KVANTROV 7

Anders

XI 6

$$E^2 = m^2c^4 + p^2c^2$$

$$\Rightarrow E = \sqrt{m^2c^4+p^2c^2} = mc^2\sqrt{1+\frac{p^2}{m^2c^2}} = mc^2\left(1+\frac{p^2}{2m^2c^2}-\frac{p^4}{8m^4c^4}\right.$$

$$\Rightarrow E \approx mc^2 + \frac{p^2}{2m} - \underbrace{\frac{p^4}{8m^3c^2}}_{=\Omega}$$

$$\Rightarrow \hat{H} = \hat{H}^{(0)} + \Omega, \quad \Omega = -\frac{p^4}{8m^3c^2}$$

Standardlösn.: Harm.osc.
$$\begin{cases} \psi_0^{(0)} = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha x^2}, & \alpha = \frac{m\omega}{\hbar} \\ E_n^{(0)} = \hbar\omega\left(n+\frac{1}{2}\right) \end{cases}$$

$$E_0 \approx E_0^{(0)} + \langle 0|\Omega|0\rangle$$

$$\langle 0|\Omega|0\rangle = \langle 0|-\frac{p^4}{8m^3c^2}|0\rangle = -\left(\frac{\alpha}{\pi}\right)^{1/2}\frac{\hbar^4}{8m^3c^2}\int_0^\infty dx\, e^{-\frac{1}{2}\alpha x^2}\left(\frac{d^4}{dx^4}\right)e^{-\frac{1}{2}\alpha x^2}$$

$$= \ldots = -\frac{3\hbar^2\omega^2}{32mc^2} \Rightarrow E_0 \approx E_0^{(0)} - \frac{3\hbar^2\omega^2}{32mc^2} = \frac{1}{2}\hbar\omega\left(1-\frac{3\hbar\omega}{16mc^2}\right)$$

Ändring: $$\frac{3\hbar^2\omega^2/(32mc^2)}{\hbar\omega/2} = \frac{3\hbar\omega}{16mc^2} = \frac{3\cdot 10\cdot 1{,}6\cdot 10^{-19}}{9{,}1\cdot 10^{-31}(3\cdot 10^8)^2} = \underline{\underline{5{,}9\cdot 10^{-6}}}$$

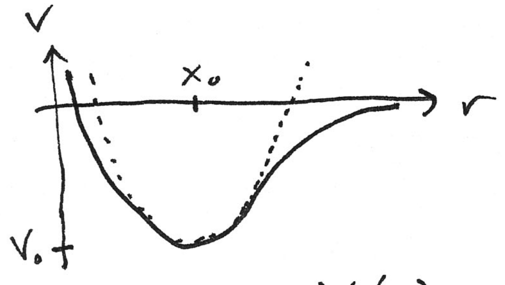
Alternativ: $\langle 0|\Omega|0\rangle$ kan räknas med stegoperatorer!

$$\begin{cases} a = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x}+\frac{i\hat{p}}{m\omega}\right) \\ a^+ = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x}-\frac{i\hat{p}}{m\omega}\right) \end{cases} \Rightarrow \hat{p} = \sqrt{\frac{\hbar m\omega}{2}}(a^+-a)i$$

och $\langle 0|\Omega|0\rangle \propto \langle 0|p^4|0\rangle \propto \langle 0|(a^+-a)^4|0\rangle =$

$$= \langle 0|aaa^+a^+ + \ldots|0\rangle = \ldots = 3\langle 0|0\rangle = 3 \qquad \text{osv...}$$

XI 8) Vibrationer i H_2-molekylen



Taylorutveckla kring $x=x_0$.
till 2:a ordn. $\Rightarrow$ harm. osc. (VII 8)
Nu: till 4:e ordn!

