$$\hat{H}_{RS} = \hat{H}_{MC} + \hat{H}_{D1} + \hat{H}_{D2} + \hat{H}_{OO} + \hat{H}_{SSC}$$

KONTAKTNA SPIN-SPIN INTERAKCIJA

$$\hat{H}_{SSC} = -\frac{8\pi\alpha^2}{3}\sum_{i<j}^{N}(\vec{s}_i\cdot\vec{s}_j)\,\delta(\vec{r}_i-\vec{r}_j)$$

ORBIT-ORBIT (TIR-TIR) INTERAKCIJA

$$\hat{H}_{OO} = -\frac{\alpha^2}{2}\sum_{i<j}^{N}\left[\frac{\vec{p}_i\cdot\vec{p}_j}{r_{ij}} + \frac{\vec{r}_{ij}\,(\vec{r}_{ij}\cdot\vec{p}_i)\,\vec{p}_j}{r_{ij}^{3}}\right]$$

$$\hat{H}_{D2} = \frac{\alpha^2}{4}\sum_{i<j}^{N}\nabla_i^2\left(\frac{1}{r_{ij}}\right)$$ ENODELČNI

$$\hat{H}_{D1} = -\frac{\alpha^2 Z}{8}\sum_{i}\nabla_i^2\left(\frac{1}{r_i}\right)$$ DVODELČNI

DARWINOV OPERATOR

$$\hat{H}_{MC} = -\frac{\alpha^2}{8}\sum_{i}(\nabla_i)^{+}\nabla_i^2$$

RELATIVISTIČNI MASNI POPRAVEK

OPERATOR RELATIVISTIČNEGA PREMIKA

$$\hat{H}_{FS} = \hat{H}_{SO} + \hat{H}_{SOO} + \hat{H}_{SS}$$

INTERAKCIJA SPIN-SPIN

$$\hat{H}_{SS} = \alpha^2 \sum_{i<j}^{N} \frac{1}{r_{ij}^3}\left[\vec{s}_i\cdot\vec{s}_j - \frac{3(\vec{s}_i\cdot\vec{r}_{ij})(\vec{s}_j\cdot\vec{r}_{ij})}{r_{ij}^2}\right]$$

INTERAKCIJA SPIN-DRUGI TIR

$$\hat{H}_{SOO} = -\frac{\alpha^2}{2}\sum_{i<j}^{N}\frac{\vec{r}_{ij}\times\vec{p}_i}{r_{ij}^3}(\vec{s}_i + 2\vec{s}_j) \equiv H_{SOO}^{(1)} + \boxed{H_{SOO}^{(2)}}$$

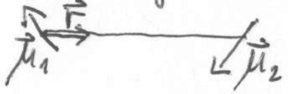
$H_{SOO}^{(1)}$: ZARADI $\vec{E}$ POLJA elektronov

$H_{SOO}^{(2)}$: MAGNETNO POLJE ZARADI GIBANJA e^-

INTERAKCIJA SPIN-TIR ZARADI $\vec{E}$ POLJA JEDRA

$$\hat{H}_{SO} = \frac{\alpha^2 Z}{2}\sum_{i}^{N}\frac{\vec{l}_i\cdot\vec{s}_i}{r_i^3}$$

Interakcija energija dveh magnetnih dipolov!



$$\frac{\mu_0}{4\pi r^3}\left[\vec{\mu}_1\cdot\vec{\mu}_2 - 3(\vec{\mu}_1\cdot\vec{r})(\mu_2\cdot\vec{r})\right]$$

$$\vec{\mu}_i \propto \vec{s}_i \longrightarrow \hat{H}_{SS}$$

● $\vec{E}_i = Z\frac{\vec{r}_i}{r_i^3} - \sum_{j}^{j\neq i}\frac{\vec{r}_{ij}}{r_{ij}^3}$ ... $\vec{E}$ polje na mestu elektrona i

$$H_{SO} + H_{SOO}^{(1)} = \frac{\alpha^2}{2}\sum_i(\vec{E}_i\times\vec{p}_i)\cdot\vec{s}_i = \frac{\alpha^2}{2}\sum_i\left[\frac{Z}{r_i^3}\vec{r}_i\times\vec{p}_i - \sum_j^{j\neq i}\frac{\vec{r}_{ij}}{r_{ij}^3}\times\vec{p}_i\right]\cdot\vec{s}_i$$

