Sedaj imamo:

$$r = \frac{r_B}{2} t, \qquad dr = \frac{r_B}{2} dt.$$

$$\langle V \rangle = -\alpha \hbar c \int_0^\infty dr\, r^{\cancel{2}} \frac{4}{r_B^3} \frac{1}{\cancel{r}} e^{-\overset{t}{\overset{\shortparallel}{\frac{2r}{r_B}}}}$$

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

$$= -\frac{\alpha \hbar c}{r_B} \int_0^\infty dt\, t e^{-t} = -\frac{\alpha \hbar c}{r_B} = -\alpha^2 m c^2$$

$$\hookrightarrow \left\langle \frac{1}{r} \right\rangle = \frac{1}{n^2 r_B}$$

$$\Rightarrow \quad 2\langle T \rangle = \alpha^2 m c^2$$

$$\text{in} \quad -\langle V \rangle = \alpha^2 m c^2 \qquad \boxed{\checkmark}$$

Poglejmo si še načelo nedoločenosti za ψ_{100}

$$\langle p \rangle = 0, \qquad \langle p^2 \rangle = 2m \langle T \rangle = \cancel{2}m \frac{\alpha^2 m c^2}{\cancel{2}}$$

$$r_B = \frac{\hbar c}{\alpha m c^2} \qquad = \frac{\alpha^2 m^2 c^4}{\hbar^2 c^2} \cdot \hbar^2 = \left(\frac{\hbar}{r_B}\right)^2.$$

Za $\langle r^p \rangle$ lahko izpeljemo splošno formulo:

$$\langle r^p \rangle = \int \psi_{100}\, r^p\, \psi_{100}\, dV = \frac{\cancel{4\pi}}{\cancel{4\pi}} \int_0^\infty dr\, r^{2+p} \frac{4}{r_B^3} e^{-\overset{t}{\overset{\shortparallel}{\frac{2r}{r_B}}}}$$

$$= \frac{4}{r_B^3} \left(\frac{r_B}{2}\right)^{p+3} \underbrace{\int_0^\infty dt\, t^{2+p} e^{-t}}_{(p+2)!} = \frac{(p+2)!}{2^{p+1}} r_B^p = \frac{(p+2)!}{2^{p+1}} r_B^p.$$

Iz splošne formule dobimo:

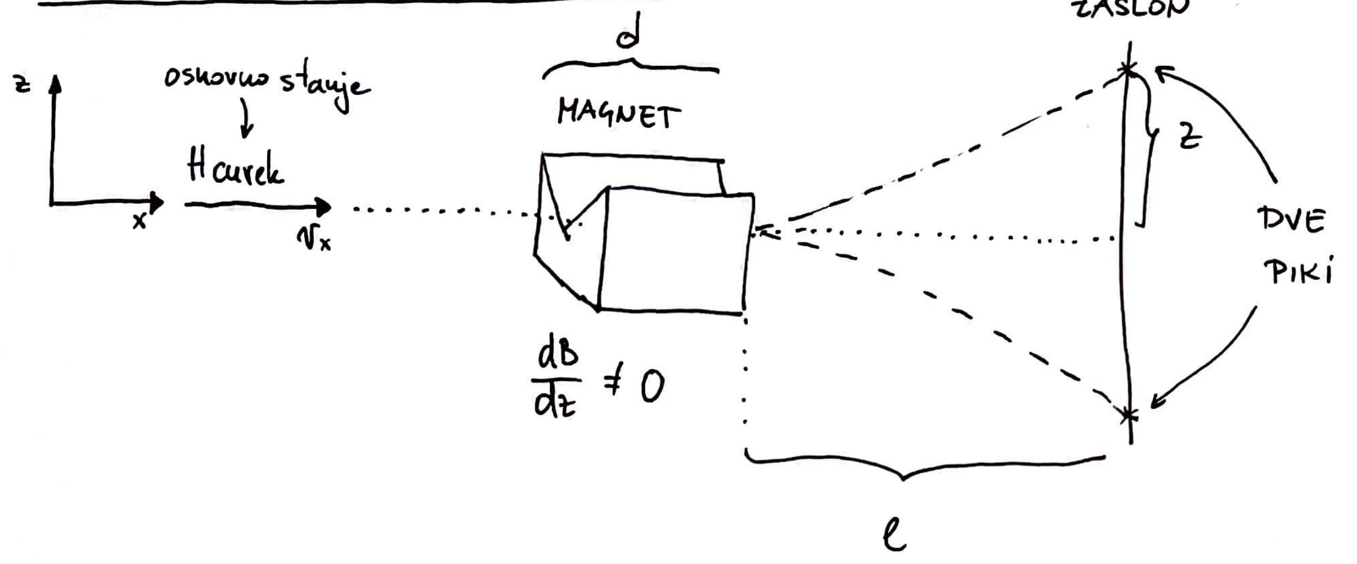
$$\langle r^2\rangle = \frac{4!}{2^3}\, r_B^2 = 3\, r_B^2 \quad \text{in} \quad \langle r\rangle = \frac{3!}{2^2}\, r_B = \frac{3}{2}\, r_B,$$

kot smo že vedeli.

