Zgodovinski uvod, Bohrov model atoma

- karakteristični atomski spektri – značilni za posamezne elemente

  - atomski spektri – spektralne črte
  - molekulski spektri – pasovi
  - trdna snov – lahko tudi zvezen spekter

- že okoli 1880 – Fraunhofer : spektralne črte He v sončni svetlobi

- Rydberg 1888 – spektralne črte vodikovega (H) atoma

$$\frac{1}{\lambda} = R\left(\frac{1}{n^2} - \frac{1}{n'^2}\right)$$

$R_\infty^{NIST} = 10973731.568160(21) \times m^{-1}$

$\tilde{\nu} = \frac{1}{\lambda}$

$\frac{hc}{\lambda} = h\nu$

1eV ⇔ 8066.54 cm^{-1} ≡ kayser

↳ posploši prejšnja dognanja

  - Balmerjeva serija (1885) : $n = 2$ (vidno področje)

    $n' = 3$, $\lambda = 656\,nm$ H_α

    $n' = 4$, $\lambda = 486\,nm$ .. H_β

– – –

  - Lymanova serija (1906) : $n = 1$ (VUV področje)

    $n' = 2, 3, \ldots$

  - Paschen : $n = 3$

...

- Rutherford 1911 ; Rutherford, Geiger, Marsden 1909–13

  sipanje na jedru

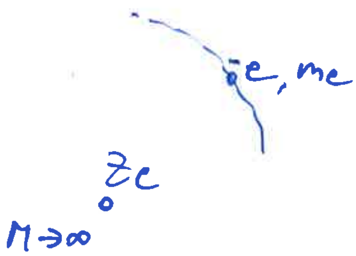
- planetarni model atoma, e^- je pospešen, a ne seva
- Bohr postulira model atoma (1913)

Bohr - Sommerfeldova teorija/model atoma

(orig. za $Z=1$)

1) obstajajo dovoljene orbite, na katerih ima e^- stalno energijo (ne seva) + do „izgube" energije e^- prihaja s prehodi med orbitami

2) gibanje je kvantizirano (vrtilna količina - večkratnik $\hbar$)



$$(i)\quad \frac{m_e v^2}{r} = \frac{Ze^2}{4\pi\varepsilon_0 r^2} \Rightarrow m_e v^2 = \frac{Ze^2}{4\pi\varepsilon_0 r}$$

$$(ii)\quad E = \frac{1}{2} m_e v^2 - \frac{Ze^2}{4\pi\varepsilon_0 r} \overset{(i)}{=} -\frac{Ze^2}{8\pi\varepsilon_0 r}$$

$$(iii)\quad m_e v r = n\hbar \Rightarrow \underline{v_n = \frac{n\hbar}{m_e r_n}}$$

$$\overset{(iii)}{\Rightarrow} \quad \frac{n^2\hbar^2}{m_e r_n^2} = m_e v_n^2 \overset{(i)}{\Rightarrow} \frac{n^2\hbar^2}{m_e r_n^2} = \frac{Ze^2}{4\pi\varepsilon_0 r_n}$$

Bohrov radij

$$\frac{1}{r_n} = \frac{Ze^2}{4\pi\varepsilon_0} \frac{m_e}{n^2\hbar^2} \Rightarrow \underline{r_n = \frac{n^2\hbar^2}{m_e} \cdot \frac{4\pi\varepsilon_0}{Ze^2}} = \boxed{\frac{\hbar^2 4\pi\varepsilon_0}{m_e e^2}} \frac{n^2}{Z}$$

$$\Rightarrow \quad E_n = -\frac{Ze^2}{8\pi\varepsilon_0 r_n} = -\frac{1}{2}\left(\frac{Ze^2}{4\pi\varepsilon_0}\right)^2 \frac{m_e}{n^2\hbar^2}$$

$$= -\frac{1}{2} \boxed{\left(\frac{e^2}{4\pi\varepsilon_0\hbar}\right)^2 m_e} \frac{Z^2}{n^2}$$