$$V(x) = V_0\left(e^{-2a(x-x_0)} - 2e^{-a(x-x_0)}\right)$$

För $x \approx x_0$: $V(x) \approx \underbrace{V(x_0) + \frac{1}{2}V''(x)(x-x_0)^2}_{V_{HO}} + \frac{1}{6}V'''(x_0)(x-x_0)^3 + \frac{1}{24}V^{(4)}(x_0)(x-x_0)^4$

$+V'(x_0)(x-x_0)$

V_{AH} (anharmonisk potential)

(VII 8) $\Rightarrow$ $V_{HO} = V_0\left(a^2(x-x_0)^2 - 1\right)$,

$$\begin{cases} k = 2V_0a^2 \Rightarrow \omega = \sqrt{\dfrac{2V_0a^2}{\mu}} \\ E_n^{(0)} = \hbar\omega(n+\frac{1}{2}) - V_0 \\ \psi_0^{(0)} = \left(\dfrac{\alpha}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha^2(x-x_0)^2} \\ \alpha = \dfrac{\mu\omega}{\hbar} = \dfrac{a\sqrt{2V_0\mu}}{\hbar} \end{cases}$$

$$\hat{H}_0 = -\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + V_{HO}(x), \quad \hat{\Omega} = V_{AH}(x) = -V_0a^3(x-x_0)^3 + \frac{7}{12}V_0a^4(x-x_0)^4$$

$$\Rightarrow \langle 0|\Omega|0\rangle = \int_{-\infty}^{\infty} dx\, \psi_0^{(0)*}(x) V_{AH}(x) \psi_0^{(0)}(x) =$$

$$= \left(\frac{\alpha}{\pi}\right)^{1/2} V_0 \int_{-\infty}^{\infty} dx \left[-a^3(x-x_0)^3 + \frac{7}{12}a^4(x-x_0)^4\right] e^{-\alpha(x-x_0)^2} = \ldots =$$

$$= \frac{7a^4V_0}{16\alpha^2} = \frac{7\hbar^2a^2}{32\mu} = \begin{Bmatrix} \mu = 0{,}84\cdot 10^{-27}\,\text{kg} \\ a = 20\,\text{nm}^{-1} \end{Bmatrix} = 0{,}007\,\text{eV}$$

$\Rightarrow$ Skillnaden $< 0{,}2\%$ av $E_0^{(0)}$

12) Centralfältsmodellen:

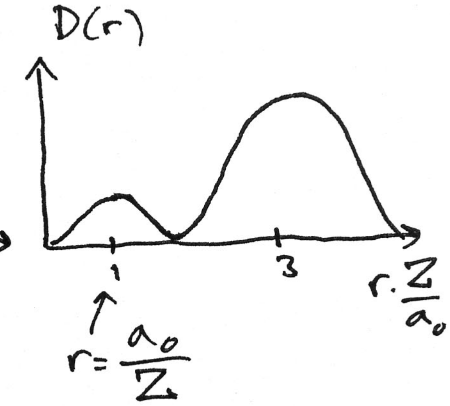
Varje e^- rör sig i ett centralfält, kärnan skärmas av de övriga e^-, ger en "effektiv kärnladdning", Z_{eff}

$$V(r) = -\frac{Z_{eff}\, e^2}{4\pi\varepsilon_0 (r+r_0)}$$

Bestäm E för en $2s$-e^- i detta fält
($2s$: $n=2$, $l=0$)

Antag $r_0 \ll a_0/Z_{eff}$. Fig. 9.3 i komp.:

dvs OK att anta $r \gtrsim \frac{a_0}{Z}$



$$r_0 \ll \frac{a_0}{Z} \lesssim r \Rightarrow \underline{\underline{r \gg r_0}}$$

$$\Rightarrow \frac{1}{r+r_0} = \frac{1}{r\left(1+\frac{r_0}{r}\right)} = \frac{1}{r}\left(1 - \frac{r_0}{r} + 2\left(\frac{r_0}{r}\right)^2 + \ldots\right)$$

$$\Rightarrow H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{Z_{eff}\, e^2}{4\pi\varepsilon_0 (r+r_0)} \approx \underbrace{-\frac{\hbar^2}{2m}\nabla^2 - \frac{Z_{eff}\, e^2}{4\pi\varepsilon_0 r}}_{\substack{= H_{väte} \\ \text{m. } e^2 \to Z_{eff} e^2}} + \underbrace{\frac{Z_{eff}\, e^2 r_0}{4\pi\varepsilon_0\, r^2}}_{= \Omega}$$

