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Kvantfröv. 9

XI. 3, 11	4/11 - tisd 2008
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XI. 3/ Part m. massan m i pot.

$V(r) = -V_0 \, e^{-r/a}$; $V_0 = \frac{4\hbar^2}{3ma^2}$

Skatta grundtillst. energin E_0 mha variations met. & ansatzen $\psi(r) = N e^{-\alpha r}$

TOSE: $H = -\frac{\hbar^2}{2m}\nabla^2 + V(r)$

$\psi(\mathbf{r}) = \psi(r) \Rightarrow \nabla^2 \longrightarrow \frac{1}{r}\frac{\partial^2}{\partial r^2} r$

Variations met: Ber $\langle H \rangle$ med ansatz

minimera $\langle H \rangle$ map param. $\alpha \Rightarrow E_0 \leq \min_\alpha \langle H \rangle$

$$\langle H \rangle = 4\pi \int_0^\infty dr \, r^2 \, \psi^* H \psi$$

$$H\psi = \left(-\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2} r + V(r) \right) N e^{-\alpha r}$$

Deriv: $\frac{1}{r}\frac{\partial^2}{\partial r^2} r \underbrace{N e^{-\alpha r}}_{\psi} = \frac{1}{r}\frac{\partial}{\partial r}(-\alpha r + 1)\psi =$

$$= \frac{1}{r}(-\alpha + \alpha^2 r - \alpha)\psi = \frac{1}{r}(\alpha^2 r - 2\alpha)\psi$$

$$\Rightarrow \langle H \rangle = 4\pi \int_0^\infty dr \, r^2 \psi^* \left[-\frac{\hbar^2}{2m}\frac{1}{r}(\alpha^2 r - 2\alpha) + V(r) \right] \psi =$$

$$= 4\pi \int_0^\infty dr \left[-\frac{\hbar^2}{2m}(\alpha^2 r^2 - 2\alpha r) - V_0 r^2 e^{-r/a} \right] N^2 e^{-2\alpha r} =$$

$$= \ldots = 4\pi N^2 \left(\frac{\hbar^2}{2m}\frac{1}{4\alpha} - V_0 \frac{2}{(2\alpha + \frac{1}{a})^3} \right)$$

Normera: $1 = 4\pi \int_0^\infty dr \, r^2 N^2 e^{-2\alpha r} = 4\pi \frac{N^2}{4\alpha^3} \Rightarrow N = \sqrt{\frac{\alpha^3}{\pi}}$

$V_0 = \frac{4\hbar^2}{3ma^2} \Rightarrow \frac{\hbar^2}{2m} = \frac{3a^2}{8} V_0$

$$\Rightarrow \langle H \rangle = 4\pi \frac{\alpha^3}{\pi} \left(\frac{3a^2}{8}\frac{V_0}{4\alpha} - V_0 \frac{2}{(2\alpha + \frac{1}{a})^3} \right) = V_0 \left(\frac{3}{8}a^2\alpha^2 - \frac{8\alpha^3}{(2\alpha + \frac{1}{a})^3} \right)$$

$\frac{d\langle H \rangle}{d\alpha} = 0 \Rightarrow \alpha = \frac{1}{2a} \Rightarrow E_0 \leq \min_\alpha \langle H \rangle = -\frac{V_0}{32}$

XI. 11 / Li-modell m. 2s-valens elektronen i effektiva pot. $V_{eff} = -\frac{e^2}{4\pi\varepsilon_0 r}\left(1 + 2e^{-3r/a_0}\right) = V_0(r) + \Omega(r)$

$V_0 = -\frac{e^2}{4\pi\varepsilon_0 r}$; $\Omega = -\frac{e^2}{4\pi\varepsilon_0 r} 2e^{-3r/a_0}$

2s tillst: $\psi_{2s} = \frac{1}{\sqrt{8\pi a_0^3}}\left[1 - \frac{r}{2a_0}\right]e^{-r/2a_0}$

m. $a_0 = \frac{\varepsilon_0 h^2}{\pi m_e e^2}$

Sökt: Grundtillst energi m. 1a ordn störn räkn

V_0 ren Coulomb pot $\Rightarrow$ $E_n^{(0)} = -\frac{Z^2\hbar^2}{2\mu a_0^2}\frac{1}{n^2}$

Här $Z=1$, $\mu \approx m_e$, $n=2$ $\Rightarrow$

$E_{2s}^{(0)} = -\frac{\hbar^2}{2m_e a_0^2}\frac{1}{4} \overset{\text{mha } a_0 = \dots}{=} -\frac{e^2}{32\pi\varepsilon_0 a_0}$

