H-szerű atomok (Z rendszám, 1 elektron – H, He^{+}, Li^{2+}, Be^{3+}, ...)

$$\boxed{\hat{H} = -\frac{1}{2}\Delta - \frac{Z}{r}}$$

Megj. $\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\Delta_{\vartheta,\varphi}$

Variációs módszerrel az alapállapot

1, Exponenciális $\qquad \psi(r) = \mathcal{N} e^{-\alpha r}$

$$\overset{!}{\langle\psi|\psi\rangle} = 1 \Rightarrow \mathcal{N}^2 \cdot \int_0^\infty dr\, 4\pi r^2 e^{-2\alpha r} = 4\pi \mathcal{N}^2 \cdot \frac{2}{(2\alpha)^3} = 1 \Rightarrow \mathcal{N} = \sqrt{\frac{\alpha^3}{\pi}}$$

mert $$\int_0^\infty r^k e^{-c\cdot r}\, dr = (-1)^k \frac{\partial^k}{\partial c^k}\left(\int_0^\infty e^{-c\cdot r} dr\right) = (-1)^k \frac{\partial^k}{\partial c^k}\left(\frac{1}{c}\right) = \frac{k!}{c^{k+1}}$$

$$\langle E_{pot}\rangle = \langle\psi|\frac{-Z}{r}|\psi\rangle = -Z\cdot\mathcal{N}^2\cdot 4\pi\int_0^\infty dr\cdot r^2\cdot\frac{1}{r}e^{-2\alpha r} = -Z\mathcal{N}^2\cdot 4\pi\cdot\frac{1}{(2\alpha)^2} = \underline{-Z\cdot\alpha}$$

$$\langle E_{kin}\rangle = \langle\psi|-\tfrac{1}{2}\Delta|\psi\rangle = -\frac{1}{2}\mathcal{N}^2\cdot 4\pi\int_0^\infty dr\cdot r^2\cdot e^{-\alpha r}\underbrace{\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}e^{-\alpha r}\right)}_{-\alpha\left(\frac{2}{r}e^{-\alpha r} - \alpha e^{-\alpha r}\right)} =$$

$$= +\frac{1}{2}\alpha\cdot\mathcal{N}^2\cdot 4\pi\int_0^\infty dr\left(2r e^{-2\alpha r} - \alpha r^2 e^{-2\alpha r}\right) =$$

$$= \frac{\alpha}{2}\mathcal{N}^2\cdot 4\pi\cdot\left[2\cdot\frac{1}{(2\alpha)^2} - \alpha\cdot\frac{2}{(2\alpha)^3}\right] = \frac{\alpha}{2}\cdot\frac{\alpha^3}{\pi}\cdot 4\pi\cdot\frac{1}{4\alpha^2} = \underline{\frac{1}{2}\alpha^2}$$

$$\Rightarrow \langle E\rangle = \frac{\alpha^2}{2} - Z\cdot\alpha$$

$$0 = \frac{d\langle E\rangle}{d\alpha} = \alpha - Z \Rightarrow \underline{\alpha_0 = Z} \quad \text{és} \quad \langle E_0\rangle = \frac{Z^2}{2} - Z\cdot Z = \underline{-\frac{1}{2}Z^2}$$

2) Gauss $\quad \psi(r) = N' \cdot e^{-\beta r^2}$

$\overset{!}{\langle \psi | \psi \rangle = 1} \Rightarrow N'^2 \cdot 4\pi \underbrace{\int_0^\infty dr\, r^2 \cdot e^{-2\beta r^2}}_{-\frac{1}{2} \cdot \frac{\partial}{\partial \beta} \underbrace{\int_0^\infty e^{-2\beta r^2} dr}_{\frac{1}{2} \cdot \sqrt{\frac{\pi}{2\beta}}}} = N'^2\, 4\pi \left(-\frac{1}{2}\right) \frac{1}{2} \left(-\frac{1}{2}\right) \sqrt{\frac{\pi}{2}}\, \beta^{-3/2} =$