Ostörda egenfkner för $2s$-tillst.:

$$\psi^{(0)}_{200} = \left\{\begin{matrix}\text{komp.} \\ (9.51)\end{matrix}\right\} = \alpha^{3/2}\, 2(1-\alpha r)e^{-\alpha r}\, Y_{00}(\theta,\varphi), \quad \alpha = \frac{Z_{eff}}{2a_0}$$

$$E_n = -\frac{Z^2\hbar^2}{2\mu a_0^2}\frac{1}{n^2} \Rightarrow E_2^{(0)} = -\frac{Z_{eff}^2\hbar^2}{8\mu a_0^2} \qquad \left(a_0 = \frac{4\pi\varepsilon_0\hbar^2}{\mu e^2}\right)$$

$$E_{200} \approx E^{(0)}_{200} + \langle 200|\Omega|200\rangle ;$$

$$\langle 200|\Omega|200\rangle = -\frac{Z_{eff}\, e^2 r_0}{4\pi\varepsilon_0} 4\alpha^3 \underbrace{\int d\Omega\, |Y_{00}|^2}_{=1} \int_0^\infty r^2 dr \frac{1}{r^2}(1-\alpha r)^2 e^{-2\alpha r} = \ldots$$

$$\ldots = -\frac{4Z_{eff}e^2 r_0}{4\pi\varepsilon_0}\alpha^3\int_0^\infty dr\,(1+\alpha^2r^2-2\alpha r)e^{-2\alpha r} =$$

$$= -\frac{4Z_{eff}e^2 r_0}{4\pi\varepsilon_0}\alpha^3\left(\frac{1}{2\alpha}-2\alpha\frac{1}{(2\alpha)^2}+\alpha^2\frac{2}{(2\alpha)^3}\right) =$$

$$= -\frac{Z_{eff}e^2 r_0}{\pi\varepsilon_0}\alpha^3\left(\cancel{\frac{1}{2\alpha}}-\cancel{\frac{1}{2\alpha}}+\frac{1}{4\alpha}\right) = -\frac{Z_{eff}e^2 r_0}{\pi\varepsilon_0}\frac{\alpha^2}{4} =$$

$$= -\frac{Z_{eff}e^2 r_0}{4\pi\varepsilon_0}\frac{Z_{eff}^2}{4a_0^2} = -\frac{Z_{eff}^3 e^2 r_0}{16\pi\varepsilon_0 a_0^2} = -\frac{Z_{eff}^3\hbar^2 r_0}{4\mu a_0^3}$$

def. av a_0

$$\Rightarrow E_{200}^{(1)} = -\frac{Z_{eff}^2\hbar^2}{8\mu a_0^2}\left(1+\underbrace{2Z_{eff}\frac{r_0}{a_0}}_{\text{litet!}}\right)$$

litet! $\left(r_0 \ll \frac{a_0}{Z_{eff}}\right)$

Kap. 12, spinn!

$$\psi_{n\ell m_\ell s m_s} = R_{n\ell}(r)\,Y_{\ell m_\ell}(\theta,\varphi)\,\chi_{sm_s}$$

$$\begin{cases}\hat{S}^2\chi = s(s+1)\hbar^2\chi \\ \hat{S}_z\chi = m_s\hbar\chi\end{cases}$$

