(59) $\psi = A(R_1 + 2R_2)$

$$\left.\begin{aligned} \psi &= A(R_1 + 2R_2) \\ \psi_\perp &= A(2R_1 - R_2) \end{aligned}\right\} \quad A = \frac{1}{\sqrt{5}} \qquad l = 0$$

$$E_n = -\frac{E_{Ry}}{n^2}, \quad E_{Ry} = 13{,}6\,eV$$

$$\frac{\langle E\rangle_\perp}{\langle E\rangle} = \frac{\frac{1}{5}(4E_1 + E_2)}{\frac{1}{5}(E_1 + 4E_2)} = \frac{4 + \frac{1}{4}}{1 + 1} = \frac{\frac{17}{4}}{2} = \frac{17}{8}$$

Povprečni radij $\langle r\rangle = \int_V \psi^* r \psi \, dV$

$$R_1 = \frac{2}{r_B^{3/2}} e^{-r/r_B}, \quad R_2 = \frac{2}{(2r_B)^{3/2}}\left(1 - \frac{r}{2r_B}\right) e^{-\frac{r}{2r_B}}$$

$$\Rightarrow \langle r\rangle = \frac{1}{5}\int_0^\infty (R_1 + 2R_2)\, r\, (R_1 + 2R_2)\, r^2 dr$$

$$= \frac{1}{5}\left(\langle 1|r|1\rangle + 4\langle 1|r|2\rangle + 4\langle 2|r|2\rangle\right)$$

- $\langle 1|r|1\rangle = \int_0^\infty \frac{4}{r_B^3} e^{-2r/r_B} r^3 dr = \ldots = \underline{\frac{3}{2} r_B}.$

- $\langle 1|r|2\rangle = \frac{\cancel{4}\sqrt{2}}{\cancel{2}\,2^{3/2}\, r_B^3}\int_0^\infty \left(1 - \frac{r}{2r_B}\right) e^{-\frac{3r}{2r_B}} r^3 dr \qquad t = \frac{3r}{2r_B}$

$$= \frac{\sqrt{2}\, r_B}{\cancel{r_B^3}}\int_0^\infty e^{-t}\left(1 - \frac{t}{3}\right)\left(\frac{2r_B}{3}\right)^4 t^3 dt$$

$$\bullet\ \langle 1|r|2\rangle = \left(\frac{2}{3}\right)^4 \sqrt{2}\, r_B \int_0^\infty \left(t^3 - \frac{t^4}{3}\right) e^{-t}\, dt$$

$$= \left(\frac{2}{3}\right)^4 \sqrt{2}\,(6-8)\, r_B = -0{,}56\, r_B$$

$$\bullet\ \langle 2|r|2\rangle = \frac{\cancel{4}}{2\cancel{8}\, r_B^3} \int_0^\infty \left(1 - \frac{r}{2r_B}\right)^2 e^{-r/r_B}\, r^3\, dr$$

$$= \frac{r_B}{2} \int_0^\infty e^{-t} \left\{ t^3 \left(1 - \frac{1}{2}t\right)^2 dt\right.$$

$$= \frac{r_B}{2} \left(3! - \cancel{3!}\overset{4!}{} + \frac{1}{4}\, 5! \right)$$

