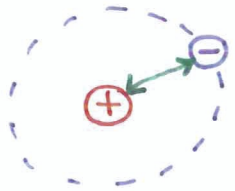
8. VÄTEATOMEN

8.1 Coulombpotentialen för elektronen i väte-atomen ges av:

$$\boxed{V(r) = -\frac{e_0^2}{r}}$$



a) Bestäm den effektiva potentialen och rita den i en figur för $l \leq 3$.

$$V_{eff} = \frac{\hbar^2 l(l+1)}{2mr^2} + V(r) = \boxed{\frac{\hbar^2 l(l+1)}{2mr^2} - \frac{e_0^2}{r}}$$

$$\text{För } l = 3 \Rightarrow V_{eff} = \frac{\hbar^2 3\cdot(3+1)}{2mr^2} - \frac{e_0^2}{r} = \boxed{\frac{6\hbar^2}{mr^2} - \frac{e_0^2}{r}}$$

b) Bestäm det klassiskt tillåtna området för det lägsta tillståndet med $l = 3$. Vad händer då l växer?

$n=4$.

$$V_{eff} \leq E_{total} \iff V_{eff} \leq -\frac{\hbar^2}{2ma_0^2}\cdot\frac{1}{n^2}$$

$$V_{eff} = \frac{\hbar^2 l(l+1)}{2mr^2} - \frac{e_0^2}{r} \leq -\frac{\hbar^2}{2ma_0^2}\cdot\frac{1}{4^2}$$

$$\overset{l=3}{\iff} \frac{6\hbar^2}{mr^2} - \frac{e_0^2}{r} \leq -\frac{\hbar^2}{2ma_0^2}\cdot\frac{1}{16}$$

Vi använder nu att $a_0 = \frac{\hbar^2}{m e_0^2} \iff e_0^2 = \frac{\hbar^2}{ma_0}$

$$\Rightarrow \frac{6\cancel{\hbar^2}}{\cancel{m}r^2} - \frac{\cancel{\hbar^2}}{\cancel{m}a_0 r} \leq \frac{\cancel{\hbar^2}}{32\cancel{m}a_0^2} \iff \frac{6}{r^2} - \frac{1}{a_0 r} \leq \frac{1}{32a_0}$$

$$\Leftrightarrow r^2 - 32a_0 r + 32 \cdot 6a_0^2 \leq 0.$$

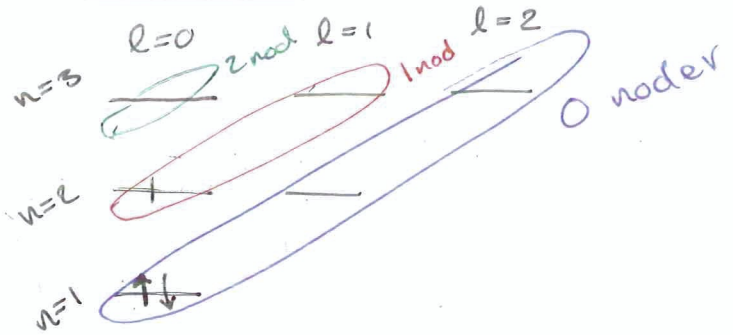
Vi löser likheten mha pq-formeln:

$$r = 16a_0 \pm \sqrt{16^2 a_0^2 - 32 \cdot 6a_0} = 16a_0 \pm \sqrt{256a_0 - 192a_0} =$$

$$= 16a_0 \pm \sqrt{64a_0} = 16a_0 \pm 8a_0$$

$$\Rightarrow (r - 8a_0)(r - 24a_0) \leq 0 \Rightarrow \boxed{8a_0 \leq r \leq 24a_0}$$

8.2 Karakterisera alla tillstånd i väteatomen med $n \leq 3$. Ange antal noder och bestäm degenerationsgraden för tillstånd med givet värde på huvudkvanttalet n.



$$N = n - l - 1$$

	$l=0$	$l=1$	$l=2$	Total deg
$n=1$	$2\cdot 1$	—	—	2
$n=2$	$2\cdot 1$	$3\cdot 2=6$	—	8
$n=3$	$2\cdot 1$	$3\cdot 2=6$	$5\cdot 2=10$	18

$$\Rightarrow \text{Degeneration } g = \sum_{l=0}^{n-1} 2(2l+1) =$$

$$= 4\sum_{l=0}^{n-1} l + 2\sum_{l=0}^{n-1} 1 = 4\,\frac{(n-1)\cdot n}{2} + 2(n-1+1) =$$

$$= 2n^2 - 2n + 2n = \boxed{2n^2}$$ (med spinn)

