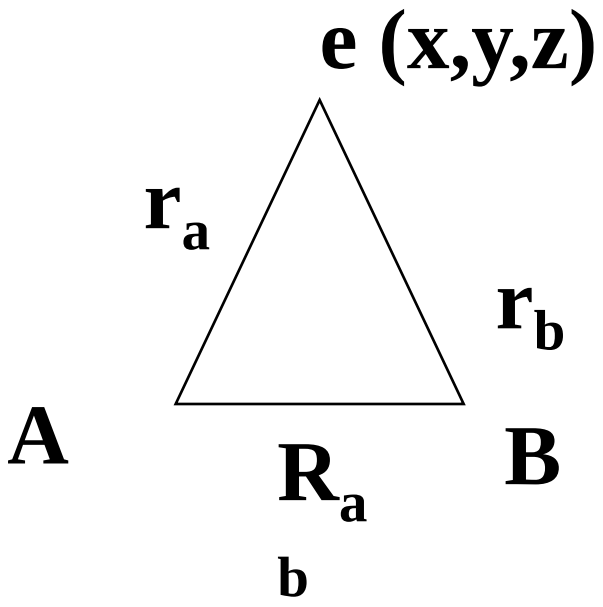
Home Work-I

$$H_2^+$$

$$\{(-h^2/8\pi^2m)\nabla^2 + V\}\,\Psi = E\,\Psi$$

H.W. 1



Solve **H.W. 2**

Work function of sodium is 2.5 eV. Predict whether the wavelength 6500Å is suitable for ejection of photoelectron or not? Guess and conclude the event.

H.W.3

- Draw the interaction of wavefunctions;
- (i) when $\psi_u = N [\psi_A + \psi_B]$
- (ii) $\psi_u = N [\psi_A - \psi_B]$

h.w.4

- If atom A and B are interact, the LCAO of their wavefunction can be $\psi_{AB} = N(c_A \psi_A + c_B \psi_B)$

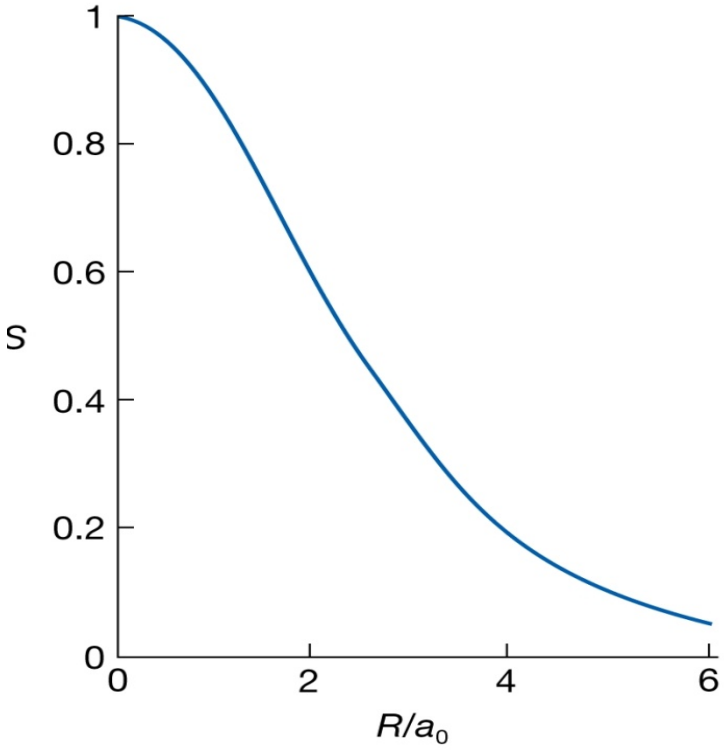
- (a) Then, how can you represent the probability density?
- (b) Which are the term(s) indicate the overlap of A and B?

h.w.5

The overlap integral, S, can be depicted as below:

■**The extent to which two atomic orbitals on different atom overlaps : the overlap integral**

$$S = \int \psi_A^{*} \psi_B d\tau$$



■**Then, continue….next page h.w.5**

■**How can you draw simple cartoon of Overalap of p-p orbital and s-p orbitals for bonding and antibonding conditions?**

S > 0 Bonding

S < 0 antibonding

S = 0 non-bonding

h.w. 6

Draw a MO diagram for B_2 and check whether it is diamagnetic?