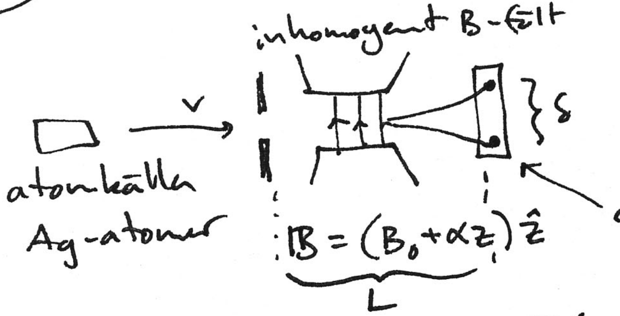
jfr. $\hat{L}^2$ & $\hat{L}_z$!

För elektronen: $s=\frac{1}{2} \Rightarrow m_s = \pm\frac{1}{2}$ (spinn upp/spinn ner)

I kompendium: spinnbankoppling etc., val av goda kvanttal

XII 1

Stern-Gerlach



strålen böjs upp eller ner, beroende på spinnet (↑ el. ↓, dvs $m_s = \pm\frac{1}{2}$) m. 50% slh var.

$v = 700$ m/s $\quad \alpha = 300$ T/m $\quad L = 0{,}1$ m

Sökt: δ

Magnetiska momentet påverkas av en kraft:

$$\mathbb{F} = (\mu\cdot\nabla)\mathbb{B} + \mu\times(\nabla\times\mathbb{B}), \quad \nabla\times\mathbb{B} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \partial_x & \partial_y & \partial_z \\ 0 & 0 & B(z) \end{vmatrix} = 0$$

$$\Rightarrow \mathbb{F} = (\mu\cdot\nabla)\mathbb{B}$$

Vad är μ för Ag-atomer? En e^- ytterst i 5s

$$\mu = \underbrace{\mu_{ban}}_{\substack{=0, \\ (\text{ty } l=0)}} + \mu_{spinn} = \mu_{spin} = -g_e \frac{\mu_B}{\hbar}\mathbb{S}$$

$g_e =$ Landaus g-faktor ≈ 2

$\mu_B =$ Bohr-magneton $= 9{,}274\cdot10^{-24}$ J/T

Beräkna kraften $\mathbb{F} = (\mu\nabla)\mathbb{B} = -2\frac{\mu_B}{\hbar} S_z\, \partial_z (B_0 + \alpha z)\hat{z} =$

$$= -2\frac{\mu_B}{\hbar}\alpha S_z \hat{z}$$

$$\Rightarrow \langle \mathbb{F}\rangle = \int \psi^* \left(-2\frac{\mu_B}{\hbar}\alpha S_z\hat{z}\right)\psi\, dV = \left\{ S_z\psi = \pm\tfrac{1}{2}\hbar \right\} =$$

$$= -2\frac{\mu_B}{\hbar}\alpha\left(\pm\tfrac{1}{2}\hbar\right)\hat{z}\int\psi^*\psi\, dV = \mp \mu_B\alpha\hat{z}$$

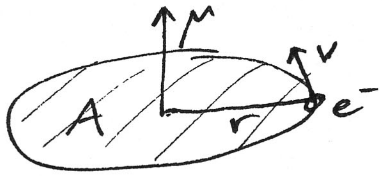
$$\text{NII: } m\ddot{z} = F = \mp\mu_B\alpha \Rightarrow z(t) = \mp\frac{\mu_B\alpha}{m}\frac{t^2}{2}$$

$$t_0 = \frac{d}{v} \Rightarrow \delta = 2\left|z\left(\frac{d}{v}\right)\right| = \frac{\mu_B\alpha}{m}\frac{d^2}{v^2} = \left\{\begin{matrix}\text{ins.} \\ \text{av} \\ \text{värden}\end{matrix}\right\} = 0{,}3 \text{ mm}$$

