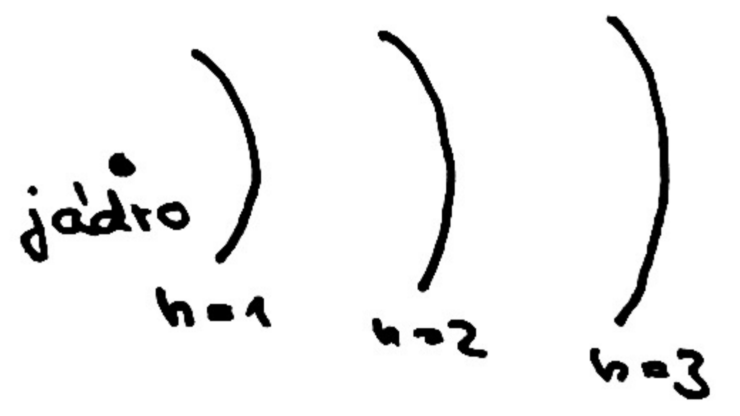
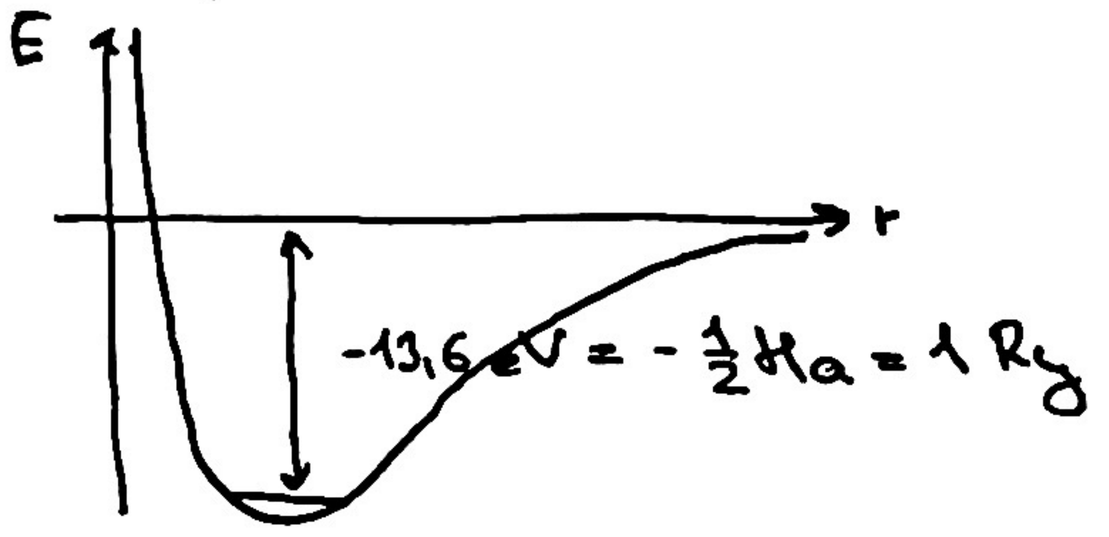
ATOM VODÍKU

① hrubá struktura

$\hat{H} = \frac{\hat{p}^2}{2} - \frac{1}{r} \Rightarrow E_n = -\frac{1}{2n^2}$ ve vodíku degenerace n^2

$\rightarrow 2n^2$ se spinem





② jemná struktura

QM + STR $\Rightarrow$ Diracova rovnice $[\vec{\sigma}\cdot(\vec{p}-e\vec{A})\frac{1}{E-e\varphi+m}\vec{\sigma}\cdot(\vec{p}-e\vec{A})]\Psi = (E-e\varphi-m)\Psi$

