TUSL for hydrogenatomet (radialdel)

$$\frac{d^2 u}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right] u$$

$$\rho = \kappa x, \quad \kappa = \frac{\sqrt{-2mE}}{\hbar}$$

$$\rho_0 = \frac{2}{a_0 \kappa}, \quad a_0 = \frac{\hbar^2}{mk}$$

Introduserer $v(\rho)$:

$$u(\rho) = \rho^{l+1} e^{-\rho} v(\rho)$$

gir riktig oppførsel for $\rho \to \infty$ og $\rho \to 0$

Finner ligning for $v(\rho)$:

$$\frac{du}{d\rho} = (l+1)\rho^l e^{-\rho} v - \rho^{l+1} e^{-\rho} v + \rho^{l+1} e^{-\rho} \frac{dv}{d\rho} = \rho^l e^{-\rho}\left[(l+1-\rho)v + \rho \frac{dv}{d\rho}\right]$$

$$\frac{d^2u}{d\rho^2} = l\rho^{l-1} e^{-\rho}\left[(l+1-\rho)v + \rho\frac{dv}{d\rho}\right] - \rho^l e^{-\rho}\left[(l+1-\rho)v + \rho\frac{dv}{d\rho}\right]$$

$$+ \rho^l e^{-\rho}\left[-v + (l+1-\rho)\frac{dv}{d\rho} + \frac{dv}{d\rho} + \rho\frac{d^2v}{d\rho^2}\right]$$

$$= \rho^l e^{-\rho}\left[\left(-2l - 2 + \rho + \frac{l(l+1)}{\rho}\right) v + 2(l+1-\rho)\frac{dv}{d\rho} + \rho\frac{d^2v}{d\rho^2}\right]$$

Radialligningen blir

$$\rho\frac{d^2v}{d\rho^2} + 2(l+1-\rho)\frac{dv}{d\rho} + [\rho_0 - 2(l+1)]v = 0$$

Anta at løsningen kan skrives som $v(\rho) = \sum_{j=0}^{\infty} c_j \rho^j$

Radiallignigen blir

$$\rho \frac{d^2 v}{d\rho^2} + 2(l+1-\rho)\frac{dv}{d\rho} + [\rho_0 - 2(l+1)]v = 0 \quad (*)$$

Anta at løsningen kan skrives som $v(\rho) = \sum_{j=0}^{\infty} c_j \rho^j$

$$\frac{dv}{d\rho} = \sum_{j=1}^{\infty} j c_j \rho^{j-1} = \sum_{j=0}^{\infty} (j+1) c_{j+1} \rho^j$$

$$\frac{d^2v}{d\rho^2} = \sum_{j=0}^{\infty} j(j+1) c_{j+1} \rho^{j-1}$$

Innsatt i $(*)$ gir dette

$$\sum_{j=0}^{\infty} \underbrace{\left[j(j+1)c_{j+1} + 2(l+1)(j+1)c_{j+1} - 2jc_j + (\rho_0 - 2(l+1))c_j \right]}_{\text{hvert av disse leddene må være } = 0} \rho^j = 0$$

$$\Rightarrow \quad c_{j+1} = \frac{2(j+l+1) - \rho_0}{j(j+1) + 2(l+1)(j+1)} c_j \quad \text{rekursjonsformel for } c_j$$

løsningen er gitt når c_0 er gitt

For å få fysisk akseptable løsninger må rekursjonen stoppe.
Det må finnes en j_{maks} slik at $c_{j_{maks}+1} = 0$. Må ha $2(j_{maks} + l + 1) - \rho_0 = 0$.
Vi kaller $\underset{n > l}{j_{maks} + l + 1}$ for n, $n = 1, 2, 3, \ldots$ (det prinsipielle/hovedkvantetallet).

Hva er kvantisert?

Har at $2n = \rho_0$. $\rho_0 = \dfrac{2}{a_0 \kappa}$ og $\kappa = \dfrac{\sqrt{-2m_e E}}{\hbar}$.

