7. Show that for H_2 molecule $\rho_{MO} > \rho_{VB}$ at the mid-point of the bond (in the ground state)

$$\rho_{MO} = \frac{(\phi_{1s}^a)^2 + (\phi_{1s}^b)^2 + 2\,\phi_{1s}^a\,\phi_{1s}^b}{1+S}$$

$$\rho_{VB} = \frac{(\phi_{1s}^a)^2 + (\phi_{1s}^b)^2 + 2S\,\phi_{1s}^a\,\phi_{1s}^b}{1+S^2}$$

Show how!

at mid-point $\phi_{1s}^a = \phi_{1s}^b$, call it ϕ_e

$$\rho_{MO} = 4\phi_e^2/(1+S) \qquad \rho_{VB} = \frac{2\phi_e^2(1+S)}{1+S^2}$$

$$\frac{\rho_{MO}}{\rho_{VB}} = 2\,\frac{1+S^2}{(1+S)^2} \quad \text{with, } 0 < S < 1 \ \ldots\ldots$$

Complete.

8. Compare the MO and VB function for the $^3\Sigma_u^+$ level of H_2.

$$\Psi_{MO} = |\sigma_g\ \sigma_u| \sim \sigma_g(1)\,\sigma_u(2) - \sigma_u(1)\,\sigma_g(2)$$

$$\ldots \sim \phi_{1s}^a(1)\,\phi_{1s}^b(2) - \phi_{1s}^b(1)\,\phi_{1s}^a(2)$$

Space part. Substituting for σ_g and σ_u and simplifying.

This is same as the space part of the VB function for the Triplet state.

~~Is it possible to~~ Can one write a simple VB function for the $^3\Sigma_u^+$ level? What about MO?