \alpha = \frac{3\hbar^2}{4}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{3\hbar^2}{4}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \underline{\underline{\frac{3\hbar^2}{4}\alpha}}$$

$\hat{S}_x = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ $\hat{S}_y = \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$ $\hat{S}_x \beta = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 0 \\ 1 \end{bmatrix} = \frac{\hbar}{2}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{\hbar}{2}\alpha$

Popravek 1. reda:

$E_{10} = \langle \beta | \hat{H}' | \beta \rangle = \langle \beta | \Omega \frac{\hbar}{2} \alpha \rangle = \Omega \frac{\hbar}{2} \langle \beta | \alpha \rangle = \underline{\underline{0}}$

os. stanje

$\hat{S}_x \alpha = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{\hbar}{2}\begin{bmatrix} 0 \\ 1 \end{bmatrix} = \frac{\hbar}{2}\beta$

$E_{1v} = \langle \alpha | \frac{\hbar}{2}\Omega \beta \rangle = \frac{\hbar}{2}\Omega \langle \alpha | \beta \rangle = \underline{\underline{0}}$ $\Big\} \langle \alpha | \hat{H}' | \alpha \rangle$

vzb. stanje

Popravki 1. reda so enaki 0

$\Downarrow$

gledamo popravek

2. reda

Popravek 2. reda:

$$E_{2n}^2 = \sum_{k \neq n} \frac{|\langle \psi_n^0 | \hat{H}' | \psi_k^0 \rangle|^2}{E_n^0 - E_k^0}$$

$$E_{20} = \frac{\langle \beta | \hat{H}' | \alpha \rangle^2}{E_0^0 - E_v^0}$$

os. stanje

$$E_{2v} = \frac{\langle \alpha | \hat{H}' | \beta \rangle^2}{E_v^0 - E_0^0}$$

vzb. stanje

E_0^0	~	β	$-\frac{1}{2}\hbar\delta$
E_v^0	~	α	$\frac{1}{2}\hbar\delta$

$\hat{S}_x \alpha = \frac{\hbar}{2}\beta$

$\hat{S}_x \beta = \frac{\hbar}{2}\alpha$

$\langle \beta | \hat{H}' | \alpha \rangle = \langle \beta | \frac{\hbar}{2}\Omega \beta \rangle = \frac{\hbar}{2}\Omega$

$\langle \alpha | \hat{H}' | \beta \rangle = \langle \alpha | \frac{\hbar}{2}\Omega \alpha \rangle = \frac{\hbar}{2}\Omega$

$$E_{20} = \frac{\frac{\hbar^2}{4}\Omega^2}{-\hbar\delta} = \underline{\underline{-\frac{\hbar\Omega^2}{4\delta}}}$$

$$E_{2v} = \frac{\frac{\hbar^2}{4}\Omega^2}{\hbar\delta} = \underline{\underline{\frac{\hbar\Omega^2}{4\delta}}}$$

brez popravkov

popravek 1. in 2. reda

$$E_0 = E_0^0 + E_{10} + E_{20} = -\frac{1}{2}\hbar\delta + 0 - \frac{\hbar\Omega^2}{4\delta}$$

$$E_v = E_0^v + E_{1v} + E_{2v} = \frac{1}{2}\hbar\delta + 0 + \frac{\hbar\Omega^2}{4\delta}$$

$\beta \qquad E_0 = -\frac{\hbar}{2}\gamma$

$\alpha \qquad E_v = \frac{\hbar\gamma}{2}$

$$\psi_n = \psi_n^0 + \psi_n^1 + \cancel{\psi_n^2} + \dots$$

$$\psi_n^1 = \sum_{n \neq j} c_{nj}\, \psi_j^0$$

$$c_{nk} = \frac{\langle \psi_k^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_k^0}$$

$$\psi_0 = \beta + c_{\beta\alpha}\,\alpha = \beta - \frac{\Omega}{2\gamma}\alpha$$

$$c_{\beta\alpha} = \frac{\langle \alpha | H' | \beta \rangle}{-\frac{\hbar}{2}\gamma - \frac{\hbar}{2}\gamma} = \frac{\frac{\hbar}{2}\Omega}{-\hbar\gamma} = -\frac{\Omega}{2\gamma}$$

$$\psi_v = \alpha + c_{\alpha\beta}\,\beta = \alpha + \frac{\Omega}{2\gamma}\beta$$

$$c_{\alpha\beta} = \frac{\langle \beta | H' | \alpha \rangle}{\frac{2\hbar}{2}\gamma} = \frac{\Omega}{2\gamma}$$

brez motnje:

$E_0 = -\frac{\hbar\gamma}{2}$; β

$E_v = \frac{\hbar\gamma}{2}$; α

motnja:

$E_0 = -\frac{\hbar\gamma}{2} - \frac{\Omega\hbar}{4\gamma}$; $\beta - \frac{\Omega}{2\gamma}\alpha$

$E_v = \frac{\hbar\gamma}{2} + \frac{\Omega\hbar^2}{4\gamma}$; $\alpha + \frac{\Omega}{2\gamma}\beta$

novi val. funkciji po upoštevanju motnje (2. reda, saj je 1. reda = 0)

He :

$1s(1)1s(2)$ ~ osnovno stanje brez popravka

$1s(1)1s(2) + \sum_i c_{0i}\psi_i$ ~ osnovno stanje s popravkom I. reda

ψ_i ... $1s(1)\,2s(2)$
$2s(1)\,1s(1)$
$1s(1)\,2p_x(2)$
$1s(1)\,2p_y(2)$
$\vdots$