Vodikov spekter

$\boxed{E_f = \Delta E}$

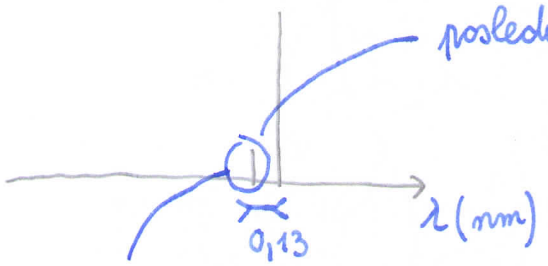
Laymanove črte:
(v UV vidnem polju)

m	izmerjene	izračunane
2	121,568	121,5664
3	102,583	102,5717
4	97,254	97,2532
5	94,974	94,9739

Balmar:

$n \to m$

$2 \to 3$



posledica devterija (^2D)

izotopska sklopitev spektralnih črt

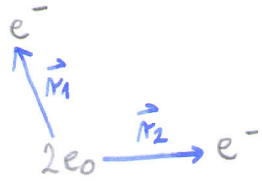
$$Ry_H = \frac{\mu e_0^4}{64\pi^3 \varepsilon_0^2 \hbar^3 c}$$

$$\mu = \frac{m_e \cdot m_p}{m_e + m_p} \ (H) \text{ - red. masa za vodik}$$

$$\mu = \frac{m_e \cdot m_d}{m_e + m_d} \ (D) \text{ - za devterij}$$

Črte v resnici niso črte - so razširjene:
- posledica Dopplerjevega pojava
⋮

Helijev atom



$$\hat{H}\psi = E\psi$$

$$\hat{H} = -\frac{\hbar^2}{2m}\vec{\nabla}_1^2 \ldots$$

$$\boxed{\begin{array}{l} 1.\ e^-: \ \vec{\nabla}_1 = \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial y_1}, \frac{\partial}{\partial z_1}\right) \\ 2.\ e^-: \ \vec{\nabla}_2 = \left(\frac{\partial}{\partial x_2}, \frac{\partial}{\partial y_2}, \frac{\partial}{\partial z_2}\right) \end{array}}$$

$\Downarrow$

$$\boxed{\hat{H} = \underbrace{-\frac{\hbar^2}{2m}\vec{\nabla}_1^2}_{\text{kin. E 1. } e^-} \underbrace{- \frac{\hbar^2}{2m}\vec{\nabla}_2}_{\text{kin. E 2. } e^-} \underbrace{- \frac{2e_0^2}{4\pi\varepsilon_0 r_1}}_{\text{pot. E 1. } e^-} \underbrace{- \frac{2e_0^2}{4\pi\varepsilon_0 r_2}}_{\text{pot. E 2. } e^-} + \underbrace{\frac{e_0^2}{4\pi\varepsilon_0 |\vec{r}_1 - \vec{r}_2|}}_{\text{odboj med 1. in 2. } e^-}}$$

Ta sistem ni več <u>ANALITIČNO REŠLJIV.</u>

Recimo, da se elektrona ne „čutita" med seboj: $\cancel{\frac{e_0^2}{4\pi\varepsilon_0|\vec{r}_1 - \vec{r}_2|}}$:

$$\hat{H} = \frac{-\hbar^2}{2m_e}\vec{\nabla}_1^2 - \frac{2e_0^2}{4\pi\varepsilon_0 r_1} - \frac{\hbar^2}{2m_e}\vec{\nabla}_2^2 - \frac{2e_0^2}{4\pi\varepsilon_0 r_2}$$

Naša val. funkcija mora biti odvisna od koordinat e^- : $\underline{\psi(\vec{r}_1, \vec{r}_2)}$

$$\psi(\vec{r}_1, \vec{r}_2) = \underset{\substack{n\,l\,m \\ 1\,1\,1}}{\psi}(\vec{r}_1)\, \underset{\substack{n\,l\,m \\ 2\,2\,2}}{\psi}(\vec{r}_2)$$

$$\boxed{\hat{H} = \hat{H}_1 + \hat{H}_2}$$

$\hat{H}_1$: Ham. operator za 1. e^- okoli $2e_0$

$\hat{H}_2$: Ham. operator za 2. e^- okoli $2e_0$

$$\hat{H}\psi(\vec{r}_1, \vec{r}_2) = (\hat{H}_1 + \hat{H}_2)(\psi_{nlm}(\vec{r}_1)\psi_{nlm}(\vec{r}_2)) =$$

