# 5.2 Kohn-Sham-Gleichungen

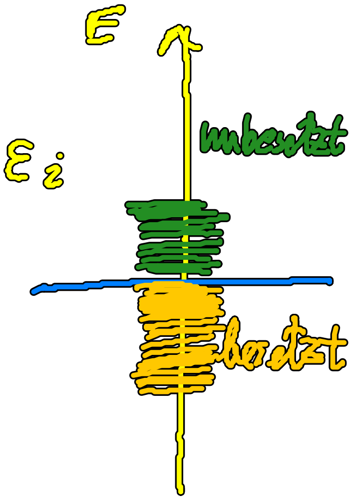
inhomogenes Elektronengas

Dichtefunktional der Grundzustandsenergie $E_g = E[n]$

$$E_g = E[n] = \langle g|\hat{T} + \hat{V}_{ee}|g\rangle + \int v(\vec{r})\, n(\vec{r})\, d^3r \quad , \langle g|g\rangle = 1$$

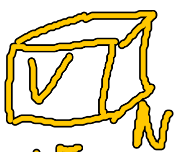
$$\frac{\delta}{\delta n(\vec{r})}\left[E[n] - \mu \int n(\vec{r})\, d^3r\right] = 0$$

Kohn-Sham-Niveaus $\varepsilon_i$




homogenes Elektronengas

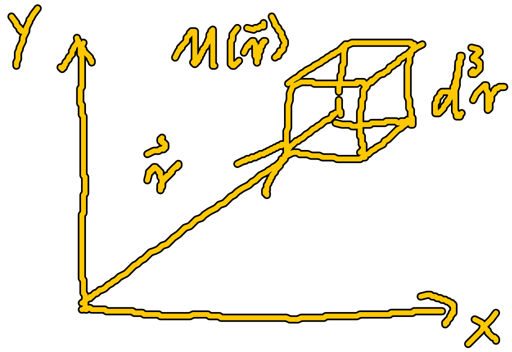
$n^{hE} = \text{konst.}$



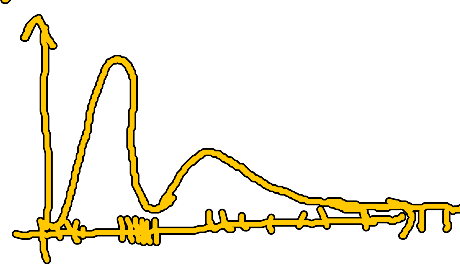

$\underline{\underline{\varepsilon^{hE}(n)}}$

$\varepsilon^{hE}$ Energie pro Elektron

$n = \frac{N}{V}$




$$\int_V \varepsilon^{hE}(n(\vec{r}))\, n(\vec{r})\, d^3r$$



$$E_g = T + V + V_{ee}$$
$$= T + V + E_H + E_{xc}$$

2 Elektronen

$\psi_{\nu_1}(1), \quad \psi_{\nu_2}(2)$

$$V_{ee} = \langle \Psi^{SD}| \frac{1}{|\vec{r}_1 - \vec{r}_2|} |\Psi^{SD}\rangle =$$

$$= \underbrace{\int \frac{|\psi_{\nu_1}(1)|^2\, |\psi_{\nu_2}(2)|^2}{|\vec{r}_1 - \vec{r}_2|}\, d^3r_1\, d^3r_2}_{\text{elektrostat. Abstoßungsenergie}} - \underbrace{\int \frac{\psi^*_{\nu_1}(1)\, \psi^*_{\nu_2}(2)\, \psi_{\nu_1}(2)\, \psi_{\nu_2}(1)}{|\vec{r}_1 - \vec{r}_2|}\, d^3r_1\, d^3r_2}_{\text{Austauschterm}}$$