XII 2

Magn. mom. från banrörelse hos e^- i väteatom gr.-tillst. enligt a) Bohr b) kvantmekaniken

a)



$$\mu_B = iA = \frac{ev}{2\pi r}\cdot \pi r^2 = \frac{1}{2}evr \text{, där:}$$

$$v = \frac{e^2}{2\varepsilon_0 h}\frac{1}{n}\ ;\ r = \frac{\varepsilon_0 h^2}{\pi m_e e^2}n^2 \overset{n=1}{\Longrightarrow}$$

$$\Rightarrow vr = \frac{h}{2\pi m_e} = \frac{\hbar}{m_e} \Rightarrow \mu_B = \frac{e\hbar}{2m_e}$$

b) $\mu_k = \left(\frac{1}{2}evr\right) = \frac{e}{2m_e}(m_e v r) = \frac{e}{2m_e}\cdot \mathbb{L}$

$\mathbb{L}^2$ är kvantiserat, $\mathbb{L}^2\psi = \hbar^2 l(l+1)\psi$

Grundtillst. $\Rightarrow l = 0 \Rightarrow \mu_k = 0$

XII 6

elektron i centralfält m. pot. $V(r)$

$\hat{H}$ innehåller spin-bankopplingsterm på formen

$$\hat{H}_{SB} = \frac{1}{2m^2c^2}\frac{1}{r}\frac{dV(r)}{dr}\hat{\mathbb{L}}\cdot\hat{\mathbb{S}}. \qquad \hat{H} = \hat{H}_0 + \hat{H}_{SB}$$

Bestäm finstrukturuppsplittringen av vätets 2p-nivå $(n=2, l=1)$.

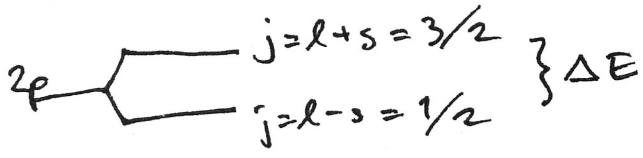
Komp., (12.34) $\Rightarrow E_{nlj} = E^0_{nl} + \frac{\hbar^2}{2}\xi_{nl}\left[j(j+1) - l(l+1) - \frac{3}{4}\right]$ (1)

$$\xi_{nl} = \frac{1}{2\mu^2c^2}\int_0^\infty \frac{dV(r)}{dr}|R_{nl}(r)|^2 r\,dr$$

$$|R_{21}(r)|^2 = \frac{1}{24}\left(\frac{1}{a_0}\right)^3\frac{r^2}{a_0^2}e^{-r/a_0} \text{ och } V(r) = -\frac{e^2}{4\pi\varepsilon_0 r} \text{ (Coulomb-pot.)}$$

$$\Rightarrow \xi_{nl} = \frac{1}{2\mu^2c^2}\frac{1}{24a_0^5}\int_0^\infty \frac{e^2}{4\pi\varepsilon_0 r^2}r^2e^{-r/a_0}r\,dr = \frac{e^2}{192\mu^2c^2\pi\varepsilon_0 a_0^3} \quad (2)$$

- e^- i 2p-nivå $\Rightarrow l=1,\ s=\frac{1}{2} \Rightarrow j=\{l+s,\ l-s\}=\{3/2,\ 1/2\}$



endast j som skiljer!

$$\Delta E = E_{2,1,3/2}-E_{2,1,1/2} = \{(1)\} = \frac{\hbar^2}{2}\xi_{21}\left[\frac{3}{2}\left(\frac{3}{2}+1\right)-\frac{1}{2}\left(\frac{1}{2}+1\right)\right] =$$

$$= \{(2)\} = \frac{\hbar^2}{2}\frac{e^2}{192\mu^2c^2\pi\varepsilon_0 a_0^3}\left(\frac{9}{4}+\frac{6}{4}-\frac{1}{4}-\frac{2}{4}\right) =$$

$$= \frac{3\hbar^2}{2}\frac{e^2}{192\mu^2c^2\pi\varepsilon_0 a_0^3} \approx 45\cdot10^{-6}\ \text{eV}$$