$$= \frac{r_B}{2} \left(6 - 24 + 30 \right) = 6\, r_B$$

$$\bullet\ \langle 1|r|1\rangle = \frac{3}{2}\, r_B$$

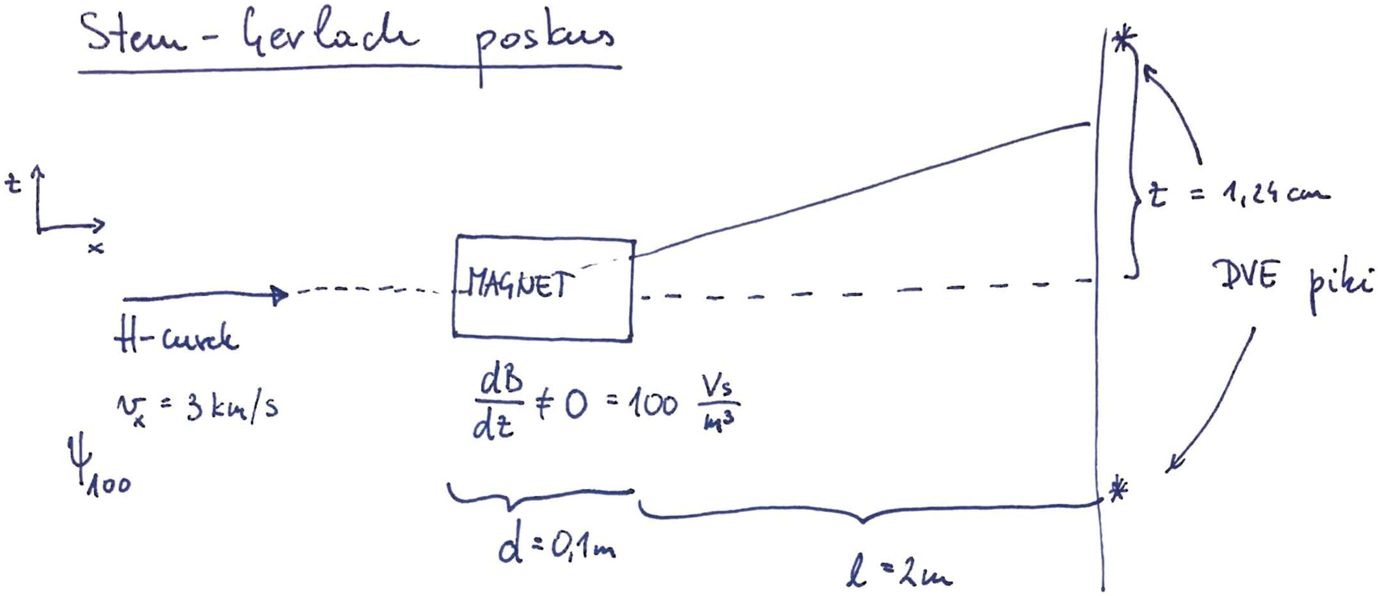
$$\langle r\rangle = \frac{1}{5}\left(\langle 1|r|1\rangle + 4\langle 1|r|2\rangle + 4\langle 2|r|2\rangle \right)$$

$$= \frac{1}{5}\left(\frac{3}{2} - 4\cdot 0{,}56 + 4\cdot 6 \right) r_B \simeq 4{,}7\, r_B$$

$$\langle r\rangle_\perp = \frac{1}{5}\Big(4\underbrace{\langle 1|r|1\rangle}_{3/2\, r_B} - 4\underbrace{\langle 1|r|2\rangle}_{-0{,}56\, r_B} + \underbrace{\langle 2|r|2\rangle}_{6\, r_B} \Big)$$

$$= \frac{r_B}{5}\left(6 + 4 \times 0{,}56 + 6 \right) \simeq 2{,}85\, r_B .$$

Stern - Gerlach poskus



$$F_z = p_{mz} \frac{dB}{dz}$$

→ gradient B-polja

magnetni dipol

Bohrov magneton

$$\mu_B = \frac{e\hbar}{2m_e}$$

klasično : $\vec{p}_m = \frac{e}{2}\, \vec{r} \times \vec{v} = \frac{e}{2m}\, \vec{l} \xrightarrow{QM} \hat{\mu}_i = -\frac{\mu_B}{\hbar}\, g_e \hat{L}_i$

ampak : $F_z = g_e \mu_B \frac{\langle L_z \rangle}{\hbar} \frac{dB}{dz} \xrightarrow{m=0} 0$

Potrebujemo novo dodatno kvantno število : spin, podobno vrtilni količini, a intrinzično – ne zaradi kroženja.