řešení v prvním řádu poruchové metody

$$\boxed{\mathcal{E}_1 = \frac{1}{2}\langle\psi_0| -(\mathcal{E}_0+\tfrac{1}{r})^2 + \pi\delta(\vec{r}) + \frac{\vec{\sigma}\cdot\vec{L}}{r^3}|\psi_0\rangle}$$

korekce ke kin. energii

kontaktní člen $\Downarrow$ nenulový pouze pro s-stavy (nenulová pst. výskytu e^- v jádře)

spin-orbitální člen $\Rightarrow$ nenulový pro ne-s-stavy (pro s-stav $L=0$)

hladina 2p

Ⓘ degenerovaná $\underline{\underline{6\times}}$: $3\times 2 = 6$

$m_\ell = -1, 0, 1$ $\quad m_s = -\frac{1}{2}, +\frac{1}{2}$

Ⓘⓘ $(\mathcal{E}_0+\frac{1}{r})^2 \rightarrow$ jen posune hladinu

$\pi\delta(\vec{r}) \rightarrow$ nepřispívá pro p-stavy

$\underline{\underline{\vec{\sigma}\cdot\vec{L} \rightarrow \text{rozštěpí p-stav}}}$

Ⓘⓘⓘ
$|I\rangle = |1\rangle|+\rangle$
$|II\rangle = |1\rangle|-\rangle$
$|III\rangle = |0\rangle|+\rangle$
$|IV\rangle = |0\rangle|-\rangle$
$|V\rangle = |-1\rangle|+\rangle$
$|VI\rangle = |-1\rangle|-\rangle$

ⒾⓋ $R_{12}(r) = \frac{1}{2\sqrt{6}} r e^{-\frac{r}{2}}$

$$\underline{\underline{\langle R_{12}|\tfrac{1}{r^3}|R_{12}\rangle}} = \int_0^\infty r^2 R_{12}^*(r)\frac{1}{r^3}R_{12}(r)\,dr = \int_0^\infty \frac{1}{2\sqrt{6}} r e^{-\frac{r}{2}} \frac{1}{r}\frac{1}{2\sqrt{6}} r e^{-\frac{r}{2}}\,dr = \frac{1}{24}\underbrace{\int_0^\infty r e^{-r}\,dr}_{=1} = \underline{\underline{\frac{1}{24}}}$$

(VI) (2')

$$\vec S\cdot\vec L = \tfrac{1}{2}(S_+L_- + S_-L_+) + S_zL_z \qquad S_\pm = S_1 \pm i S_2,\quad L_\pm = L_1 \pm i L_2$$

obecně $J_\pm |j,m\rangle = \sqrt{j(j+1)-m(m\pm1)}\,|j,m\pm1\rangle$

$J_3|j,m\rangle = m\,|j,m\rangle$

$\Rightarrow$ $S_\pm|\pm\rangle = 0$, $S_\mp|\pm\rangle = |\mp\rangle$, $S_z|\pm\rangle = \pm\tfrac12|\pm\rangle$

$\Rightarrow$ $L_+|1\rangle = 0$, $L_-|-1\rangle = 0$

$L_+|0\rangle = \sqrt2|1\rangle$, $L_-|0\rangle = \sqrt2|-1\rangle$

$L_+|-1\rangle = \sqrt2|0\rangle$, $L_-|1\rangle = \sqrt2|0\rangle$

$L_z|-1\rangle = -1\,|-1\rangle$, $L_z|0\rangle = 0\,|0\rangle$, $L_z|1\rangle = +1\,|1\rangle$

(VI')

$$\vec S\cdot\vec L\,|I\rangle = \vec S\cdot\vec L\,|1\rangle|+\rangle = \tfrac12(\underbrace{S_+|+\rangle}_{0} L_-|1\rangle + S_-|+\rangle \underbrace{L_+|1\rangle}_{0}) + \underbrace{S_z|+\rangle}_{+\frac12}\underbrace{L_z|1\rangle}_{+1} =$$

$$= \tfrac12|1\rangle|+\rangle = \tfrac12|I\rangle$$

$$\vec S\cdot\vec L\,|VI\rangle = \vec S\cdot\vec L\,|-1\rangle|-\rangle = \dots = \tfrac12|VI\rangle$$

$$\vec S\cdot\vec L\,|II\rangle = \vec S\cdot\vec L\,|1\rangle|-\rangle =$$

$$= \tfrac12(\underbrace{S_+|-\rangle}_{|+\rangle}\underbrace{L_-|1\rangle}_{\sqrt2|0\rangle} + \underbrace{S_-|-\rangle}_{0}\underbrace{L_+|1\rangle}_{0}) + \underbrace{S_z|-\rangle}_{-\frac12|-\rangle}\underbrace{L_z|1\rangle}_{1|1\rangle}$$