Rydbergova energija

$$\boxed{\alpha = \frac{e^2}{4\pi\varepsilon_0 \hbar c} \approx \frac{1}{137}}$$

$$= -\frac{1}{2}\left(\frac{e^2}{4\pi\varepsilon_0 \hbar c}\right)^2 m_e c^2 \cdot \frac{Z^2}{n^2}$$

$$= -\frac{1}{2} \boxed{\alpha^2 m_e c^2} \frac{Z^2}{n^2}$$

$$E_0 = \alpha^2 m_e c^2 = \frac{e^2}{4\pi\varepsilon_0 a_0} = \left(\frac{e^2}{4\pi\varepsilon_0\hbar}\right)^2 m_e$$

$$a_0 = \frac{4\pi\varepsilon_0 \hbar^2}{m_e e^2} = \frac{\hbar}{\alpha m c}$$

$$E_0 = 4.359\,744\,722\,2071\,(85) \times 10^{-18}\ J$$

$$= 27.211\,386\,245\,988\,(53)\ eV$$

$$a_0 = 5.291\,772\,109\,03\,(80) \times 10^{-11}\ m$$

- - - -

- $m_e v_n r_n = n\hbar$

$$\Rightarrow m_e v_n a_0 \frac{n^2}{Z} = n\hbar$$

$$\Rightarrow \boxed{v_n = \frac{Z}{n} \alpha c}$$

- S tem že razložimo Rydbergovo formulo:

$$-E_n + E_{n'} = \frac{1}{2}\alpha^2 m_e c^2 \left(\frac{Z^2}{n^2} - \frac{Z^2}{n'^2}\right) \equiv h\nu \equiv \frac{hc}{\lambda}$$

$$\equiv hcR_\infty \left(\frac{Z^2}{n^2} - \frac{Z^2}{n'^2}\right)$$

$$hcR_\infty = \frac{1}{2}\alpha^2 m_e c^2$$

$$\boxed{R_\infty = \frac{1}{2}\alpha^2 m_e \frac{c}{h}}$$

- spektri so odvisni od mase jedra, saj za $M \not\to \infty$ nadomestimo → izotopski premik

$$m_e \to \frac{m_e M}{m_e + M} = \mu$$

Pri vodiku

$$\mu = \frac{m_e m_p}{m_e + m_p}, \quad \frac{m_p}{m_e} \approx 1836$$

$$R_H = \frac{\mu}{m_e} R_\infty = \frac{m_p}{m_e + m_p} R_\infty$$

— Moseley: v rentgenskih spektrih

$$\sqrt{\nu} \propto Z$$

\+ senčenje $\quad Z \to Z - \sigma$

- odvisen od lupine
- se da razložiti le s kvantno teorijo

\+ emisijske črte K_α, K_β (ta vrzel se zapolni)

$L \ldots$

$M \ldots$

– relativistični efekti/učinki

$$E = \gamma m c^2$$

$$T = (\gamma - 1) m c^2 \approx \Delta E \qquad \gamma = \frac{1}{\sqrt{1-\frac{v^2}{c^2}}} \approx 1 + \frac{1}{2}\frac{v^2}{c^2} + \ldots$$

$$\frac{\Delta E}{E} \sim \frac{v^2}{c^2} \sim \frac{Z^2 \alpha^2}{n^2}$$

Bohr: $\boxed{v_n = \frac{Z}{n} \alpha c}$

Pomembni za težje atome

⇒ Z njimi je povezana fina struktura

Na svetilka, Na dublet

589.0, 589.6 nm

$$\Delta E = 2.1 \cdot 10^{-3} \, eV = 17 \, cm^{-1}$$

Za to je odgovorna interakcija spinov z B poljem, ki ga čutijo e^-!

$$\mu_B = \frac{e\hbar}{2m_e} \approx 9.27 \cdot 10^{-24} \frac{J}{T}$$

– hiperfina struktura: $\mu_N \approx \frac{\mu_B}{2000}$

$$\frac{m_p}{m_e} \approx 1836 \, !$$

↳ še 1000× manjša

vodik: $\lambda = 21 \, cm$

$$h\nu = 6 \cdot 10^{-6} \, eV = 0.05 \, cm^{-1}$$

Vodikov atom

SE: $\left\{-\frac{\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{4\pi\varepsilon_0 r}\right\}\psi = E\psi$

a.u.: $\left\{-\frac{1}{2}\nabla^2 - \frac{Z}{r}\right\}\psi = E\psi$ — izpustimo vijugice