■ $\vec{j}_i(\vec{r}) = \vec{v}_i\rho_i(\vec{r}) = -e\vec{v}_i\delta(\vec{r}-\vec{r}_i)$ ... električni tok e^-

$$\vec{B}_{ij} = \frac{\mu_0}{4\pi}\int\vec{j}_i\times\frac{\vec{r}_{ij}}{r_{ij}^3}\,d\vec{r} = -\frac{\mu_0}{4\pi}e\vec{v}_i\times\frac{\vec{r}_{ij}}{r_{ij}^3} = -\alpha^2\vec{p}_i\times\frac{\vec{r}_{ij}}{r_{ij}^3}$$

$$H_{SOO}^{(2)} = \alpha^2\sum_{i<j}\left(\vec{p}_i\times\frac{\vec{r}_{ij}}{r_{ij}^3}\right)\cdot\vec{s}_j$$

V približku centralnega polja lahko spin-tir interakcijo upoštevamo z obliko:

$$H_{SO}^{eff} = \sum_i \xi_i \, \vec{l}_i \cdot \vec{s}_i$$ ... vsota teče le po elektronih v odprtih podlupinah

SPIN-ORBIT (TIR) PARAMETER $\xi_i = \frac{\alpha^2}{2}\left\langle \frac{1}{r}\frac{dU}{dr}\right\rangle$ ... U je efektivni enodelčni potencial

Po potrebi dodamo še $H_{SOO}^{(2)}$ in H_{SS}, kjer vsota spet le po odprtih podlupinah

MAGNETNI MOMENT

$|\mu| = \frac{e\hbar}{2m_e}\sqrt{l(l+1)}$ $\quad \vec{\mu} = I\vec{S} = -\left(\frac{e}{T}\right)\pi r^2$, $T = \frac{2\pi r}{v}$ $\rightarrow \vec{\mu} = -\frac{e}{2m_e}\vec{l}$

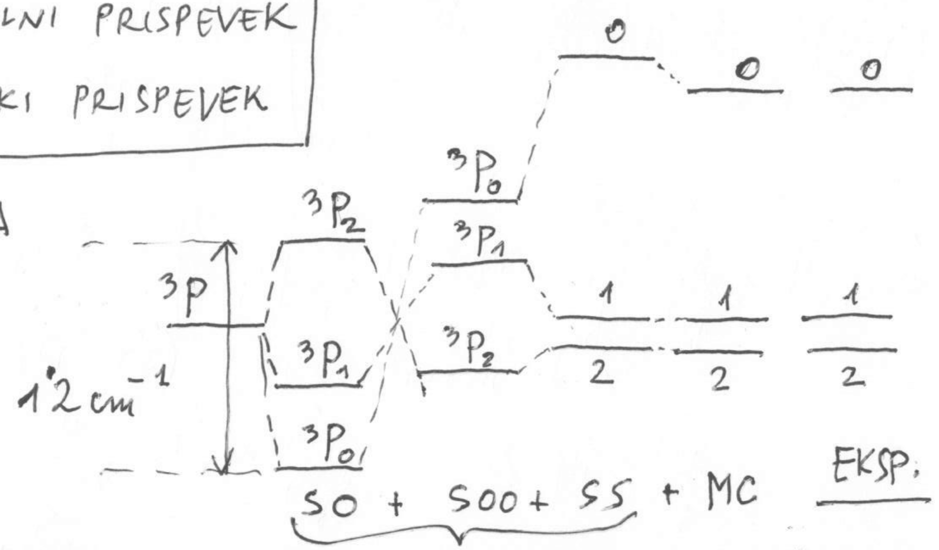
$= \mu_B \sqrt{l(l+1)}$ $\quad \mu_B$ .. BOHROV MAGNETON $\frac{e\hbar}{2m_e} = 9.27 \cdot 10^{-24}\,\mathrm{Am}^2$