1a ordn störn. räkn:

$E_{2s}^{Li} \approx E_{2s}^{(0)} + \langle\psi_{2s}|\Omega|\psi_{2s}\rangle$

$\langle\psi_{2s}|\Omega|\psi_{2s}\rangle = 4\pi\int_0^\infty dr\, r^2 \psi_{2s}^* \Omega \psi_{2s} =$

$= 4\pi\int_0^\infty dr\, r^2 \frac{1}{8\pi a_0^3}\left[1 - \frac{r}{2a_0}\right]^2 e^{-r/a_0}\left(\frac{-e^2}{4\pi\varepsilon_0 r}\right)2e^{-3r/a_0}$

$= \dots = -\frac{e^2}{32\pi\varepsilon_0 a_0}\left(\frac{19}{64}\right)$

(Väte gs. energi:)

$\Rightarrow E_{2s}^{Li} = -\frac{e^2}{32\pi\varepsilon_0 a_0}\left(1 + \frac{19}{64}\right) \approx -\frac{13{,}6\,\text{eV}}{\underbrace{2^2}_{n=2}}\left(1 + \frac{19}{64}\right) \approx$

$\approx 4{,}4$ eV

XII. 3/ Vad är vinkeln mellan tot. rörelsemängdsmom. $\mathbb{J}$ & ban rörelsemängdsmom $\mathbb{L}$ för tillst. $^2P_{3/2}$

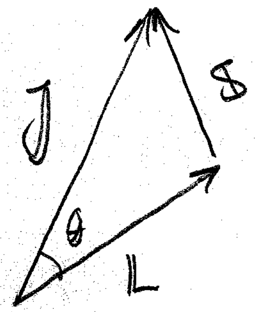
<u>Givet:</u> $l = 1$; $j = \frac{3}{2}$; $s = \frac{1}{2}$

$^2P_{3/2}$ $\quad 2 = 2s+1$

Längder på motsv. vekt: $|\mathbb{J}| = \hbar\sqrt{j(j+1)}$

$\mathbb{J} = \mathbb{L} + \mathbb{S} \implies$ $|\mathbb{L}| = \hbar\sqrt{l(l+1)}$

$|\mathbb{S}| = \hbar\sqrt{s(s+1)}$



<u>Cosinus satsen:</u>

$$|\mathbb{S}|^2 = |\mathbb{L}|^2 + |\mathbb{J}|^2 - 2|\mathbb{L}||\mathbb{J}|\cos\theta$$

$$\cos\theta = \frac{|\mathbb{L}|^2 + |\mathbb{J}|^2 - |\mathbb{S}|^2}{2|\mathbb{L}||\mathbb{J}|} =$$

$$= \frac{l(l+1) + j(j+1) - s(s+1)}{\sqrt{l(l+1)\,j(j+1)}} = \ldots = \frac{5}{2}\sqrt{\frac{2}{15}}$$

$$\implies \underline{\underline{\theta \approx 24^\circ}}$$

XII.5/ Atom m valensel. i s-tillst utanför slutet elektronskal. Homogent magn. fält.
$B = 0{,}4\,T$ ber. vägl. motsv. mot spinn-flip resonans.

Slutet el. skal: $L=0,\ J=0,\ S=0$

+ en s-elektron $\Rightarrow L=0,\ S=\frac{1}{2} \Rightarrow J=\frac{1}{2}$

$$m_J = \pm\frac{1}{2}$$

Energibidrag från magn. fält. $E_B = g_j \mu_B B m_j$

spinn-flip $m_j \ -\frac{1}{2} \rightarrow \frac{1}{2} \Rightarrow$

$$\Delta E_B = g_j \mu_B B = \Big/ \underset{\text{för en el.}}{\overset{\text{Landé fkt.}}{g_j = 2}} \Big/ = 2\mu_B B$$

$$g_j = 1 + \frac{j(j+1) - \ell(\ell+1) + s(s+1)}{2j(j+1)} = \Big/ \begin{matrix} \ell=0 \\ s=\frac{1}{2}\ j=\frac{1}{2} \end{matrix} \Big/ = 2$$

motsv. vägl. $\frac{hc}{\lambda} = \Delta E_B \Rightarrow \lambda = \frac{hc}{\Delta E_B} = \frac{hc}{2\mu_B B} =$