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{r^2}\vec{l}^{\,2}$$

$$\vec{l}^{\,2} = -\left\{\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right\}$$

$\vec{l} = \vec{r}\times\vec{p} = \vec{r}\times(-i\nabla)$

$$\left(\nabla = \hat{r}\frac{\partial}{\partial r}\cdot + \hat{\vartheta}\frac{1}{r}\frac{\partial}{\partial\vartheta}\cdot + \hat{\varphi}\frac{1}{r\sin\vartheta}\frac{\partial}{\partial\varphi}\cdot\right)$$

- $\psi(\vec{r}) = \psi(r,\vartheta,\varphi) = R(r)\,Y(\vartheta,\varphi)$

- sferne harmonike = harmonske funkcije, ki jih poznamo

$$\vec{l}^{\,2}\,Y_{lm}(\vartheta,\varphi) = l(l+1)\,Y_{lm}(\vartheta,\varphi)$$

$$l_z\,Y_{lm}(\vartheta,\varphi) = m\,Y_{lm}(\vartheta,\varphi)$$

$l_z = -i\frac{\partial}{\partial\varphi}$

normirani so takole: $d\Omega = \sin\vartheta\, d\vartheta\, d\varphi = d(\cos\vartheta)\, d\varphi$ $\quad \vartheta\in[0,\pi]$, $\varphi\in[0,2\pi]$

$$\int d\Omega\; Y^*_{l'm'}(\Omega)\,Y_{lm}(\Omega) = \delta_{ll'}\,\delta_{mm'}$$

$$\int d\Omega\,|Y_{lm}(\Omega)|^2 = 1$$

l, m sta celi števili: $l = 0, 1, 2, \ldots$ — tirno kv. število

$-l \le m \le l$ — magnetno kv. število (tirno)

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

$Y_{10} = \sqrt{\frac{3}{4\pi}}\cos\vartheta$

$Y_{1,\pm1} = \mp\sqrt{\frac{3}{8\pi}}\sin\vartheta\, e^{\pm i\varphi}$

$Y_{2,0} = \sqrt{\frac{5}{16\pi}}\left(3\cos^2\vartheta - 1\right)$

$Y_{2,\pm1} = \mp\sqrt{\frac{15}{8\pi}}\sin\vartheta\cos\vartheta\, e^{\pm i\varphi}$

$Y_{2,\pm2} = \sqrt{\frac{15}{32\pi}}\sin^2\vartheta\, e^{\pm 2i\varphi}$

...

Kako do sem ? $\psi = R(r)Y(\vartheta,\varphi)$

$$\Rightarrow \quad \frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) - 2r^2\left\{-\frac{Z}{r} - E\right\} = \frac{1}{Y}\vec{\ell}^{\,2}Y$$

obe strani sta konstanti $\equiv \lambda$

$$\vec{\ell}^{\,2}Y = \lambda Y$$

- spet lahko pišemo : $Y(\vartheta,\varphi) = \Theta(\vartheta)\,\phi(\varphi)$

$$\frac{\sin^2\vartheta}{\Theta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial\Theta}{\partial\vartheta}\right) + \lambda\sin^2\vartheta = -\frac{1}{\phi}\frac{\partial^2\phi}{\partial\varphi^2} \quad (\equiv m^2)$$

obe strani sta konstanti

$$\left.\begin{aligned} -\frac{1}{\phi}\frac{\partial^2\phi}{\partial\varphi^2} &= m^2 \\ \phi'' + m^2\phi &= 0 \end{aligned}\right\} \text{harmonska enačba}$$

$$\phi = Ae^{im\varphi} + Be^{-im\varphi}$$

- zahtevamo $\phi(\varphi) = \phi(\varphi+2\pi) \Rightarrow$ m je celo število
- z algebrajskim pristopom pokažemo, da je m omejen $(m_{max} = \ell)$
  $\hookrightarrow \ell_+, \ell_-$