$\boxed{8.3}$ $\boxed{\text{Hamiltonoperatorn ges av:}}$

$$\boxed{H = -\frac{\hbar^2}{2m_e}\nabla^2 - Z\frac{e_0^2}{r}}$$

$$e_0^2 = \frac{\hbar^2}{m_e a_0}, \quad E_1 = -\frac{Z\hbar^2}{2m_e a_0^2} = -\frac{Ze_0^2}{2}$$

a) Visa att vågfunktion $\phi(r)$ är normerad och satisfierar S.E. Vilka kvanttal svarar denna vågfunktion mot?

$$\boxed{\phi(r) = \sqrt{\frac{Z^3}{\pi a_0^3}} \cdot e^{-\frac{Z}{a_0}r}}$$

Normering:

$$\iiint |\phi|^2 dr d\theta d\varphi = [\text{vinkeloberoende}] =$$

$$= \int_{-\infty}^{\infty} \frac{Z^3}{\cancel{\pi} a_0^3} \cdot e^{-\frac{2Z}{a_0}r} \cdot 4\cancel{\pi} r^2 dr = [\text{jämn}] =$$

$$= \int_0^{\infty} \frac{4Z^3}{a_0^3} \cdot r^2 \cdot e^{-\frac{2Z}{a_0}r} dr = \frac{4Z^3}{a_0^3} \cdot \frac{2!}{\left(\frac{2Z}{a_0}\right)^3} = 1 \quad \square$$

Schrödingerekvationen.

$$H\phi = E\phi$$

$$\Leftrightarrow \underbrace{-\frac{\hbar^2}{2m_e}\nabla^2\phi}_{1} - Z\frac{e_0^2}{r}\phi = E\phi$$

$$1 \quad -\frac{\hbar^2}{2m_e}\nabla^2\phi = -\frac{\hbar^2}{2m_e} \cdot \frac{1}{r}(r\phi)''_{rr} = -\frac{\hbar^2}{2m_e r}(\phi + r\phi'_r)'_r =$$

$$-\frac{\hbar^2}{2m_e r}\left(\phi_r' + \phi_r' + r\phi_{rr}''\right) = \boxed{-\frac{\hbar^2}{2m_e r}\left(2\phi' + r\phi''\right)} \quad *$$

Vi använder att $\phi(r) = \sqrt{\frac{Z^3}{\pi a_0^3}} \cdot e^{-\frac{Z}{a_0} r}$

$$\Rightarrow \phi'(r) = \sqrt{\frac{Z^3}{\pi a_0^3}} \cdot \left(-\frac{Z}{a_0}\right) e^{-\frac{Z}{a_0} r}$$

$$\Rightarrow \phi''(r) = \sqrt{\frac{Z^3}{\pi a_0^3}} \left(-\frac{Z}{a_0}\right)^2 e^{-\frac{Z}{a_0} r}$$

Insatt i $*$ får vi:

$$= -\frac{\hbar^2}{2m_e r}\left(2\sqrt{\frac{Z^3}{\pi a_0^3}}\left(-\frac{Z}{a_0}\right) + r\sqrt{\frac{Z^3}{\pi a_0^3}}\left(-\frac{Z}{a_0}\right)^2\right) e^{-\frac{Z}{a_0} r} =$$

$$= -\frac{\hbar^2}{2m_e r}\left(2 - r\frac{Z}{a_0}\right)\underbrace{\sqrt{\frac{Z}{\pi a_0^3}}\left(-\frac{Z}{a_0}\right) e^{-\frac{Z}{a_0} r}}_{\phi} =$$

$$= \frac{\hbar^2}{2m_e}\left(\frac{2Z}{a_0 r} - \frac{Z^2}{a_0^2}\right)\phi(r) = \boxed{\left(Z\frac{e_0^2}{r} + E_1\right)\phi(r)}$$

Insatt i S.E. får vi:

$$\cancel{Z\frac{e_0^2}{r}\phi(r)} + E_1\phi(r) - \cancel{Z\frac{e_0^2}{r}\phi(r)} = E\phi(r) \qquad \square$$

$$\Leftrightarrow \boxed{H\phi(r) = E_1\phi(r)} \qquad \frac{1}{a_0 K} = n \Rightarrow$$

Huvudkvanttalen: $n = 1$, $l = 0$, $m = 0$

b) $\boxed{\text{Bestäm förväntningsvärdet av } T \text{ och } V}$

$\boxed{n=2,\ l=1,\ m=1}$ $E_{total} = E_2 = -hcR\frac{Z^2}{n^2} = \boxed{-13.6\cdot\frac{1}{8}\ eV.}$

