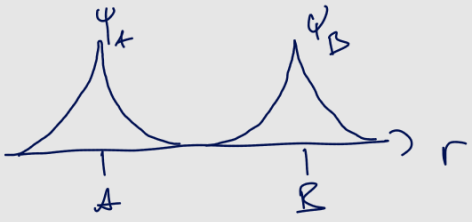
Produktansatz: $\Psi = \Psi(r)\,\phi(\theta,\varphi)$ ($\neq$)

$\Psi(r)$: Radialteil; $\phi(\theta,\varphi)$: Winkelteil

Superposition: $\Psi = \Psi_A(\vec{r}) + \Psi_B(\vec{r})$ ($=$)



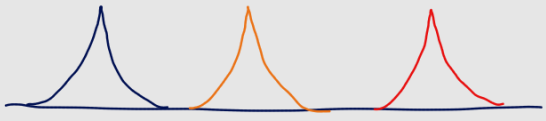
$S = 0$

$= \langle \Psi_A | \Psi_B \rangle$

$H_{AA} = \langle \Psi_A | \hat{H} | \Psi_A \rangle$

$H_{AB} = \langle \Psi_A | \hat{H} | \Psi_B \rangle$

LCAO:



$\Psi(\vec{r}) = c_A \phi_A(\vec{r}) + c_B \phi_B(\vec{r}) + c_C \phi_C(\vec{r})$