$$\Rightarrow \quad \delta r = \sqrt{\langle r^2\rangle - \langle r\rangle^2} = r_B \sqrt{\underbrace{3 - \frac{9}{4}}_{\frac{3}{4}}} = \frac{\sqrt{3}}{2}\, r_B \,, \quad \delta p = \frac{\hbar}{r_B}$$

$$\delta p\, \delta r = \frac{\sqrt{3}}{2}\hbar = \frac{\hbar}{2}\cdot\sqrt{3} \approx 1.73 \cdot \frac{\hbar}{2}.$$

STERN-GERLACHOV POSKUS



Začetni vpadni curek so atomi vodika H v osnovnem stanju z $l=0$, $m=0$ in $n=1$, t.j. ψ_{100}

Sila na magnetni dipol v z smeri je $F_z = p_{mz} \frac{dB}{dz}$

dipolni magnetni moment — gradient gostote magnetnega polja

KLASIČNO : $p_{mz} = \frac{e}{2m_e}(\vec{r}\times\vec{p})_z = \frac{e}{2m_e} L_z$, $\vec{L} = \vec{r}\times\vec{p}$, $\vec{p} = m_e\vec{v}$

KVANTNO : $\hat{\mu}_z = -g_e \frac{e}{2m_e}\langle \hat{L}_z\rangle = -g_e \underbrace{\frac{e\hbar}{2m_e}}_{\mu_B} \frac{\langle L_z\rangle}{\hbar} = -\frac{\mu_B}{\hbar} g_e \langle L_z\rangle$

konvencija

μ_B ... Bohrov magneton

$$F_z = -\langle \mu_z\rangle \frac{dB}{dz} = -\frac{\mu_B}{\hbar} g_e \langle L_z\rangle \frac{dB}{dz}$$

Za lastna stanja ψ_{nlm} velja $\hat{L}_z \psi_{nlm} = \hbar m \psi_{nlm}$, $\langle L_z\rangle = \hbar m$.

Sila na dipol je torej $F_z = -m g_e \frac{dB}{dz}$, a v osnovnem stanju je $m=0$ in je $F_z = 0$. A opazimo dve piki, torej $F_z \neq 0$. Uvedemo novo kvantno število, spin:

$$\hat{\mu} = -\frac{\mu_B}{\hbar}\left(g_e \hat{L} + g_s \hat{S}\right)$$

giromagnetna faktorja

Spin se obnaša tako kot vrtilna količina in ima svoje operatorje $\hat{S}_{i, i=x,y,z}$, $\hat{S}^2$. Valovni funkciji ψ_{nem} moramo dodati dve kvantni števili : s... celoten spin in m_s... projekcija spina na z-os. Torej: $\psi_{nem} \rightarrow \psi_{nem_e s m_s}$

in velja : $\hat{S}_z \psi_{nem_e s m_s} = \hbar s \, \psi_{nem_e s m_s}$ in : $\hat{S}^2 \psi_{nem_e s m_s} = \hbar^2 s(s+1) \psi_{nem_e s m_s}$.

Število stanj (degeneracije) za posamezen s je $2s+1$.

Opazimo 2 piki = 2 stanji. Sledi : $2s+1 = 2 \Rightarrow s = \frac{1}{2}$.

[Delcem s spinom $\frac{1}{2}, \frac{3}{2}, \ldots$ pravimo fermioni, tistim s spinom $0, 1, 2, \ldots$ pa bosoni.]

Vrnimo se na SG poskus in izvrednotimo silo za stanja $\psi_{nem_e s m_s}$

$$F_z = \frac{\mu_B}{\hbar}\left(g_e \langle L_z \rangle + g_s \langle S_z \rangle\right)\frac{dB}{dz} = \mu_B \left(g_e m_e + g_s m_s\right)\frac{dB}{dz} = \underline{\underline{\pm \frac{1}{2}\mu_B g_s \frac{dB}{dz}}}$$

Tako dobimo silo na atom H kot posledico sklopitve spina e^- z gradientom B. Neznani faktor g_s dobimo iz eksperimenta.

