Sheet 4

Aufgabe 3

$$\left(-\frac{\hbar^2\nabla^2}{2m} + V_{ext}\right)\psi = E\psi$$

$$\nabla^2\psi_0 = -\frac{2m\overbrace{(E - V_{ext})}^{\tilde{E}}}{\hbar^2}\psi$$

→ because $\tilde{E}$ uniquely determines the solution to this PDE, two different V_{ext} will yield different GS wavefunctions.

Because if this was true, that would mean that

$$\nabla^2\psi_0 = -\frac{2m\tilde{E}'}{\hbar^2}\psi_0 \quad \text{and} \quad \nabla^2\psi_0 = -\frac{2m\tilde{E}}{\hbar^2}\psi_0$$

and this implies $E' = \tilde{E}$, but that would mean $V_{ext}' = \tilde{V}_{ext}$

↯

Aufgabe 2

$$(\hat{T} + \hat{V}_{en} + \hat{V}^{\varepsilon}_{HF})\,\varphi_\varepsilon = \epsilon_\varepsilon\varphi_\varepsilon(x)$$

$$\hat{V}^{\varepsilon}_{HF}(\vec{r}) = \sum_{\nu}\int dx'\,\frac{e^2}{|r-r'|}\left[|\varphi_\nu(x')|^2| - \frac{\varphi_\nu^*(x')\,\varphi_\varepsilon(x')\,\varphi_\nu(x)}{\varphi_\varepsilon(x)}\right]$$

assuming a single electron: $\nu = \varepsilon$

$$V^{\varepsilon}_{HF} = \int dx'\,\frac{e^2}{|r-r'|}\left[|\varphi_\varepsilon(x')|^2| - \frac{\varphi_\varepsilon^*(x')\,\varphi_\varepsilon(x')\,\varphi_\varepsilon(x)}{\varphi_\varepsilon(x)}\right]$$

$$= \int dx'\,\frac{e^2}{|r-r'|}\left[|\varphi_\varepsilon(x')|^2 - |\varphi_\varepsilon(x')|^2\right] = 0$$

$\Rightarrow (\hat{T} + \hat{V}_{en})\,\varphi_\varepsilon(x) = E_\varepsilon\,\varphi_\varepsilon(x)$ → Normal Schrödinger