$$= N'^2 \left(\frac{\pi}{2\beta}\right)^{3/2} = 1 \qquad \Rightarrow N' = \left(\frac{2\beta}{\pi}\right)^{3/4}$$

$$\langle E_{pot} \rangle = \langle \psi | -\frac{Z}{r} | \psi \rangle = -Z N'^2 \cdot 4\pi \int_0^\infty dr\, r^2 e^{-\beta r^2} \cdot \frac{1}{r} e^{-\beta r^2} =$$

$$= -Z N'^2 \cdot 4\pi \cdot \int_0^\infty dr \cdot \underbrace{r \cdot e^{-2\beta r^2}}_{\frac{1}{-4\beta} \frac{\partial}{\partial r}\left(e^{-2\beta r^2}\right)} = -Z N'^2 \cdot 4\pi \cdot \frac{-1}{4\beta} \left[e^{-2\beta r^2} \right]_0^\infty = \underline{-Z \sqrt{\frac{8\beta}{\pi}}}$$

$$\langle E_{kin} \rangle = \langle \psi | -\frac{1}{2} \Delta | \psi \rangle = -\frac{1}{2} N'^2 \cdot 4\pi \int_0^\infty dr\, r^2 e^{-\beta r^2} \left[\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \underbrace{\frac{\partial}{\partial r} e^{-\beta r^2}}_{-2\beta r\, e^{-\beta r^2}} \right] =$$

$$= -\frac{1}{2} N'^2 \cdot 4\pi (-2\beta) \int_0^\infty dr\, e^{-\beta r^2} \Big[\underbrace{3 r^2 e^{-\beta r^2}}_{3\left(-\frac{1}{2}\right) \frac{\partial}{\partial \beta}\left(e^{-2\beta r^2}\right)} + \underbrace{r^3 (-2\beta r) e^{-\beta r^2}}_{-2\beta \cdot \frac{1}{4} \frac{\partial^2}{\partial \beta^2}\left(e^{-2\beta r^2}\right)} \Big] =$$

$$\overset{!}{=} -\frac{1}{2} N'^2 \cdot 4\pi (-2\beta)\left(-\frac{1}{2}\right) \Big[\underbrace{3 \frac{\partial}{\partial \beta} \left(\frac{1}{2} \sqrt{\frac{\pi}{2\beta}} \right)}_{3 \cdot \frac{1}{2} \sqrt{\frac{\pi}{2}} \left(-\frac{1}{2}\right) \beta^{-3/2}} + \underbrace{\beta \frac{\partial^2}{\partial \beta^2} \left(\frac{1}{2} \sqrt{\frac{\pi}{2\beta}} \right)}_{\beta \cdot \frac{1}{2} \sqrt{\frac{\pi}{2}} \left(-\frac{1}{2}\right)\left(-\frac{3}{2}\right) \beta^{-5/2}} \Big] =$$

$$= -\frac{1}{2} \frac{2\beta}{\pi} \sqrt{\frac{2\beta}{\pi}} \cdot 4\pi \cdot \beta \cdot \left(-\frac{3}{4}\right) \sqrt{\frac{\pi}{2}} \cdot \beta^{-3/2} \cdot \left[1 - \frac{1}{2} \right] = \underline{\frac{3}{2} \beta}$$

$$\Rightarrow \langle E \rangle = \frac{3}{2} \beta - Z \sqrt{\frac{8\beta}{\pi}}$$

$$0 = \frac{\partial \langle E \rangle}{\partial \beta} = \frac{3}{2} - Z \sqrt{\frac{8}{\pi}} \cdot \frac{1}{2} \cdot \frac{1}{\sqrt{\beta}} \Rightarrow \underline{\beta_0 = \frac{8 \cdot Z^2}{9\pi}}$$

$$\Rightarrow E_0 = \frac{3}{2} \cdot \frac{8 \cdot Z^2}{9\pi} - Z \cdot \frac{8 \cdot Z}{3\pi} = \underline{-\frac{4 \cdot Z^2}{3\pi}}$$

H $\quad Z = 1 \rightarrow E_0 = -0{,}424$

$> -\frac{1}{2}$