in da je $m_{min} = -\ell$ $\quad \}\ \ell_\pm = \ell_x \pm i\ell_y$

- pokažemo, da je za $m = m_{max} = \ell$ $\quad Y \propto \sin^\ell\vartheta\, e^{i\ell\varphi}$

in da je $\lambda = \ell(\ell+1)$ $\quad$ enačba za $\Theta(\vartheta)$

$$\left\{ P_{\ell,-m} = (-1)^m\frac{(\ell-m)!}{(\ell+m)!}P_{\ell m} \right.$$

$$\boxed{m \geq 0}$$

$$\boxed{Y_{\ell m}(\vartheta,\varphi) = (-1)^m\sqrt{\frac{(2\ell+1)(\ell-m)!}{4\pi\ (\ell+m)!}}\, P_{\ell m}(\cos\vartheta)\, e^{im\varphi}}$$

posplošeni Legendreovi polinomi

izbira faze : Condon – Shortley (1935) $\quad \boxed{Y^*_{\ell m} = (-1)^m Y_{\ell,-m}}$

$P_{\ell,0}(\cos\vartheta) = P_\ell(\cos\vartheta)$ } „navadni" L.p.

- radialna enačba: $R(r) = \frac{P(r)}{r}$

$$\underbrace{\left[-\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \frac{Z}{r}\right] P(r) = E\,P(r)}$$

↳ $E<0$: vezana stanja

$E>0$: nevezana stanja — Coulombski val

(i) vezana stanja: $(E<0)$

$$\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} - \frac{2Z}{r}\right] P = 2E\,P$$

$$\left\{ 0 = \left[\frac{d^2}{d\rho^2} - \frac{1}{4} + \frac{n}{\rho} - \frac{l(l+1)}{\rho^2}\right] P \right.$$

↳ nova spremenljivka: $\rho = \frac{2Zr}{n}$

in se: $2E = -\frac{Z^2}{n^2}$,

kjer n še ni znan.

zahteve: $\rho \to \infty$: $P \to e^{-\rho/2}$

$\rho \to 0$: $P \to \rho^{l+1}$

zahtevamo

$$\boxed{\begin{aligned} P(0) &= 0 \\ P(\infty) &\to 0 \end{aligned}}$$

v $\rho \to \infty$: $\frac{d^2}{d\rho^2}P - \frac{1}{4}P = 0 \Rightarrow P = A\,e^{\rho/2} + B\,e^{-\rho/2}$

v $\rho \to 0$: $\frac{d^2}{d\rho^2}P - \frac{l(l+1)}{\rho^2}P = 0 \Rightarrow P = A\,r^{l+1} + B\,r^{-l}$

Zato lahko pišemo: $P_{nl} = \rho^{l+1} e^{-\rho/2} f(\rho)$

$$\Rightarrow \boxed{f'' + \left(\frac{2l+2}{\rho} - 1\right) f' + \frac{n-l-1}{\rho} f = 0}$$

Rešujemo z vrsto: število členov je končno le za $n \geq l+1$ in $n \in \mathbb{Z}$.

* **Dobimo**

$$P_{n\ell}(r) = \sqrt{\frac{(n-\ell-1)!\,Z}{(n+\ell)!\,n^2}} \left(\frac{2Zr}{n}\right)^{\ell+1} \underbrace{L_{n-\ell-1}^{2\ell+1}\left(\frac{2Zr}{n}\right)} \exp\left(-\frac{Zr}{n}\right)$$

realne funkcije

posplošeni Laguerreovi polinomi; stopnja $n-\ell-1$ } Abramowitz, Stegun

Normalizacija: $\int_0^\infty R_{n'\ell}(r)\, R_{n\ell}(r)\, r^2 dr =$

$$\int_0^\infty P_{n'\ell}(r)\, P_{n\ell}(r)\, dr = \delta_{nn'}$$

Tabela: $\rho = \frac{Zr}{n}$

$$P_{1,0}(r) = 2\sqrt{Z}\,\rho\, e^{-\rho}$$

$$P_{2,0}(r) = \sqrt{\frac{Z}{2}}\,\rho\,(2-2\rho)\, e^{-\rho}$$

$$P_{2,1}(r) = \sqrt{\frac{2Z}{3}}\,\rho^2\, e^{-\rho}$$

$$P_{3,0}(r) = \frac{2}{3}\sqrt{\frac{Z}{3}}\,\rho\,(3-6\rho+2\rho^2)\, e^{-\rho}$$

$$P_{3,1}(r) = \frac{1}{3}\sqrt{\frac{2Z}{3}}\,\rho^2\,(4-2\rho)\, e^{-\rho}$$

$$P_{3,2}(r) = \frac{2}{3}\sqrt{\frac{2Z}{15}}\,\rho^3\, e^{-\rho}$$

- Kontinuumske rešitve — reševali smo enačbo za parcialne valove (Y_{lm}!)