$Z=1$

$$\phi(r,\theta,\phi) = R(r)\cdot U(\theta,\phi) = -\left(\frac{1}{2a_0}\right)^{3/2}\cdot\frac{2}{\cancel{\sqrt{8}}}\cdot\frac{r}{\cancel{2}a_0}e^{-\frac{r}{2a_0}}\cdot\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\varphi} =$$

$$= \frac{r}{\sqrt{8a_0^3\cdot 8\pi}\,a_0}e^{-\frac{r}{2a_0}}\cdot\sin\theta\cdot e^{i\varphi} =$$

$$= \boxed{\frac{r}{8\sqrt{a_0^3\pi}\,a_0}e^{-\frac{r}{2a_0}}\cdot\sin\theta\cdot e^{i\varphi}}\ \phi_{211}$$

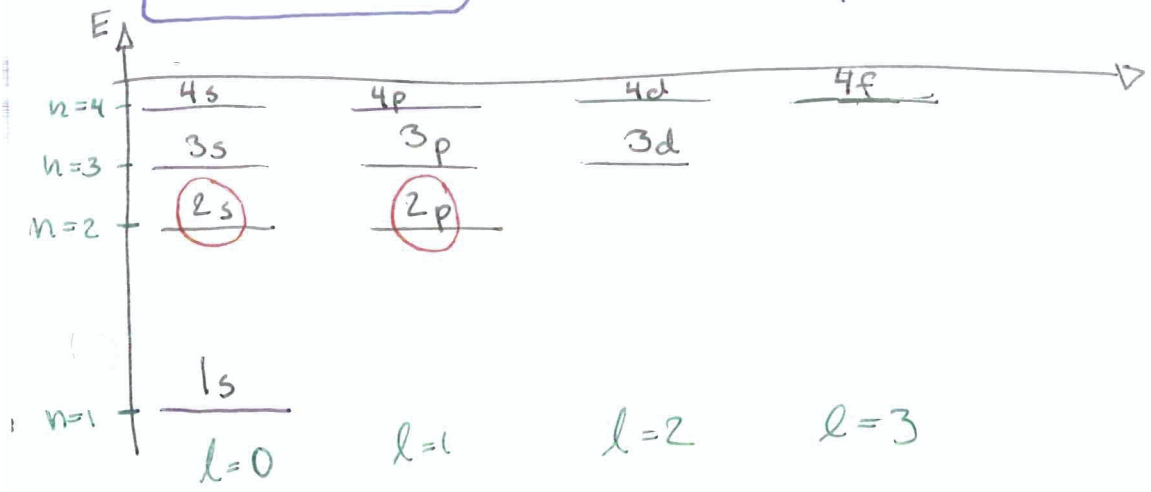
$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e_0^2}{r} = \underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r}r}_{T} + \underbrace{\frac{L^2}{r^2} - \frac{e_0^2}{r}}_{V_{eff}}$$

$$\langle V\rangle = -e_0^2\left\langle\phi_{211}\middle|\frac{1}{r}\phi_{211}\right\rangle = \text{Maple} = \underline{-13.6\cdot 2} = \boxed{2E_2}\ eV$$

$$\langle T\rangle = E_{tot} - \langle V\rangle = E_2 - 2E_2 = -E_2 = \boxed{13.6\cdot\frac{1}{8}\ eV}$$

8.4 Bestäm r_{rms} för 2s och 2p i väte.

$$\boxed{r_{rms} = \sqrt{\langle r^2 \rangle}}$$ Root mean square



För 2s

$m = 0, \pm l$

$l=0,\ n=2,\ m=0 \Rightarrow (2,0,0)$

$$\boxed{\phi_{200} = \frac{1}{\sqrt{8\pi a_0^3}}\left(1-\frac{r}{2a_0}\right)e^{-\frac{r}{2a_0}}}$$

$$\langle r \rangle = \langle \phi_{200} | \phi_{200} \cdot r^2 \rangle = \frac{1}{8\pi a_0^3}\int_0^\infty r^2\left(1-\frac{r}{2a_0}\right)^2 e^{-\frac{r}{a_0}} \cdot 4\pi r^2 dr$$

