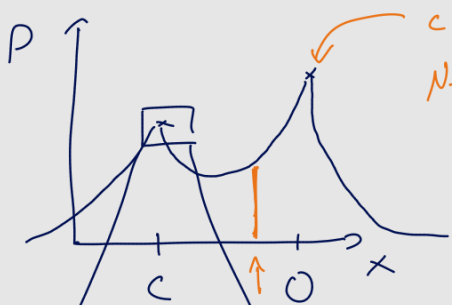
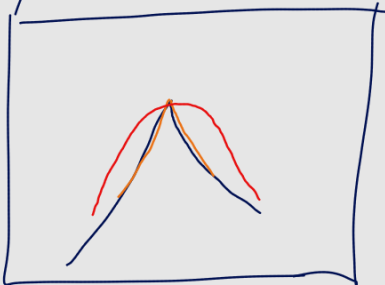
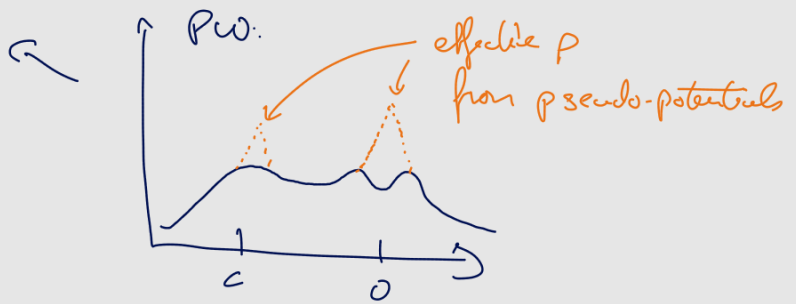


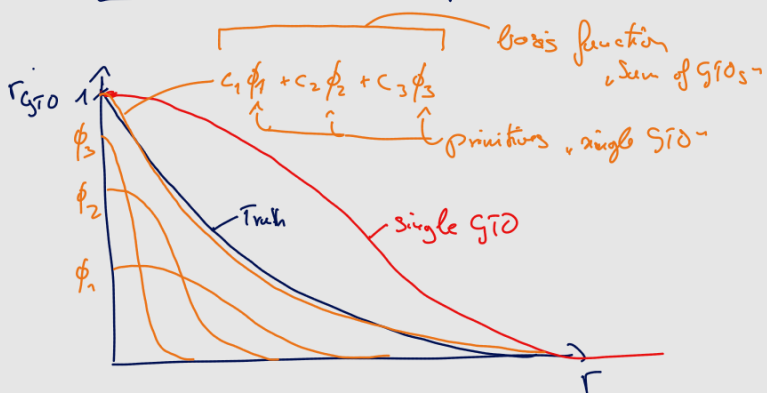


cusp $N-c$ $\xrightarrow{\text{analog}}$ $e-e$ cusp



$$STD: \exp(-\alpha r)$$

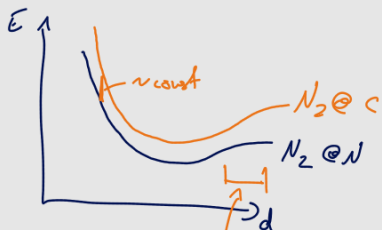
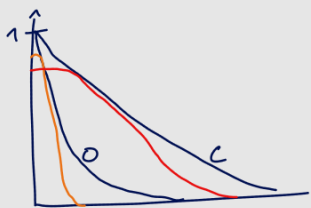
$$STD: \exp(-\alpha r^2) \leftarrow \text{preferred: } \int \phi_i^* \phi_j dr$$



$$\begin{array}{c|cc} \textcircled{3}s & \textcircled{2}p & \textcircled{1}d \\ m & 0 & 0 \\ & \pm 1 & \pm 1 \\ & & \pm 2 \end{array}$$

$$\textcircled{3} \cdot \textcircled{1} + \textcircled{2} \cdot \textcircled{3} + \textcircled{1} \cdot \textcircled{5} = 14$$

$$\psi = \begin{vmatrix} X_1(x_1) & X_2(x_1) \\ X_1(x_2) & X_2(x_2) \end{vmatrix} = \begin{vmatrix} - & / \\ - & / \end{vmatrix} = X_1(x_1)X_2(x_2) - X_1(x_2)X_2(x_1)$$

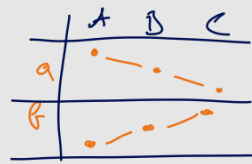


$$E(z; \vec{R} | \text{method}, \text{basis set})$$

$\uparrow$ "always HF"
 $\uparrow$ $\alpha \dots$

$$\Rightarrow \frac{\partial E}{\partial \alpha} (\text{frozen } z, \vec{R}, \text{method})$$

def2-TZVP



Contraction: $X = \sum_i w_i \phi_i$

A: $0.8a + 0.2b$

Flexible coefficients:

C: $0.2a + 0.8b$

"decontract" $\Rightarrow$

each primitive is one sole box

UGBS