$v_x = 3\frac{km}{s}$, $z = 1{,}24\,cm$, $d = 0{,}1\,m$, $l = 2m$, $\frac{dB}{dz} = 100\frac{Vs}{m^3}$, $\mu_B = \frac{e\hbar}{2m_e}$

sila v z-smeri je konstantna, čas preleta dobimo iz d in v_x: $t = \frac{d}{v_x}$

$$\int_0^t F_z \, dt = \int_0^{v_z} m_p \, dv_z \Rightarrow \frac{1}{2}\mu_B g_s \frac{dB}{dz}\cdot\frac{d}{v_x} = m_p v_z = m_p v_x \frac{z}{l} \quad \text{ker: } \frac{v_z}{z} = \frac{v_x}{l}$$

$$\Rightarrow g_s = \frac{2 m_p v_x^2 z}{\mu_B \frac{dB}{dz} d l} = \frac{2 m_p c^2 \, 2 m_e c^2 \, \beta_x^2 \, z}{e \frac{dB}{dz} \hbar c \, d l \cdot c} = \frac{2\,GeV \; 1\,MeV \left(\frac{3\cdot 10^3}{3\cdot 10^8}\right)^2 1{,}2\cdot 10^{-2}\,m}{200\,eV\,nm \; 100\frac{eVs}{m^3}\; 3\cdot 10^8\frac{m}{s}\; 0{,}2\,m^2}$$

$$= 2 \quad \text{(v okviru napake)}$$

L-S oz. Spin-tirna sklopitev

Poleg sile na dipolni moment, ima spin elektrona vpliv tudi na energijske nivoje v atomu vodika. Spin elektrona se namreč lahko sklopi z induciranim dipolom, ki je posledica tirne vrtilne količine $\hat{L}$.

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

Povprečja $\langle r^p \rangle$ že znamo izračunati, sedaj si poglejmo kako dobimo $\langle LS \rangle$ za določena stanja. V ta namen uvedemo celotno vrtilno količino $\hat{J} = \hat{L} + \hat{S}$ in preidemo iz ene baze v drugo: $\psi_{nlm_l s m_s} \xrightarrow[\text{baznih stanj}]{\text{linearna sprememba}} \psi_{nlsjm_j} = \psi_x$. Za ta stanja velja:

$$\begin{aligned}
\hat{L}^2 \psi_x &= \hbar^2 l(l+1)\, \psi_x \\
\hat{S}^2 \psi_x &= \hbar^2 s(s+1)\, \psi_x \\
\hat{J}^2 \psi_x &= \hbar^2 j(j+1)\, \psi_x \\
\hat{J}_z \psi_x &= \hbar m_j\, \psi_x
\end{aligned}$$

so lastna stanja teh štirih operatorjev s temi lastnimi vrednostmi

Nas zanima skalarni produkt, ki ga dobimo iz

$$J = L + S \Rightarrow J^2 = L^2 + 2LS + S^2 \quad / \langle\ \rangle$$

$$\langle LS \rangle = \frac{\langle J^2 \rangle - \langle L^2 \rangle - \langle S^2 \rangle}{2}$$

$$= \frac{\hbar^2}{2}\left(j(j+1) - l(l+1) - s(s+1) \right).$$

Poglejmo si, kako določimo j in kako se prerazporedijo stanja med tema dvema bazama.

Kvantna števila j in m_j dobimo takole:

a) Določimo maksimalno $j_{max} = l+s$,

b) Minimalno vrednost $j_{min} = |l-s|$,

c) Gremo od j_{min} do j_{max} v korakih po 1,

d) Za vsak j gredo m_j od $\underbrace{-j \text{ pa do } +j}_{2j+1 \text{ stanj (degeneracija)}}$ v korakih po 1.

Poglejmo kako se to napravi za atom H, kjer ima e^- $s = 1/2$ in projekciji $m_s = \pm 1/2$. Gremo po vrsti za poljubne $n = 1, 2, \ldots$ in $l = 0, 1, 2, \ldots$

$\boxed{l=0}$ $\quad j_{max} = l + s = 0 + \frac{1}{2} = \frac{1}{2}$, $\quad j_{min} = |0 - \frac{1}{2}| = \frac{1}{2}$, samo en $j = \frac{1}{2}$.

$$\psi_{nlm_lsm_s} = \underbrace{\psi_{n00\frac{1}{2}\pm\frac{1}{2}}}_{2 \text{ stanji},\ m_s = \pm\frac{1}{2}} \Longrightarrow \psi_{nlsjm_j} = \underbrace{\psi_{n0\frac{1}{2}\frac{1}{2}\pm\frac{1}{2}}}_{2 \text{ stanji},\ m_j = \pm\frac{1}{2}}.$$

