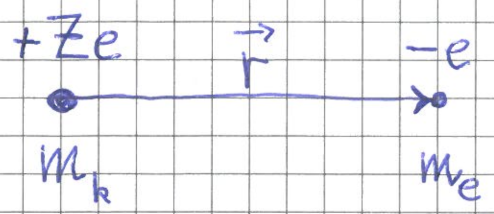
Coulombpotensialet; repetisjon (++)



$$V(r) = -\frac{Ze^2}{4\pi\varepsilon_0 r}$$

$$\mu = m_e m_k / (m_e + m_k)$$

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi(\vec{r}) + V(r)\psi(\vec{r}) = E\psi(\vec{r})$$

$$\psi(r,\theta,\varphi) = R(r)\cdot Y(\theta,\varphi)$$

$$Y_{\ell m}(\theta,\varphi) = P_\ell^m(\cos\theta)\cdot e^{im\varphi}$$

$$\ell = 0, 1, 2, \ldots \quad ; \quad m = 0, \pm 1, \ldots, \pm \ell$$

$$Y_{00} \sim 1, \quad Y_{10} \sim \cos\theta, \quad Y_{20} \sim 3\cos^2\theta - 1, \ldots$$

$$Y_{1,\pm 1} \sim \sin\theta \; e^{\pm i\varphi}$$

$$Y_{2,\pm 1} \sim \sin\theta \cos\theta \; e^{\pm i\varphi}$$

$$Y_{2,\pm 2} \sim \sin^2\theta \; e^{\pm 2i\varphi} \qquad \text{osv}$$

$$R(r) = u(r)/r$$

$$-\frac{\hbar^2}{2\mu}\frac{d^2u}{dr^2} + V^{\ell}_{\text{eff}}(r)\,u(r) = E\,u(r)$$

$$V^{\ell}_{\text{eff}}(r) = -\frac{Ze^2}{4\pi\varepsilon_0 r} + \frac{\hbar^2\ell(\ell+1)}{2\mu r^2}$$

$$\rho = \sqrt{-8\mu E/\hbar^2}\; r \qquad (\text{dim. los})$$

$$\Rightarrow \frac{d^2u}{d\rho^2} + \left\{\frac{\lambda}{\rho} - \frac{\ell(\ell+1)}{\rho^2} - \frac{1}{4}\right\}u = 0$$

$$\lambda = \frac{Ze^2}{4\pi\varepsilon_0\hbar}\sqrt{\frac{\mu}{-2E}} \qquad (\text{dim. los})$$

$$u(\rho) = e^{-\rho/2}\cdot v(\rho)$$

$$\Rightarrow \frac{d^2v}{d\rho^2} - \frac{dv}{d\rho} + \frac{\lambda}{\rho}v - \frac{\ell(\ell+1)}{\rho^2}v = 0$$

$$v(\rho) = \sum_{k=0}^{\infty} c_k\,\rho^{\ell+1+k}$$

$$\Rightarrow c_k = c_{k-1}\cdot\frac{\ell+k-\lambda}{k(2\ell+1+k)}\;; \qquad k=1,2,\ldots$$

Avbruddskrav:

$$\lambda = n = l + 1 + n_r \quad ; \quad n_r = 0, 1, 2, \ldots$$

Energikvantisering:

Hovedkvantetallet

$$\lambda = \frac{Ze^2}{4\pi\varepsilon_0 \hbar}\sqrt{\frac{\mu}{-2E}} = Z \cdot \alpha \cdot \sqrt{\frac{\mu c^2}{-2E}} = n$$

$$\left(\alpha = e^2/4\pi\varepsilon_0 \hbar c \approx 1/137 = \text{finstrukturkonstanten}\right)$$

$$\Rightarrow E_n = -\frac{1}{2}(Z\alpha)^2 \cdot \frac{\mu c^2}{n^2} \quad ; \quad n = 1, 2, 3, \ldots$$

Hydrogen: $Z = 1$, $\mu \approx m_e \Rightarrow E_n \approx -\frac{13.6\,\text{eV}}{n^2}$

$E_n \ll \mu c^2$ (= relativistisk hvileenergi) $\Rightarrow$ ikke-relativistisk behandling OK.

Degenerasjon: $g_n = n^2$

(utledet s. 113)

Andre 1-elektron-systemer (ioner):

He^+ : $Z = 2$, $E_n \approx -\frac{4 \cdot 13.6\,\text{eV}}{n^2} = -\frac{54.4\,\text{eV}}{n^2}$

osv.

Tunge atomer: Mange elektroner, men $E_n^{(Z)} \sim Z^2 \cdot E_n^H$

$\Rightarrow$ av størr. orden 100 keV hvis $Z \sim 10^2$

$\Rightarrow$ relativistisk teori blir etterhvert nødvendig (for nøyaktige beregninger)

Noen eksplisitte radialfunksjoner $R_{n\ell}(r)$:

n	ℓ	$R_{n\ell}(r)$	"Navn"
1	0	$R_{10} \sim e^{-r/a}$	1s
2	0	$R_{20} \sim \left(1-\frac{r}{2a}\right) e^{-r/2a}$	2s
	1	$R_{21} \sim \frac{r}{a}\, e^{-r/2a}$	2p
3	0	$R_{30} \sim \left(1-\frac{2r}{3a}+\frac{2r^2}{27a^2}\right) e^{-r/3a}$	3s
	1	$R_{31} \sim \frac{r}{a}\left(1-\frac{r}{6a}\right) e^{-r/3a}$	3p
	2	$R_{32} \sim \left(\frac{r}{a}\right)^2 e^{-r/3a}$	3d

med

$$a = \frac{1}{Z}\,\frac{m_e}{\mu} \cdot a_0 \;; \quad a_0 = \frac{4\pi\varepsilon_0 \hbar^2}{e^2 m_e} \simeq 0.529\,\mathring{A}$$

(= Bohr-radien)

$$\Psi_{n\ell m}(r,\theta,\varphi) = R_{n\ell}(r)\cdot Y_{\ell m}(\theta,\varphi)$$
$$= \frac{u_{n\ell}(r)}{r}\cdot Y_{\ell m}(\theta,\varphi)$$

$(n=0,1,2\cdots;\ \ell=0,\cdots,n-1;\ m=0,\pm1,\cdots,\pm\ell)$

Normering:

$$\int|\Psi_{n\ell m}|^2 d^3r = \int_0^\infty [R_{n\ell}(r)]^2 r^2 dr \cdot \int |Y_{\ell m}(\theta,\varphi)|^2 d\Omega$$
$$= \int_0^\infty [u_{n\ell}(r)]^2 dr = 1$$

$\Rightarrow$ Sanns. for å finne elektronet i avstand mellom r og $r+dr$ fra kjernen er

$$[u_{n\ell}(r)]^2 dr$$

$\Rightarrow$ "Radialtetthet": $P_{n\ell}(r) = [u_{n\ell}(r)]^2 = r^2[R_{n\ell}(r)]^2$

Eks: $$\left\langle\frac{1}{r}\right\rangle_{n\ell m} = \int \frac{1}{r}|\Psi_{n\ell m}|^2 d^3r = \int_0^\infty \frac{1}{r}[u_{n\ell}(r)]^2 dr = \ldots\ldots = \frac{1}{n^2 a}$$

$\Rightarrow$ Orbitalens utstrekning:

$$\left\langle\frac{1}{r}\right\rangle_{n\ell m}^{-1} = n^2 a = \frac{n^2}{Z}\frac{m_e}{\mu}a_0$$

Dvs: Øker kraftig med n