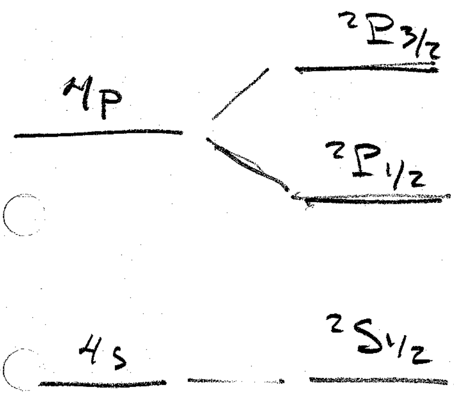
$$= \Big/ \mu_B = \frac{e\hbar}{2m_e} \Big/ = \frac{c m_e}{eB} 2\pi \approx \underline{2{,}7\,\text{cm}}$$

XII.11 / Hyperfinstruktur, Kalium 4p & 4s

Om atomkärnan har ett rörelsemängds mom. $\mathbb{I}$ $|\mathbb{I}| = \hbar\sqrt{I(I+1)}$ så kopplar det till tot. el. rör.m.mom $\mathbb{J}$ enl.

$$H_{HFS} = \frac{2\pi}{\hbar} A\, \mathbb{I}\cdot\mathbb{J}$$; A hyperfinstr. konst i frekv.

Kalium 4p & 4s



a) Hur många HFS-niv. splittras de tre niv. i? $I = \frac{3}{2}$

b) Ber. storl. i uppsplittring mellan HFS-niv. givet:

$A(^2S_{1/2}) = 230{,}0\,MHz$

$A(^2P_{1/2}) = 29{,}0\,MHz$

$A(^2P_{3/2}) = 6{,}1\,MHz$

Ledn: Def tot. rör.m.mom $\mathbb{F} = \mathbb{I} + \mathbb{J}$ =>
$|\mathbb{F}| = \hbar\sqrt{F(F+1)}$ => $F \in \{|I-J|, |I-J|+1, \ldots, I+J\}$

a) $I = \frac{3}{2}$

$^2S_{1/2}$ & $^2P_{1/2}$ => $J = \frac{1}{2}$ => $\left.\begin{array}{l} F_{min} = |I-J| = 1 \\ F_{max} = I+J = 2 \end{array}\right\}$ => $\underline{2\text{ niv!}}$

$^2P_{3/2}$ => $J = \frac{3}{2}$ => $\left.\begin{array}{l} F_{min} = |I-J| = 0 \\ F_{max} = I+J = 3 \end{array}\right\}$ => $\underline{4\text{ niv!}}$

b) Ber ΔE_{HFS}: $\mathbb{F} = \mathbb{I} + \mathbb{J}$ => $\mathbb{F}^2 = \mathbb{I}^2 + 2\mathbb{I}\cdot\mathbb{J} + \mathbb{J}^2$

=> $H_{HFS} = \frac{\pi}{\hbar} A(\mathbb{F}^2 - \mathbb{I}^2 - \mathbb{J}^2) = \pi\hbar A(F(F+1) - I(I+1) - J(J+1))$

Eg. $\Delta E_{HFS}(^2S_{1/2}) = \Big/\underset{\text{samma}}{I, J}\Big/ = E_{HFS}(F=2) - E_{HFS}(F=1) =$

$= \pi\hbar A(^2S_{1/2})(2(2+1) - 1(1+1)) =$

$= \pi\hbar A(^2S_{1/2})\, 4 \approx \underline{1{,}9\,\mu eV}$ små energisplittringar!

XIII. 3/ $t \leq 0$ väteatom i grundtillst ψ_{100}

$t > 0$ pålagd yttre störn: $V(\mathbf{r},t) = V_0 z e^{-t/\tau} \sin \omega t$

Ber $P(2p)$ för $t \to \infty$.

Flera 2p tillst: $n=2,\ l=1 \Rightarrow m = -1, 0, 1$

Grundtillst: $\psi_{100} = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$

$$P(2p) = |c_{21}(t)|^2 = |c_{21,-1}(t)|^2 + |c_{210}(t)|^2 + |c_{211}(t)|^2$$

Tids ber störn teori:

$$c_{21}(t) = -\frac{i}{\hbar}\int_0^t \langle 21|V(\mathbf{r},t')|100\rangle e^{i\omega_{2p1s}t'}dt'$$

där $\langle 21| = \langle 21-1| + \langle 210| + \langle 211|$

obs! $V(\mathbf{r},t) = V(z,t) = V(r,\theta,t)$ dvs φ ober.

$$\Rightarrow \langle \underbrace{21\pm1}_{\varphi_{1\pm1} \propto e^{\pm i\varphi}}|V(r,\theta,t)|100\rangle \propto \int_0^{2\pi} e^{\pm i\varphi}d\varphi = 0$$