$\Rightarrow \hat{\mu} = -\frac{\mu_B}{\hbar}\left(g_L \hat{L} + g_s \hat{S}\right)$; degeneracija je vedno $2s+1$,

ker opazimo dve piki $\Rightarrow 2s+1 = 2 \Rightarrow s = 1/2$

$$F_z = g_s \mu_B \frac{\langle \hat{S}_z \rangle}{\hbar} \frac{dB}{dz} = \pm \frac{g_s \mu_B}{2} \frac{dB}{dz} \quad ; \quad g_s = ?$$

• določimo g_s iz v_z

$$\int F_z \, dt = m_p \int dv_z = m_p v_z \qquad ; \qquad \frac{v_z}{v_x} = \frac{z}{l}$$

$$\|$$

$$F_z \cdot \frac{d}{v_x} = \underbrace{\mu_B \frac{g_s}{2} \frac{dB}{dz} \frac{d}{v_x} = m_p v_z}$$

$$g_s = \frac{2 m_p v_x^2 z}{\mu_B \frac{dB}{dz} d l} = \frac{2 m_p c^2 \, 2 m_e c^2 \, \beta_x^2 \, z}{e \hbar c \frac{dB}{dz} c \quad dl}$$

$$= \frac{2 \,\text{GeV} \quad \text{MeV} \quad (3 \cdot 10^3 / 3 \cdot 10^8)^2 \quad 1{,}2 \cdot 10^{-2} \,\text{m}}{200 \,\text{eV nm} \quad 100 \,\frac{\text{eV s}}{\text{m}^3} \cdot 3 \cdot 10^8 \,\frac{\text{m}}{\text{s}} \quad 0{,}2 \,\text{m}^2}$$

$\longrightarrow$ 2 v okviru napake.

Ključna posledica SG poskusa je obstoj spina velikosti $\frac{1}{2}$. Obnaša se kot vrtilna količina in ga moramo dodati v valovno funkcijo elektrona.

$$\psi_{nlm_l} \rightarrow \psi_{nlm_l s m_s}$$

$$\hat{S}^2 \psi_{\dots s m_s} = \hbar^2 s(s+1) \,, \quad \hat{S}_z \psi_{\dots s m_s} = \hbar m_s \psi_{\dots s m_s}$$

L-S sklopitev

Poleg magnetne sile na dipol v gradientu magnetnega polja, se zaradi obstoja spina spremenijo energijski nivoji atoma vodika.

$$\Delta E_{ls} = \frac{\alpha \hbar c}{2(mc)^2} \left\langle \frac{1}{r^3} \right\rangle \langle ls \rangle$$

Če želimo določiti $\langle ls \rangle$ je dobro uvesti celotno vrtilno količino : $\hat{j} = \hat{l} + \hat{s}$, $\hat{j}^2 = \hat{l}^2 + 2\hat{l}\hat{s} + \hat{s}^2$

tako da : $\langle ls \rangle = \frac{1}{2} \left(\langle j^2 \rangle - \langle l^2 \rangle - \langle s^2 \rangle \right)$

$$\psi_{nlm_l s m_s} \xrightarrow[\text{baze}]{\text{sprememba}} \psi_{nlsjm_j} \quad : \quad \hat{j}^2 \psi_{nlsjm_j} = \hbar^2 j(j+1) \psi_{\dots}$$

$$\hat{j}_z \psi_{nlsjm_j} = \hbar m_j \psi_{nlsjm_j}$$

Orbitalna in spinska vrtilna količina, ~~A~~ kvantni števili l in s, se seštejeta v celotno vrtilno količino j.

SEŠTEVANJE
$$\begin{cases} j_{max} = l + s \\ j_{min} = |l - s| \end{cases}$$
in $m_j = -j, -j+1, \dots, j-1, j$

• za elektron je $s = 1/2$, $m_s = \pm \frac{1}{2}$. Kako sedaj seštejemo v j za nek fiksen ℓ?

$\boxed{\ell = 0}$, $m_\ell = 0$, $s = 1/2$, $m_s = \pm \frac{1}{2}$ $\Rightarrow$ DVE stanji

$$\left.\begin{aligned} j_{max} &= \ell + s = 0 + \tfrac{1}{2} = \tfrac{1}{2} \\ j_{min} &= |\ell - s| = |0 - \tfrac{1}{2}| = \tfrac{1}{2} \end{aligned}\right\} \quad j = 1/2 \,, \quad m_j = \tfrac{1}{2}$$

$\Rightarrow$ DVE stanji

$$\underset{n\,\ell\,m_\ell\,s\,m_s}{\psi_{n 0 0 \frac{1}{2} \pm\frac{1}{2}}} \longrightarrow \underset{n\,\ell\,s\,j\,m_j}{\psi_{n 0 \frac{1}{2} \frac{1}{2} \pm\frac{1}{2}}}$$