$\boxed{l=1}$ $\quad j_{max} = 1 + \frac{1}{2} = \frac{3}{2}$, $\quad j_{min} = |1 - 1/2| = \frac{1}{2}$ $\Rightarrow$ 2 možnosti za $j = \frac{1}{2}, \frac{3}{2}$

$\psi_{nlm_lsm_s}$: $\quad [l = 0 \quad m_l = 0]$

$\qquad l = 1 \quad m_l = \pm 1, 0$,

$\qquad s = \frac{1}{2} \quad m_s = \pm \frac{1}{2}$

ψ_{nlsjm_j}: $\quad j = \frac{1}{2}$, $m_j = \pm \frac{1}{2}$

$\qquad j = \frac{3}{2}$, $m_j = \pm \frac{3}{2}, \pm \frac{1}{2}$

št. stanj $\# = (2l+1)(2s+1) = 3 \cdot 2 = 6$, $\quad \# = 2j+1$, torej: $(2\,\frac{1}{2} + 1) + (2 \cdot \frac{3}{2} + 1)$

$= 2 + 4 = 6.$

Sedaj, ko poznamo l, s in j, lahko izvrednotimo $\langle LS \rangle$

$\boxed{l=0}$, $s=\frac{1}{2}$, $j=\frac{1}{2}$: $\langle LS\rangle = \frac{\hbar^2}{2}\left(j(j+1) - \cancel{l(l+1)}^{\,0} - s(s+1)\right) = 0$

↳ NI RAZCEPA ZA $l=0$

$\boxed{l=1}$, $s=\frac{1}{2}$, $j=\begin{cases}\frac{1}{2} \\ \frac{3}{2}\end{cases}$, $\langle LS\rangle = \frac{\hbar^2}{2}\begin{cases} \cancel{\frac{1}{2}}\left(\frac{3}{2}\right) - 2 - \cancel{\frac{3}{4}} = -2 \\ \frac{3}{2}\,\frac{5}{2} - 2 - \frac{3}{4} = \frac{15-8-3}{4} = 1 \end{cases}$

LS razcep na dve veji

→ .... $\langle LS\rangle = \hbar^2 \begin{cases} -1, & \text{za } j=\frac{1}{2}, \\ \frac{1}{2}, & \text{za } j = \frac{3}{2}. \end{cases}$

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

izgine, ko vzamemo $\psi^* \frac{1}{r^3}\psi$

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

$$\left\langle\frac{1}{r^3}\right\rangle = \frac{1}{2^6\pi r_B^3}\underbrace{\int_0^{2\pi} d\varphi}_{2\pi}\int_{-1}^{1} d(\cos\theta)\int_0^\infty \cancel{r^2}\,dr\,\underbrace{(1-\cos^2\theta)}_{\sin^2\theta}\left(\frac{r}{r_B^2}\right)^{\cancel{2}}\frac{1}{\cancel{r^3}}\,e^{-\overbrace{\frac{r}{r_B}}^{t}}, \quad dr = r_B\,dt$$

$$= \frac{1}{2^5 r_B^3}\underbrace{\int_{-1}^{1} dc\,(1-c^2)}_{2-\frac{2}{3}=\frac{4}{3}}\underbrace{\int_0^\infty dt\, e^{-t}\,t}_{1!} = \frac{1}{2^3\cdot 3 r_B^3} = \frac{1}{24 r_B^3} = \underline{\frac{1}{24}\left(\frac{\alpha mc^2}{\hbar c}\right)^3}.$$

$$\langle LS\rangle = \hbar^2\begin{cases} -1 & \text{za } j=1/2 \\ \frac{1}{2} & \text{za } j=3/2\end{cases}$$

$$\Rightarrow \Delta E_{es} = \frac{\alpha\,\cancel{\hbar c}\,\alpha^3 m^{\cancel{3}} c^{\cancel{6}}\,\cancel{\hbar^2 c^2}}{2\,\cancel{m^2c^2}\cdot 24\,\cancel{(\hbar c)^3}\,\cancel{c^2}}\begin{cases}-1 \\ \frac{1}{2}\end{cases} = \frac{\alpha^4 mc^2}{48}\times\begin{cases}-1, & j=1/2 \\ \frac{1}{2}, & j=3/2\end{cases} = \begin{cases}-30\,\mu\text{eV}, \\ 15\,\mu\text{eV}.\end{cases}$$