Da er $\underline{E_n} = -\dfrac{\hbar^2\kappa^2}{2m_e} = -\dfrac{\hbar^2}{2m_e}\left(\dfrac{2}{a_0\rho_0}\right)^2 = -\dfrac{2\hbar^2}{m_e a_0^2 \rho_0^2} = \underline{-\dfrac{\hbar^2}{2m_e a_0^2}\dfrac{1}{n^2}}$

Numerisk

$$E_n = -\frac{h^2c^2}{8\pi^2 m_e c^2 a_0^2}\frac{1}{n^2} = -\frac{(1240\ \mathrm{eV\,nm})^2}{8\pi^2 \cdot 0{,}511\ \mathrm{MeV}\cdot(0{,}0529\ \mathrm{nm})^2}\cdot\frac{1}{n^2} = -13{,}6\ \mathrm{eV}\ \frac{1}{n^2}$$

Hvordan ser løsningene ut?

<u>Grunntilstanden</u> har $n=1$, $\ell=0$, $m=0$

$E_1 = -13{,}6\ \mathrm{eV}$, $Y_0^0 = \dfrac{1}{\sqrt{4\pi}}$

Radialdel: $R_{n\ell}(r) = \dfrac{u(r)}{r} = \dfrac{1}{r}\rho^{\ell+1}e^{-\rho}v(\rho)$

$= \dfrac{1}{r}(\kappa r)^{\ell+1}e^{-\kappa r}v(\kappa r)$

$= \dfrac{1}{r}\left(\dfrac{r}{a_0 n}\right)^{\ell+1}e^{-r/a_0 n}\,v\!\left(\dfrac{r}{a_0 n}\right)$

| $\rho = \kappa r$; $\kappa = \dfrac{2}{a_0\rho_0} = \dfrac{1}{a_0 n}$

demper for $r \to 0$ — demper for $r \to \infty$

$R_{10}(r) = \dfrac{1}{r}\left(\dfrac{r}{a_0}\right)^{0+1}e^{-r/a_0}\,v\!\left(\dfrac{r}{a_0}\right) = \dfrac{c_0}{a_0}e^{-r/a_0}$

c_0 finnes fra normering $\Rightarrow c_0 = \dfrac{2}{\sqrt{a_0}}$

$$R_{10}(r) = \frac{2}{\sqrt{a_0^3}} e^{-r/a_0} \qquad Y_0^0 = \frac{1}{\sqrt{4\pi}}$$

$$\underline{\psi_{100}(r,\theta,\varphi) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}} \qquad \Big| \; \psi_{nlm}(r,\theta,\varphi)$$

Neste energinivå: $n = 2$, da er $l = 0$ og $m = 0$, eller $l = 1$ og $m = -1, 0, 1$

Altså fire tilstander ψ_{nlm} som har samme energi. <u>Degenerasjon</u>, med <u>degenerasjonsgrad</u> 4.

For hvert energinivå (hver n) er det n forskjellig verdier for l, $l = 0, 1, 2, \ldots, n-1$, for en gitt l så er det $2l+1$ mulige verdier av m, $m = -l, -l+1, \ldots, l-1, l$.

Da er degenerasjonsgraden

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

Det generelle uttrykket for $v(\rho)$ er gitt ved det assosierte <u>Laguerre polynomet</u>

$$v(\rho) = L^{2l+1}_{n-l-1}(2\rho) \quad \text{hvor}$$

$$L^{p}_{q-p}(x) \equiv (-1)^p \left(\frac{d}{dx}\right)^p L_q(x) \quad \text{og}$$

$$L_q(x) \equiv e^x \left(\frac{d}{dx}\right)^q \left(e^{-x} x^q\right).$$

Med normering er bølgefunksjonen for hydrogen

$$\psi_{nlm}(r,\vartheta,\varphi) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n[(n+1)!]^3}}\; e^{-r/a_0 n} \left(\frac{2r}{na_0}\right)^l L^{2l+1}_{n-l-1}\left(\frac{2r}{na_0}\right) Y_l^m(\vartheta,\varphi)$$

Disse er <u>ortonormale</u>

$$\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \psi^*_{nlm}\,\psi_{n'l'm'}\, r^2 \sin\vartheta \, dr\, d\vartheta\, d\varphi = \delta_{nn'}\,\delta_{ll'}\,\delta_{mm'}$$