

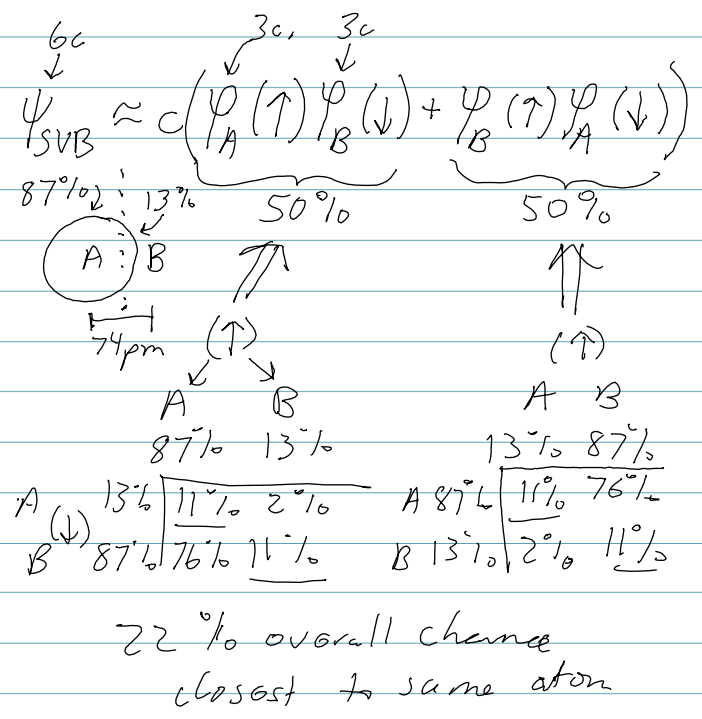
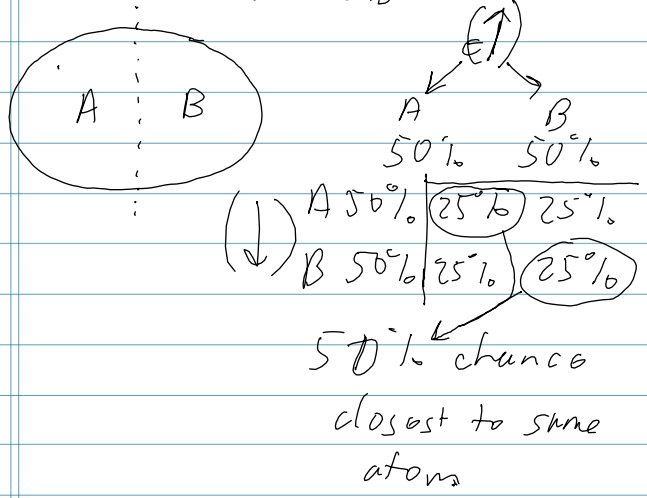
Ionic Resonance Structures in VB Theory

simple MO: e⁻ independent move simple VB: strong correlation

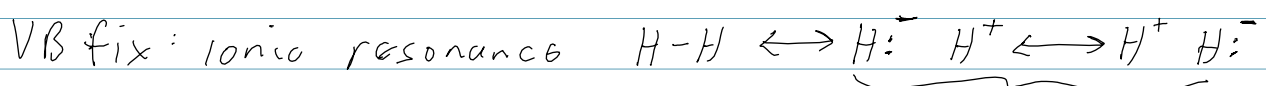
What is chance that both e⁻ are closest to same atom of H₂ molecule?

$\psi^2 \Rightarrow$ probabilities

MO Theory $\psi_{6ls} \approx c(\psi_A + \psi_B)$



Pauling: 22% < True ans. < 50%
(VB) (MO)



$\psi_{VB} = \psi_{SVB} + \lambda_A (\psi_A(\uparrow)\psi_A(\downarrow)) + \lambda_B (\psi_B(\uparrow)\psi_B(\downarrow))$ ionic res. structures

H₂ and F₂: $\lambda_A = \lambda_B \approx 0.25c$

if A has higher EN than B: $\lambda_A > \lambda_B$