$$= \hat{H}_1\psi_{n_1l_1m_1}(\vec{r}_1)\underbrace{\psi_{n_2l_2m_2}(\vec{r}_2)}^{\text{konst.}} +$$

$$\hat{H}_2\underbrace{\psi_{n_1l_1m_1}(\vec{r}_1)}_{\text{konst.}}\psi_{n_2l_2m_2}(\vec{r}_2) =$$

$$= \psi_{n_2l_2m_2}(\vec{r}_2)E_{n_1}\psi_{n_1l_1m_1}(\vec{r}_1) +$$

$$\psi_{n_1l_1m_1}(\vec{r}_1)E_{n_2}\psi_{n_2l_2m_2}(\vec{r}_2) =$$

$$= \underline{(E_{n_1} + E_{n_2})\psi_{n_1l_1m_1}(\vec{r}_1)\psi_{n_2l_2m_2}(\vec{r}_2)}$$

dokazali smo :

$$\boxed{\hat{H}\psi(\vec{r}_1, \vec{r}_2) = (E_{n_1} + E_{n_2})\psi(\vec{r}_1, \vec{r}_2)}$$

Če zanemarimo odboj med e^-, lahko enačbo rešimo ANALITIČNO - naredili smo

PRIBLIŽEK GOLEGA JEDRA

Približek golega jedra

$$\boxed{\Psi(\vec{r}_1, \vec{r}_2 \ldots \vec{r}_n) = \phi_1(\vec{r}_1)\phi_2(\vec{r}_2)\ldots\phi_n(\vec{r}_n)}$$

$\phi_n(\vec{r}_n)$ ... ENODELČNA FUNKCIJA

$E = E_1 + E_2 \ldots + E_n$ – energija sistema je enaka vsoti energij enodelčnih funkcij

$$E_n = \frac{-13{,}6\,eV\,z^2}{n^2}$$

> Fermioni so delci, ki ne morejo imeti enakih vseh 5 kv. števil – primer e^- v atomu.

H (vodik): $E_n = -13{,}6\,eV$ $\uparrow$ 1s $\underline{E_n = E_{ion\,1}}$ (1. ionizacijska energija)

He (helij): $\uparrow\downarrow$ 1s

$$E_n = -\frac{13{,}6eV\cdot 4}{1} - \frac{13{,}6eV\cdot 4}{1} = -108{,}8\,eV \qquad \underline{E_{ion\,1} \doteq 54{,}4\,eV}$$

Li (litij): $\uparrow$ 2s — — — $2p^6$

$\uparrow\downarrow$ 1s

$$E_n = 2\cdot\left(-\frac{13{,}6eV\cdot 9}{1}\right) + \underline{\left(-\frac{13{,}6eV\cdot 9}{4}\right)} = -275{,}4\,eV$$

$E_{ion\,1} = 30{,}6\,eV$

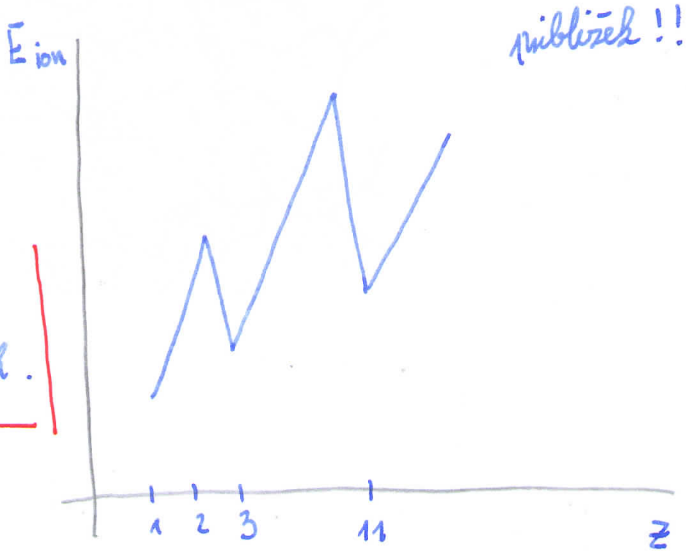
Be (berilij): $E_{ion\,1} = \frac{13{,}6\cdot 4^2}{2^2}$

Na (natrij): $E_{ion\,1} = \frac{13{,}6\cdot 11^2}{3^2}$

B (bor): $E_{ion\,1} = \frac{13{,}6\cdot 5^2}{2^2}$

Ne (neon): $E_{ion\,1} = \frac{13{,}6\cdot 10^2}{2^2}$

približek!!



> Odboj med e^- smo zanemarili, zato se ionizacijske energije (izmerjene) razlikujejo od izračunanih.