Bara ett matris el. behöver ber. $\langle 210|V|100\rangle$

$$\psi_{210} = \frac{1}{4\sqrt{2\pi a_0^3}}\frac{r}{a_0}e^{-r/2a_0}\cos\theta$$

$$|c_{21}(t)|^2 = \left|-\frac{i}{\hbar}\int_0^t dt' \langle 210|V(z,t')|100\rangle e^{i\omega_{2p1s}t'}\right|^2 =$$

$$= \ldots = \xrightarrow[t\to\infty]{} \frac{2^{15}a_0^2V_0^2}{3^{10}\hbar^2}\cdot\frac{\omega^2}{\left(\frac{1}{\tau^2}+\omega_{2p1s}^2+\omega^2\right)^2}$$

$\Rightarrow P(2p)$ ber på frekv. ω & dämpn. τ. dch!

X.11/ sp^3-hybridisering ger el. vågfunk.

$$\psi = \frac{1}{2} R(r) \left[Y_{00} - i\frac{\sqrt{3}}{2} \left(Y_{11} + Y_{1,-1} \right) \right]$$

$R(r)$ radiella vågfunk. $Y_{\ell m}$ klotytefunk.

Ber: $\langle x\rangle, \langle y\rangle$ & $\langle z\rangle$ antaget: $\langle r\rangle = r_0$

Skriv om ψ: $Y_{11} + Y_{1,-1} = -\sqrt{\frac{3}{8\pi}} \frac{2iy}{r}$

$$Y_{00} = \frac{1}{\sqrt{4\pi}}$$

$$\Rightarrow \psi = \frac{R(r)}{2} \frac{1}{\sqrt{4\pi}} \left[1 - \frac{3}{\sqrt{2}} \frac{y}{r} \right] = \frac{1}{\sqrt{4\pi}} \frac{R(r)}{2} \left[1 - \frac{3}{\sqrt{2}} \sin\theta \sin\varphi \right]$$

$$\langle r\rangle = \int_0^\infty dr \int_0^{\pi} d\theta \int_0^{2\pi} d\varphi \, r^2 \sin\theta \, \psi^* r \psi =$$

$$= \frac{1}{4\pi} \underbrace{\int_0^\infty dr \, r^3 \frac{R^2(r)}{4}}_{A} \underbrace{\int_0^\pi d\theta \int_0^{2\pi} d\varphi \sin\theta \left[1 - \frac{3}{\sqrt{2}} \sin\theta \sin\varphi \right]^2}_{4\pi \frac{5}{2}}$$

$$= \frac{5}{2} A = r_0 \Rightarrow A = \frac{2}{5} r_0$$

$$\langle x\rangle = \int dr \, \psi^* x \psi = \int dr \frac{1}{4\pi} \frac{R^2(r)}{4} x \left[1 - \frac{3}{\sqrt{2}} \frac{y}{r} \right]^2 =$$

$$= \int dr \frac{1}{4\pi} \frac{R^2(r)}{4} \left[\underset{\uparrow \text{udda}}{x} - \sqrt{2}\, 3 \underset{\text{udda m } x \neq y}{\frac{yx}{r}} + \frac{9}{2} \underset{\text{udda i } x}{\frac{y^2 x}{r^2}} \right] = 0$$

$\langle z\rangle = 0$ genom samma arg.

$$\langle y\rangle = \int dr \frac{1}{4\pi} \frac{R^2(r)}{4} \left[\underset{\text{udda}}{y} - \sqrt{2}\, 3 \underset{\text{jämn!}}{\frac{y^2}{r}} + \frac{9}{2} \underset{\text{udda}}{\frac{y^3}{r^2}} \right] =$$

$$= \frac{1}{4\pi} \underbrace{\int_0^\infty dr \, r^2 \frac{R^2(r)}{4} r}_{A} \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \underbrace{\sin\theta}_{} (-\sqrt{2}\, 3) \frac{y^2}{r^2} =$$

$$= \frac{1}{4\pi} \frac{2}{5} r_0 (-\sqrt{2}\, 3) \underbrace{\int_0^\pi d\theta \sin^3\theta}_{4/3} \underbrace{\int_0^{2\pi} d\varphi \sin^2\varphi}_{\pi} =$$

$$= -\frac{\sqrt{2}\, 2}{5} r_0 \frac{1}{4\pi} 3 \frac{4}{3} \pi = \underline{\underline{-\frac{2\sqrt{2}}{5} r_0}}$$