$= \ldots$ Maple $= \boxed{42\, a_0^2}$

För 2p

$n=2,\ l=1,\ m=-1,0,1$

$$\phi_{210} = \frac{1}{\sqrt{24a_0^5}}\, r e^{-\frac{r}{2a_0}} \cdot Y_1^0(\theta,\varphi)$$

$$\phi_{21\pm1} = \frac{\mp 1}{8\sqrt{\pi a_0^3}} \cdot \frac{r}{a_0} e^{-\frac{r}{2a_0}} \cdot \sin(\theta) e^{\pm i\varphi} = \frac{1}{\sqrt{24a_0^5}}\, r e^{-\frac{r}{2a_0}} \cdot Y_1^{\pm 1}(\theta,\varphi)$$

$$\langle r \rangle = \frac{1}{24a_0^5}\int_0^\infty r^4 e^{-\frac{r}{a_0}} \cdot r^2 dr = \ldots = \boxed{30a_0^2}$$

8.5 Hur ser spektrumet för en myonväteatom ut?

Samma struktur men annan energiskala.

$$\boxed{E_n \approx -\frac{\hbar^2}{2 \cdot 200 m_e \cdot a_0^2} \cdot \frac{1}{n^2}}$$

8.7 Viralteoremet

a) Argumentera för att det i 3D gäller att

$$2\langle E_{kin} \rangle = \langle \bar{r} \cdot \nabla V \rangle$$

Allmänt gäller: $\boxed{\frac{d}{dt}\langle A \rangle = \frac{i}{\hbar}\langle [H, A] \rangle}$ se s. 118.

där H är Hamiltonoperatorn i 3D:

$$[H, A] = -\left[\bar{r} \cdot \bar{p}, \frac{p^2}{2m} + V(\bar{r})\right] = -\left[\bar{r} \cdot \bar{p}, \frac{p^2}{2m}\right] - \left[\bar{r} \cdot \bar{p}, V(\bar{r})\right] =$$

$$= -\left[xp_x + yp_y + zp_z, \frac{(p_x^2 + p_x^2 + p_z^2)}{2m}\right] - \left[xp_x + yp_y + zp_z, V(\bar{r})\right] =$$

$$= -\frac{i\hbar}{m}(p_x^2 + p_x^2 + p_z^2) + i\hbar(xV_x' + yV_y' + zV_z') =$$

$$\boxed{= -2i\hbar E_{kin} + i\hbar(r \cdot \nabla V)}$$

$A = \bar{r}\cdot\bar{p}$ är ej tidsberoende

$$\Rightarrow \frac{d}{dt}\langle A\rangle = \frac{d}{dt}\langle \bar{r}\cdot\bar{p}\rangle = 0 = \cancel{\frac{i}{\hbar}}\left(\cancel{-2i\hbar} E_{kin} + \cancel{i\hbar}(r\cdot\nabla V)\right)$$

$$\Rightarrow \boxed{2\langle E_{kin}\rangle = \langle r\cdot\nabla V\rangle} \quad \square \quad \text{QED.}$$

b) Använd detta teorem för att finna ett allmänt uttryck för:

$$\boxed{\left\langle \frac{1}{r}\right\rangle_{nl} = \left\langle \phi_{nlm} \middle| \frac{1}{r}\phi_{nlm}\right\rangle}$$

$$\nabla V(r) = V_r' \cdot \hat{r} = \frac{e_0^2}{r^2}\hat{r}$$

$$\Rightarrow \bar{r}\cdot\nabla V(r) = \frac{e_0^2}{r} = -V(r) \Rightarrow \langle \bar{r}\cdot\nabla V\rangle = \langle -V\rangle$$

Viralteoremet: $2\langle E_{kin}\rangle = \langle r\cdot\nabla V(r)\rangle = \langle -V(r)\rangle$

$$\Leftrightarrow \langle E_{kin}\rangle = \frac{1}{2}\langle -V\rangle = -\frac{1}{2}\langle V\rangle$$

$$\langle H\rangle = \langle E_{kin} + V\rangle = \langle E_{kin}\rangle + \langle V\rangle =$$

$$= -\frac{1}{2}\langle V\rangle + \langle V\rangle = \frac{1}{2}\langle V\rangle = E_n = \boxed{-\frac{\hbar^2}{2m_e a_0^2}\cdot\frac{1}{n^2}}$$

$$\Rightarrow \left\langle \frac{1}{r}\right\rangle = -\frac{1}{e_0^2}\langle V\rangle = -\frac{2}{e_0^2}\langle H\rangle = \frac{2}{e_0^2}\cdot\frac{\hbar^2}{2m_e a_0^2 n^2} = \boxed{\frac{1}{a_0 n^2}}$$