→ ravni val : normalizacija : $\delta^3(\vec{k}-\vec{k}')$

$$(2\pi)^{-3/2} e^{i\vec{k}\cdot\vec{r}} = \langle \vec{r}|\vec{k}\rangle = \left(\frac{2}{\pi}\right)^{1/2} \sum_{l,m} i^l j_l(kr) Y_{lm}(\hat{r}) Y_{lm}^*(\hat{k})$$

→ podobno :

$$\phi^{(+)}(\vec{k},\vec{r}) = \left(\frac{2}{\pi}\right)^{1/2} \sum_{l,m} i^l e^{i\sigma_l} \frac{F_l(r;k)}{kr} Y_{lm}(\hat{r}) Y_{lm}^*(\hat{k})$$

$$F_l(r;k) \sim \sin\left(kr + \frac{Z}{k}\ln(2kr) - \frac{l\pi}{2} + \sigma_l\right)$$

$$\sigma_l = \arg \Gamma\left(l+1-i\frac{Z}{k}\right)$$

coulombska valovna (radialna) funkcija za $E = \frac{k^2}{2} > 0$

$$F_l(\rho;\eta) = \frac{2^l e^{-\pi\eta/2} |\Gamma(l+1+i\eta)|}{(2l+1)!} \rho^{l+1} e^{i\rho} \times$$

$$\times M(l+1+i\eta,\ 2l+2,\ -2i\rho)$$

$$\begin{cases} \eta = -\frac{Z}{k} & : \text{Sommerfeldov parameter} \\ \rho = kr \end{cases}$$

$$M(a,b;z) = {}_1F_1(a,b;z)$$

= konfluentna hipergeometrijska funkcija

podobno kot $j_l(r)$, je $\frac{F_l(r)}{r}$ rešitev radialnega dela („mirujoči" valovi)

⇒ $F_l(r,k)$ ustreza $P_{nl}(r)$

<u>Mimogrede</u>

$$M(-n,\ a+1,\ x) = \frac{n!}{(a+1)_n} L_n^a(x)$$

$$(a)_n = \frac{\Gamma(a+n)}{\Gamma(a)}$$

1. Atomske enote

Schrödingerjeva enačba — $\vec{r}$ oblika!

$$\left\{ -\frac{\hbar^2}{2m_e}\nabla^2 - \frac{Z e_0^2}{4\pi\varepsilon_0 r} \right\} \psi(\vec{r}) = E\psi(\vec{r})$$

a) vpeljemo
$$\vec{r} = a_0 \tilde{\vec{r}}$$
$$E = E_0 \tilde{E}$$

b) za normirano valovno funkcijo velja

$$\int \psi^*(\vec{r})\psi(\vec{r})\, \overset{d^3r}{dV} = \int \psi^*(a_0\tilde{\vec{r}})\, \psi(a_0\tilde{\vec{r}})\, \overbrace{\frac{dV}{d\tilde{V}}}^{a_0^3} d\tilde{V}$$

$$= \int \underbrace{\psi^*(a_0\tilde{\vec{r}})\psi(a_0\tilde{\vec{r}})\, a_0^3}_{\substack{\parallel\\ \tilde{\psi}^*(\tilde{\vec{r}})\tilde{\psi}(\tilde{\vec{r}})}} d\tilde{V}$$

$$\Rightarrow \quad \psi(a_0\tilde{\vec{r}})\, a_0^{+3/2} = \tilde{\psi}(\vec{r})$$
$$[m^{-3/2} \cdot m^{+3/2} = 1]$$