$$= \tfrac{1}{\sqrt2}|+\rangle|0\rangle - \tfrac12|-\rangle|1\rangle =$$

$$= \tfrac{1}{\sqrt2}|III\rangle - \tfrac12|II\rangle$$

$$\vec S\cdot\vec L\,|III\rangle = \vec S\cdot\vec L\,|0\rangle|+\rangle = \dots = \tfrac{1}{\sqrt2}|II\rangle$$

$$\vec S\cdot\vec L\,|IV\rangle = \vec S\cdot\vec L\,|0\rangle|-\rangle = \dots = \tfrac{1}{\sqrt2}|V\rangle$$

$$\vec S\cdot\vec L\,|V\rangle = \vec S\cdot\vec L\,|-1\rangle|+\rangle = \dots = \tfrac{1}{\sqrt2}|IV\rangle - \tfrac12|V\rangle$$

$\Rightarrow$ $|I\rangle$ a $|VI\rangle$ jsou vl. stavy $\vec L\cdot\vec S$,

ale $|II\rangle$ a $|III\rangle$ se míchají } musíme najít vhodné LK

a $|IV\rangle$ a $|V\rangle$

(VII)

$c_2|II\rangle + c_3|III\rangle$

$$\vec S\cdot\vec L\,(c_2|II\rangle + c_3|III\rangle) = \lambda(c_2|II\rangle + c_3|III\rangle)$$

$$c_2\left(\tfrac{1}{\sqrt2}|III\rangle - \tfrac12|II\rangle\right) + c_3\left(\tfrac{1}{\sqrt2}|II\rangle\right) = \lambda(c_2|II\rangle + c_3|III\rangle)$$

$$\begin{pmatrix} -\frac12 & \frac{1}{\sqrt2} \\ \frac{1}{\sqrt2} & 0 \end{pmatrix}\begin{pmatrix} c_2 \\ c_3 \end{pmatrix} = \lambda\begin{pmatrix} c_2 \\ c_3 \end{pmatrix} \Rightarrow -\lambda(-\tfrac12-\lambda) - \tfrac12 = 0 \Rightarrow \lambda = \begin{cases} \frac12 : & c_2 = \frac{1}{\sqrt3},\ c_3 = \sqrt{\frac23} \\ -1 : & c_2 = \sqrt{\frac23},\ c_3 = -\frac{1}{\sqrt3} \end{cases}$$

+ normalizace $|c_2|^2 + |c_3|^2 = 1$

$$|\widetilde{II}\rangle = \tfrac{1}{\sqrt3}|II\rangle + \sqrt{\tfrac23}|III\rangle \quad (\lambda = \tfrac12)$$

$$|\widetilde{III}\rangle = \sqrt{\tfrac23}|II\rangle - \tfrac{1}{\sqrt3}|III\rangle \quad (\lambda = -1)$$

$\Uparrow$

a analogicky pro $|IV\rangle$ a $|V\rangle$:

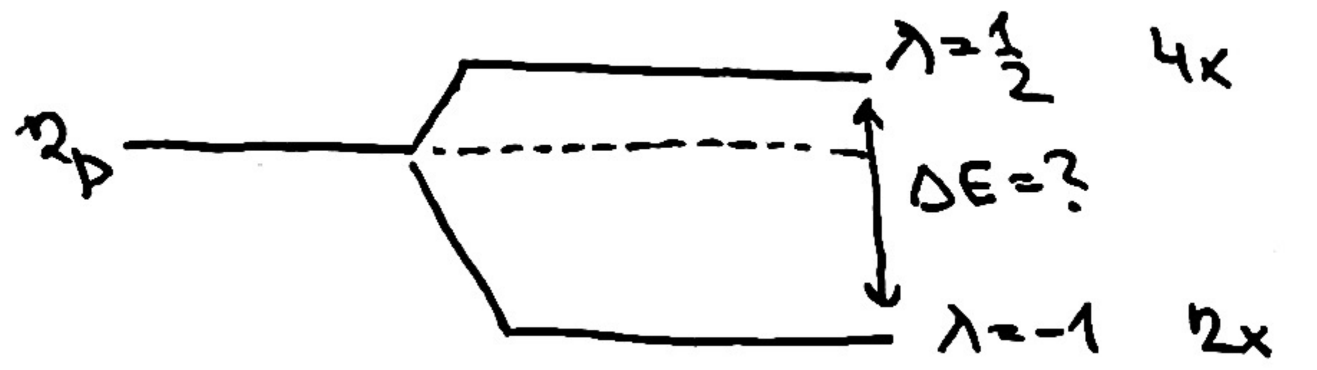
$$|\widetilde{IV}\rangle = -\frac{1}{\sqrt{3}}|IV\rangle + \sqrt{\frac{2}{3}}|V\rangle \qquad (\lambda = -1)$$

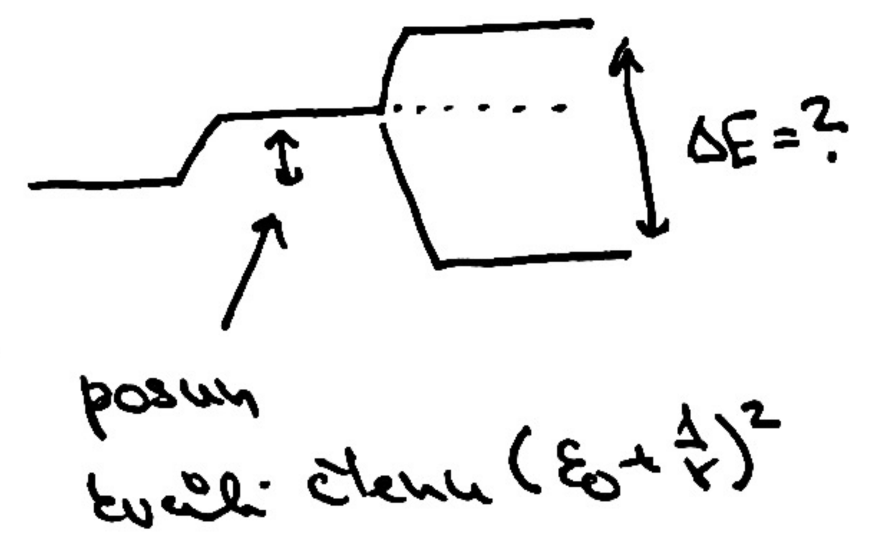
$$|\widetilde{V}\rangle = \sqrt{\frac{2}{3}}|IV\rangle + \frac{1}{\sqrt{3}}|V\rangle \qquad (\lambda = \tfrac{1}{2})$$

(IX)

sextet $\longrightarrow$ kvadruplet $\lambda = \frac{1}{2}$ $\quad |I\rangle, |\widetilde{II}\rangle, |\widetilde{V}\rangle, |VI\rangle$

$\searrow$ dublet $\lambda = -1$ $\quad |\widetilde{III}\rangle, |\widetilde{IV}\rangle$





$$\Delta E = \frac{1}{48}\left(\frac{1}{2} - (-1)\right) = \frac{1}{32} \text{ Ha}$$

$$\Delta E = \Delta \mathcal{E}\, m (Z\alpha)^4$$

$$\Delta\nu = R_\infty Z^4 \alpha^{-1}\, 2\Delta\mathcal{E} \longrightarrow \text{teor. } 10949 \text{ MHz}$$

(10969 MHz exp.) $\quad \Delta\lambda \doteq 2{,}7$ cm

(X) zavedení celkového momentu hybnosti $\vec{J}$ $\qquad \vec{J}^2 |j,m\rangle = j(j+1)|j,m\rangle$