$\mu_z = -\mu_B m_l$ ... ORBITALNI PRISPEVEK

$\mu_z = -\overset{\approx 2}{g_s}\mu_B m_s$ ... SPINSKI PRISPEVEK

PRIMER: FINA STRUKTURA

He $1s2p\,^3P$



ODVISNOST MATRIČNIH ELEMENTOV FINE STRUKTURE OD J

4

$$E_{so} = \langle \gamma LSJM | \hat{H}_{so} | \gamma LSJM \rangle = \frac{\alpha^2 Z}{2} \langle \gamma LSJM | \sum_i \frac{\vec{l}_i \cdot \vec{s}_i}{r_i^3} | \gamma LSJM \rangle$$

$$= \frac{\alpha^2 Z}{2} (-1)^{J-M} \begin{pmatrix} J & 0 & J \\ -M & 0 & M \end{pmatrix} \langle \gamma LSJ \| \sum_i \frac{\vec{l}_i \cdot \vec{s}_i}{r_i^3} \| \gamma LSJ \rangle \rightarrow \sum_i \{ u_i^1(\text{prostor})\, t_i^1(\text{spin}) \}^0_0$$

$$= \frac{\alpha^2 Z}{2} (-1)^{J-M} \frac{(-1)^{J-M}}{\sqrt{[J]}} (-1)^{L+S+J} \sqrt{[J]} \begin{Bmatrix} L & S & J \\ S & L & 1 \end{Bmatrix}$$

$$\times \sum_i \langle \gamma_L L \| \vec{l}_i \| \gamma_L L \rangle \langle \gamma_s S \| \vec{s}_i \| \gamma_s S \rangle$$

$$\propto (-1)^{L+S+J} \begin{Bmatrix} L & S & J \\ S & L & 1 \end{Bmatrix} \propto J(J+1) - L(L+1) - S(S+1)$$

$$E_{so} = \xi_{so} [J(J+1) - L(L+1) - S(S+1)]$$

$$E_{soo} = \langle \gamma LSJM | H_{soo} | \gamma LSJM \rangle = -\frac{\alpha^2}{2} \langle \gamma LSJM | \sum_{i<j}^{N} \left(\frac{\vec{r}_{ij} \times \vec{p}_i}{r_{ij}} \right) (\vec{s}_i + 2\vec{s}_j) | \gamma LSJM \rangle$$

$$\propto \sum_{i>j} \{ \text{vektor}(\text{prostor}) \cdot \text{vektor}(\text{spin}) \}^0_0$$

$$E_{soo} \propto (-1)^{L+S+J} \begin{Bmatrix} L & S & J \\ S & L & 1 \end{Bmatrix} \propto J(J+1) - L(L+1) - S(S+1)$$

$$= \xi_{soo} [(J+1)J - L(L+1) - S(S+1)]$$

$$E_{ss} = \alpha^2 \langle \gamma LSJ | \sum_{i<j} \frac{1}{r_{ij}} \left[\vec{s}_i \cdot \vec{s}_j - \frac{3(\vec{s}_i \cdot \vec{r}_{ij})(\vec{s}_j \cdot \vec{r}_{ij})}{r_{ij}^2} \right] | \gamma LSJ \rangle \propto A + B (-1)^{L+S+J} \begin{Bmatrix} L & S & J \\ S & L & 2 \end{Bmatrix}$$

$$\langle \gamma_L L \| \tfrac{1}{r_{ij}} \| \gamma_L L \rangle \langle \gamma_S S \| \vec{s}_i \cdot \vec{s}_j \| \gamma_S S \rangle$$

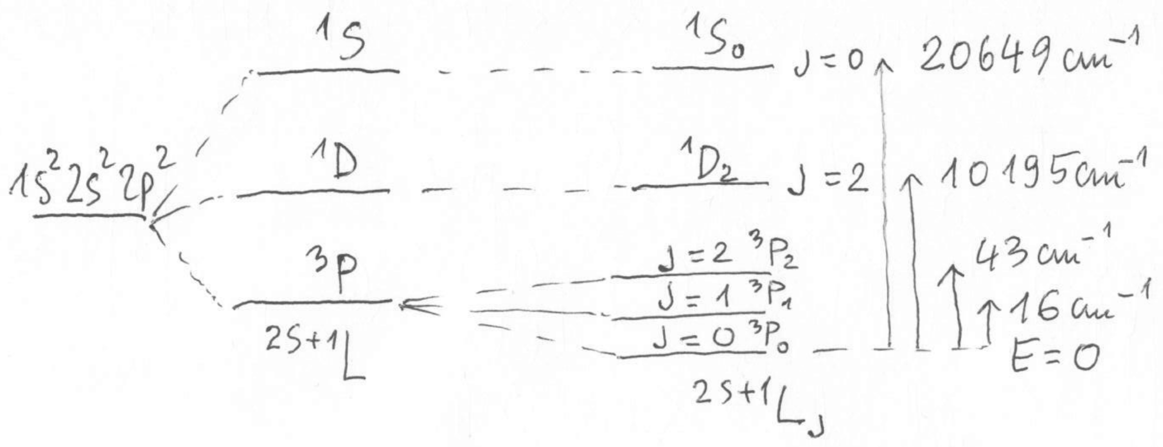
$$\langle \gamma_L L \| \vec{r}_{ij} \otimes \vec{r}_{ij} \| \gamma_L L \rangle \langle \gamma_S S \| \vec{s}_i \otimes \vec{s}_j \| \gamma_S S \rangle$$