$\boxed{\ell = 1}$, $m_\ell = 0, \pm 1$, $s = 1/2$, $m_s = \pm \frac{1}{2}$ $\Big\}$ $\underset{m_\ell = 0,1 \;\; m_s = \pm\frac{1}{2}}{3 \cdot 2} = 6$ stanj

$(2\ell+1) \times (2s+1) = 3 \cdot 2$

$$j_{max} = 1 + \tfrac{1}{2} = \tfrac{3}{2} \qquad j = \left(\tfrac{1}{2}, \tfrac{3}{2}\right)$$

$$j_{min} = |1 - \tfrac{1}{2}| = \tfrac{1}{2} \qquad m_j = \pm\tfrac{1}{2} \qquad m_j = \pm\tfrac{1}{2}, \pm\tfrac{3}{2}$$

2 + 4 stanj = 6 stanj

$$\langle \ell s \rangle = \tfrac{1}{2}\left(\langle j^2 \rangle - \langle \ell^2 \rangle - \langle s^2 \rangle\right)$$

$$= \frac{\hbar^2}{2}\left(j(j+1) - \ell(\ell+1) - s(s+1)\right) = \frac{\hbar^2}{2} \begin{cases} \cancel{\tfrac{1}{2} \cdot \tfrac{3}{2}} - 1 \cdot 2 - \cancel{\tfrac{1}{2} \cdot \tfrac{3}{2}} = -2 \\ \tfrac{3}{2}\,\tfrac{5}{2} - 2 - \tfrac{3}{4} = \tfrac{12-8}{4} = +1 \end{cases}$$

$$= \begin{cases} -\hbar^2 & \text{za } j = \tfrac{1}{2} \\ +\frac{\hbar^2}{2} & \text{za } j = \tfrac{3}{2} \end{cases}$$

(60) Določi ΔE_{ls} za $\psi_{211} = \frac{1}{8\sqrt{\pi r_B^3}} \frac{r}{r_B} S_\theta e^{-\frac{r}{2r_B}} e^{i\varphi}$

$$\Delta E_{ls} = \frac{\alpha \hbar c}{2(mc)^2} \left\langle \frac{1}{r^3} \right\rangle \langle ls \rangle$$

$$S_\theta^2 = 1 - C_\theta^2$$

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{\cancel{64}_{32}\, \pi r_B^3} \int_0^\infty \cancel{r^2} dr \int_{-1}^{1} dC_\theta\, \cancel{2\pi} \left(\frac{r}{r_B}\right)^2 \frac{1}{\cancel{r^3}} e^{-\frac{r}{r_B}} S_\theta^2 \cdot 1$$

$$= \frac{1}{32\, r_B^3} \underbrace{\left(2 - \frac{2}{3}\right)}_{\frac{4}{3}} \underbrace{\int_0^\infty \frac{r}{r_B} e^{-\frac{r}{r_B}} \frac{dr}{r_B}}_{1!} = \frac{1}{24 r_B^3} = \frac{(\alpha mc^2)^3}{24(\hbar c)^3}$$

$$\Delta E_{ls} = \frac{\alpha \cancel{\hbar c} \cdot \cancel{c^2}}{2(m\cancel{c^2})^{\cancel{2}}} \cdot \frac{\alpha^3 (mc^2)^{\cancel{3}}}{24 \cancel{(\hbar c)^3}} \cdot \cancel{\hbar^2} \cdot \begin{cases} \frac{1}{2} & j = 3/2 \\ -1 & j = 1/2 \end{cases}$$

$$= \frac{\alpha^4}{96} mc^2 \cdot \begin{cases} 1 \\ -2 \end{cases} = \begin{cases} 1{,}5 \cdot 10^{-5}\,\text{eV} = 15\,\mu\text{eV}, \\ -3 \cdot 10^{-5}\,\text{eV} = -30\,\mu\text{eV}. \end{cases}$$

Torej se $E_2 = -\frac{13{,}6\,\text{eV}}{4}$ črta razcepi za $\sim 10^{-5}$ eV na dve črti ena nad in druga 2x pod originalno vrednostjo.