$\vec{J} = \vec{S} + \vec{L}$ $\qquad J_z |j,m\rangle = m|j,m\rangle$

$$J^2 = (\vec{S}+\vec{L})^2 = S^2 + L^2 + 2\vec{S}\cdot\vec{L}$$

$$\Rightarrow \vec{S}\cdot\vec{L} = \frac{1}{2}(J^2 - S^2 - L^2) \longrightarrow \frac{1}{2}\left[j(j+1) - s(s+1) - l(l+1)\right] =$$

$$= \frac{1}{2}\left[j(j+1) - \frac{1}{2}\left(\frac{1}{2}+1\right) - 1(1+1)\right] =$$

(XI)

$$= \frac{1}{2}\left[j(j+1) - \frac{3}{4} - 2\right] =$$

$$= \frac{1}{2}\left[j(j+1) - \frac{11}{4}\right] = \begin{cases} \frac{1}{2} \Rightarrow j = \frac{3}{2} \\ -1 \Rightarrow j = \frac{1}{2} \end{cases}$$

$$|I\rangle = |1\rangle|+\rangle: \quad J_z|I\rangle = (S_z + L_z)|I\rangle = S_z|+\rangle|1\rangle + L_z|1\rangle|+\rangle =$$

$$= \frac{1}{2}|1\rangle|+\rangle + 1\,|1\rangle|+\rangle =$$

$$= \frac{3}{2}|I\rangle$$

~~$|II\rangle = |1\rangle|-\rangle$ $J_z|II\rangle$~~

$$|\widetilde{II}\rangle = \frac{1}{\sqrt{3}}|II\rangle + \sqrt{\frac{2}{3}}|III\rangle: \quad J_z|\widetilde{II}\rangle = (S_z + L_z)\Big(\frac{1}{\sqrt{3}}\underbrace{|II\rangle}_{|1\rangle|-\rangle} + \sqrt{\frac{2}{3}}\underbrace{|III\rangle}_{|0\rangle|+\rangle}\Big) =$$

$$= \frac{1}{\sqrt{3}}\left(-\frac{1}{2}+1\right)|II\rangle + \sqrt{\frac{2}{3}}\left(\frac{1}{2}+0\right)|III\rangle =$$

$$= \frac{1}{2}|\widetilde{II}\rangle$$

a analogicky pro zbylé stavy

$$J_z|\mathrm{I}\rangle = \tfrac{3}{2}|\mathrm{I}\rangle \qquad J^2|\mathrm{I}\rangle = \tfrac{3}{2}(\tfrac{3}{2}+1)|\mathrm{I}\rangle$$

$$J_z|\widetilde{\mathrm{II}}\rangle = \tfrac{1}{2}|\widetilde{\mathrm{II}}\rangle \qquad J^2|\widetilde{\mathrm{II}}\rangle = \tfrac{3}{2}(\tfrac{3}{2}+1)|\widetilde{\mathrm{II}}\rangle$$

$$J_z|\widetilde{\mathrm{III}}\rangle = \tfrac{1}{2}|\widetilde{\mathrm{III}}\rangle \qquad J^2|\widetilde{\mathrm{III}}\rangle = +\tfrac{1}{2}(+\tfrac{1}{2}+1)|\widetilde{\mathrm{III}}\rangle$$

$$J_z|\widetilde{\mathrm{IV}}\rangle = -\tfrac{1}{2}|\widetilde{\mathrm{IV}}\rangle \qquad J^2|\widetilde{\mathrm{IV}}\rangle = \tfrac{1}{2}(\tfrac{1}{2}+1)|\widetilde{\mathrm{IV}}\rangle$$

$$J_z|\widetilde{\mathrm{V}}\rangle = -\tfrac{1}{2}|\widetilde{\mathrm{V}}\rangle \qquad J^2|\widetilde{\mathrm{V}}\rangle = \tfrac{3}{2}(\tfrac{3}{2}+1)|\widetilde{\mathrm{V}}\rangle$$

$$J_z|\mathrm{VI}\rangle = -\tfrac{3}{2}|\mathrm{VI}\rangle \qquad J^2|\mathrm{VI}\rangle = \tfrac{3}{2}(\tfrac{3}{2}+1)|\mathrm{VI}\rangle$$

XV např. v magnetickém poli lze dále sejmout degeneraci

→ Zeemanův jev