c) zdaj določimo konstanti a_0 in E_0

$$\left\{ -\frac{\hbar^2}{2m_e}\frac{1}{a_0^2}\tilde{\nabla}^2 - \frac{Z e_0^2}{4\pi\varepsilon_0}\frac{1}{a_0}\frac{1}{\tilde{r}} \right\} \tilde{\psi}(\tilde{\vec{r}}) = E_0\tilde{E}\,\tilde{\psi}(\tilde{\vec{r}}) \quad / : E_0$$

$$\left\{ -\frac{\hbar^2}{2m_e}\frac{1}{a_0^2}\frac{1}{E_0}\tilde{\nabla}^2 - \frac{Z e_0^2}{4\pi\varepsilon_0}\frac{1}{a_0}\frac{1}{E_0}\frac{1}{\tilde{r}} \right\} \tilde{\psi}(\tilde{\vec{r}}) = \tilde{E}\,\tilde{\psi}(\tilde{\vec{r}})$$

c.1) $\dfrac{\hbar^2}{m_e}\dfrac{1}{a_0^2}\dfrac{1}{E_0} = 1$ c.2) $\dfrac{e_0^2}{4\pi\varepsilon_0 a_0 E_0} = 1$

$$\frac{c.1)}{c.2)} = \frac{\hbar^2}{m_e a_0^2 \cancel{E_0}} \cdot \frac{4\pi\varepsilon_0 \cancel{a_0 E_0}}{e_0^2} = 1$$

$$\Rightarrow \boxed{a_0 = \frac{4\pi\varepsilon_0 \hbar^2}{m_e e_0^2}}$$

Bohrov radij:

$a_0 \approx 5.29177 \times 10^{-11}\,m$

$\Rightarrow$ c.2) $\Rightarrow$

$$\frac{e_0^2}{4\pi\varepsilon_0 a_0 E_0} = 1 \Rightarrow \quad E_0 = \frac{e_0^2}{4\pi\varepsilon_0 a_0} = \frac{e_0^2}{4\pi\varepsilon_0}\,\frac{m_e e_0^2}{4\pi\varepsilon_0 \hbar^2}$$

$$\boxed{E_0 = \left(\frac{e_0^2}{4\pi\varepsilon_0}\right)^2 \frac{m_e}{\hbar^2}}$$

$E_0 \approx 4.35974 \times 10^{-18}\,J$ Hartree-jeva energija (hartree)

$\approx 27.2114\,eV$

Omeni rydberge

$$\boxed{E_0 = \underbrace{\left(\frac{e_0^2}{4\pi\varepsilon_0}\right)^2 \frac{m_e}{\hbar^2}\cdot\frac{c^2}{c^2}}_{\alpha^2} = \alpha^2 m_e c^2}$$

d) časovna enota

$$\Psi(\vec{r},t) = \int \psi(\vec{r},E)\, e^{-iEt/\hbar}\, dE$$

$$\exp\left(-\frac{iEt}{\hbar}\right) = \exp\left(-\frac{iE_0\tilde{E}\, t_0\tilde{t}}{\hbar}\right)$$

$$\frac{E_0\cdot t_0}{\hbar} = 1 \quad \Rightarrow \quad \boxed{t_0 = \frac{\hbar}{E_0}}$$

$t_0 \approx 2.41888 \times 10^{-17}\,s$

e) hitrost

$$v_0 = \frac{a_0}{t_0} = \frac{a_0 E_0}{\hbar} = \frac{e_0^2}{4\pi\varepsilon_0\hbar}\cdot\frac{c}{c} = \alpha\cdot c$$

konstanta fine strukture : $\boxed{\alpha = \frac{e_0^2}{4\pi\varepsilon_0\hbar c}}$ $\quad \boxed{v_0 = \alpha\cdot c}$

$v_0 \simeq 2.18769 \times 10^{+6}\,m/s$

f) Naraj la c. 2) :

$$\frac{e_0^2}{4\pi\varepsilon_0 a_0 E_0} = 1 \quad , \qquad E_0 = \alpha^2 m_e c^2$$

$$a_0 = \left(\frac{e_0^2}{4\pi\varepsilon_0}\right) \cdot \alpha^{-2} \left(\frac{1}{m_e c^2}\right)$$

