Atomové jednotky

Bohrův poloměr

$$a_0 = \frac{4\pi \varepsilon_0 \hbar^2}{e^2 m_e} \quad \leftarrow \text{měřítko vzdálenosti}$$

$$r = a_0 r' \;;\; x = a_0 x'$$

$$\frac{\partial}{\partial x} = \frac{1}{a_0}\frac{\partial}{\partial x'} \qquad x' \longrightarrow x \qquad r' \longrightarrow r$$

Ve Schrödingerově rovnici:

$$-\frac{\hbar^2}{2m_e}\nabla^2 - \frac{Ze^2}{4\pi\varepsilon_0 r} \longrightarrow -\frac{\hbar^2}{2m_e a_0^2}\nabla^2 - \frac{Ze^2}{4\pi\varepsilon_0 a_0}\frac{1}{r}$$

$$= -\underbrace{\frac{e^4 m_e}{(4\pi\varepsilon_0)^2\hbar^2}}_{E_h \text{ ... Hartreeho energie}}\frac{1}{2}\nabla^2 - \frac{Ze^4 m_e}{(4\pi\varepsilon_0)^2\hbar^2}\frac{1}{r}$$

$$\left(-\frac{E_h}{2}\nabla^2 - ZE_h\frac{1}{r}\right)\Psi(\vec{r}) = E\Psi(\vec{r}) \quad \Big/ : E_h \qquad \frac{E}{E_h} \to E$$

$$\boxed{\left(-\frac{1}{2}\nabla^2 - \frac{Z}{r}\right)\Psi(\vec{r}) = E\Psi(\vec{r})}$$

alternative

$$-\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial r^2} - \frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{r} \qquad r = \lambda r'$$

$$-\frac{\hbar^2}{2m_e}\frac{1}{\lambda^2}\frac{\partial^2}{\partial r'^2} - Z\frac{e^2}{4\pi\varepsilon_0}\frac{1}{\lambda}\frac{1}{r'} \Longrightarrow E_{jid} = 2E_h$$

$$\lambda = \frac{a_0}{2}$$