$$\{\text{skalar}(P)\ \text{skalar}(S)\}^0_0 \qquad \{\text{matrika}(P)\ \text{matrika}(S)\}^0_0$$

$$\propto A + \xi_{ss} \left[\frac{3}{4} C(C+1) - L(L+1) - S(S+1) \right]$$

$$C \equiv J(J+1) - L(L+1) - S(S+1)$$

PRIMER: FINA STRUKTURA V OSNOVNEM STANJU OGLJIKA:



$E_{SS} \approx 0$

$$\Delta E_{FS} = E_{FS}^{J} - E_{FS}^{J-1}$$

$$= 2\left[\xi_{SO}(\gamma LS) + \xi_{SOO}(\gamma LS)\right] J$$

$$\equiv 2\xi J$$

$\xi > 0$ ... normalna FS

$\xi < 0$ ... obrnjena FS

EFEKT KONČNEGA JEDRA S SPINOM NA ATOMSKE NIVOJE

(1) IZOTOPSKI PREMIK. UPOŠTEVANJE REDUCIRANE MASE SISTEMA JEDRO-e^- NAMESTO MASE e^- m_e

VODIK:

$$E_n = -\frac{1}{2}\left(\frac{m_R}{m_e}\right)\frac{Z^2}{n^2} \qquad m_R = m_e \frac{m_j}{m_e + m_j}$$

$$= -\frac{1}{2}\frac{Z^2}{n^2} \cdot X_j \qquad X_H = 0{,}9995 \quad X_D = 0{,}9998$$

Opazimo majhne premike spektralnih črt, če opazujemo različne izotope istega elementa.

(2) HIPERFINA STRUKTURA. INTERAKCIJA MED MAGNETNIM DIPOLOM JEDRA, KI JE SORAZMEREN S SPINOM TER MAGNETNIM POLJEM e^- NA OBMOČJU JEDRA

(6)

$$\vec{\mu}_j = \gamma_j \vec{I} = g_j \mu_N \vec{I}$$

vrtilna količina jedra

jedrski Bohrov magneton

giromagnetno razmerje jedra
neutron : -3.8261
proton : 5.5857

$$\mu_N = \frac{e\hbar}{2m_p} = 5.05 \cdot 10^{-27}\,\mathrm{Am}^2 \approx \frac{\mu_B}{2000}$$

$$H_{HFS} = -\vec{\mu}_j \cdot \vec{B}_e \propto \langle \vec{I} \cdot \vec{J} \rangle$$

... KOMUTIRA S CELOTNO VRTILNO KOLIČINO ATOMA $\vec{F} = \vec{J} + \vec{I}$

$$\Delta E_{HFS} \propto \left(F(F+1) - I(I+1) - J(J+1)\right)$$

OSNOVNO STANJE VODIKA:

$I = 1/2 \quad J = 1/2 \; ({}^2S_{1/2})$

$$F = \begin{cases} \uparrow_p \; \uparrow_{e^-}, & 1 \\ \uparrow_p \; \downarrow_{e^-}, & 0 \end{cases}$$

$1s\,{}^2S_{1/2}$ — $F=1$, $F=0$

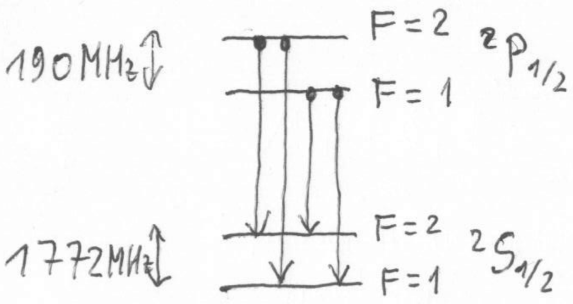
$1420\,\mathrm{MHz} = \Delta E_{HFS} = 0.00475\,\mathrm{cm}^{-1}\;(5{,}9 \cdot 10^{-6}\,\mathrm{eV})$