$\hookrightarrow$ klasični radij elektrona $\quad \frac{e_0^2}{4\pi\varepsilon_0 r_e} = m_e c^2$

$$\boxed{r_e = \frac{e_0^2}{4\pi\varepsilon_0} \frac{1}{m_e c^2}}$$

$$\Rightarrow \quad \boxed{a_0 = \alpha^{-2} r_e} \qquad r_e \approx 2.81794 \times 10^{-15}\, m$$

SI enote: $\quad \left\{ -\frac{\hbar^2}{2m_e}\nabla^2 - \frac{Z e_0^2}{4\pi\varepsilon_0} \frac{1}{r} \right\} \psi(\vec{r}) = E\psi(\vec{r})$

atomske enote: $\quad \left\{ -\frac{1}{2}\tilde{\nabla}^2 - \frac{Z}{\tilde{r}} \right\} \tilde{\psi}(\tilde{\vec{r}}) = \tilde{E}\, \psi(\tilde{\vec{r}})$

$\Rightarrow$ vrtilno količino bomo merili v enotah $\hbar$

$$\Rightarrow \quad \hbar \longrightarrow 1$$

maso $\qquad m_e$

$$m_e \longrightarrow 1$$

naboj $\qquad e_0$

$$e_0 \longrightarrow 1$$

Ostane $\quad 4\pi\varepsilon_0$

$$4\pi\varepsilon_0 \longrightarrow 1$$

$\rightarrow$ hitrosti bomo merili v enotah v_0

kolikšna bo potem svetlobna hitrost v a.u.?

$$\frac{c}{v_0} = \frac{c}{\alpha \cdot c} = \alpha^{-1}$$

$$c \longrightarrow \alpha^{-1}$$

g) enota za el. poljsko jakost

$$\boxed{F_0 = \frac{e_0}{4\pi\varepsilon_0 a_0^2}}$$

$$F_0 \approx 5.14221 \times 10^{11} \, \frac{V}{m}$$

h) enota za gostoto magn. polja

$$\Delta H = \frac{1}{2} \frac{e_0 \hbar}{m_e} \cdot g_e \cdot \tilde{\vec{\ell}} \cdot \vec{B}$$

$$\boxed{B_0 = \frac{E_0 m_e}{e_0 \hbar}} \approx 2.35052 \times 10^5 \, T \approx B_0$$

$$\Delta H_{orb} = -\vec{p}_m \cdot \vec{B} = +\frac{1}{2} \frac{e_0 \hbar}{m_e} \tilde{\ell} B_z \cdot g_e$$

$\hookrightarrow \vec{B} \parallel \hat{z}$

$$\Delta \tilde{E} \, E_0 = \frac{1}{2} \frac{e_0 \hbar}{m_e} B_0 \, \tilde{\ell} \tilde{B}_z g_e$$

$$g_e = 1$$

$$E_0 = \frac{e_0 \hbar}{m_e} B_0$$

$$\Delta H_{spin} = +\frac{1}{2} \frac{e_0 \hbar}{m_e} \cdot \tilde{s} B_z \cdot g_s$$

$$g_s \approx 2$$

$$m_e \cdot v_p \cdot r_p = \tilde{\ell} \hbar$$

$$m_e \, \omega_p \, r_p^2 = \tilde{\ell} \hbar$$

$$m_e \frac{2\pi}{t_p} r_p^2 = \tilde{\ell} \hbar$$

$$\Rightarrow \frac{r_p^2}{t_p} = \frac{\tilde{\ell} \hbar}{m_e 2\pi}$$

$$p_m = I \cdot S$$
$$= -\frac{e_0}{t_p} \cdot \pi r_p^2$$
$$= -e_0 \cancel{\pi} \cdot \frac{\tilde{\ell} \hbar}{m_e 2\cancel{\pi}}$$
$$= -\frac{e_0 \hbar}{2 m_e} \cdot \tilde{\ell}$$

$$\mu_B = \frac{e_0 \hbar}{2 m_e} \approx 5.78838 \times 10^{-5} \frac{eV}{T}$$

$$\approx 9.27401 \times 10^{-24} \frac{J}{T}$$