$\downarrow$

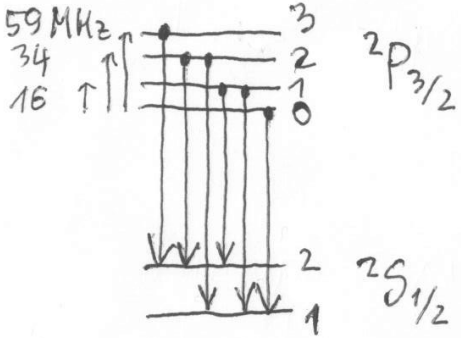
$\lambda = 21\,\mathrm{cm}$

HIPERFINA STRUKTURA PREHODA V Na: $3p\,^2P_{1/2,\,3/2} \rightarrow 3s\,^2S_{1/2}$

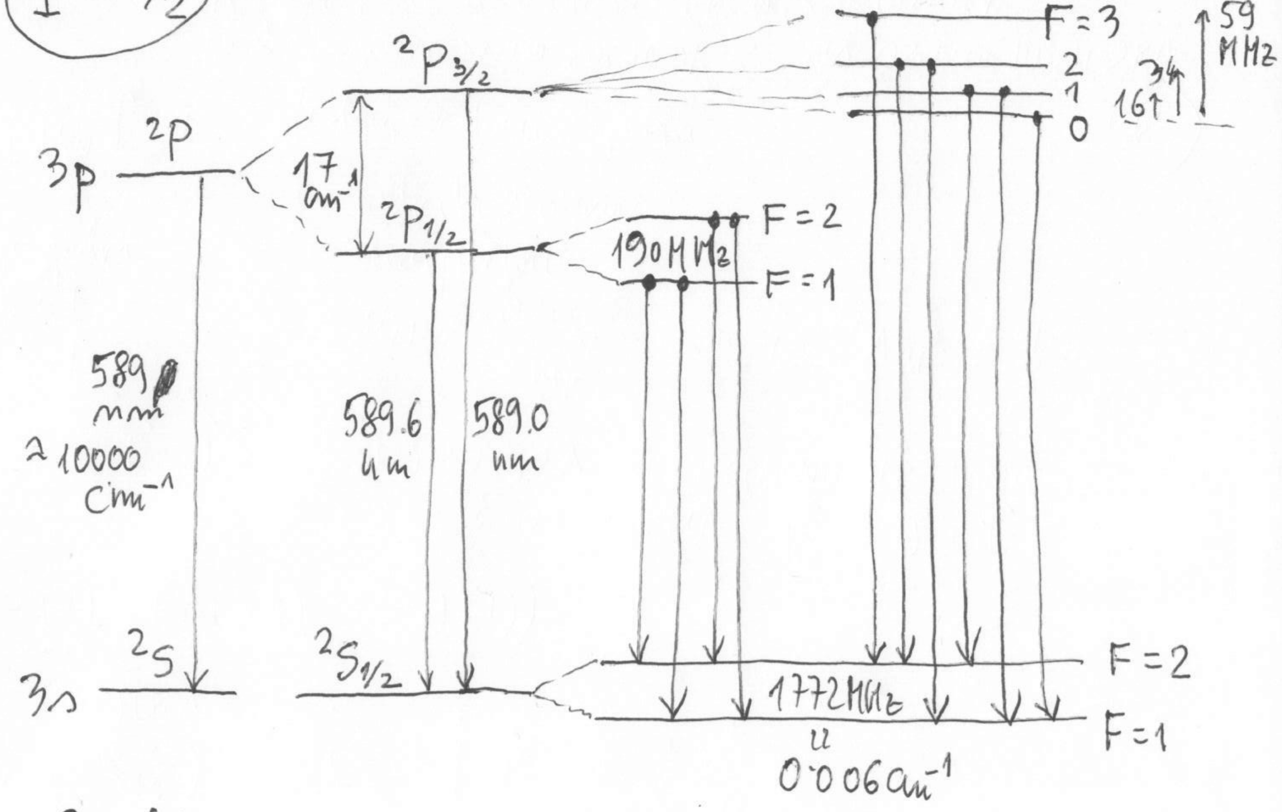
$I = 3/2$



4 črte



6 črt



Prehoda $3 \rightarrow 1$ ter $0 \rightarrow 2$ sta dipolno prepovedana.

Spekter