Tutorial - 5 additional questions

A1. Justify or contradict the following statements about sp3 hybridization:
Contribution of
(A) each of px, py and pz orbitals is necessarily 25%
(B) s orbital is 25%
(C) all p orbitals combined is 75%
(D) pz orbital may be 0%

A) Statement is wrong

B) statement is correct

c) statement is correct

D) statement is correct.

A3. For a spx hybrid orbital,
$\psi = 0.625\phi\ 2s + 0.312\phi\ 2px + 0.417\phi\ 2py + 0.625\phi\ 2pz$
What is the percentage of p-contribution in this orbital?

Percentage of p contribution = 62.92

A4. For BeH2 molecule aligned along x-axis
(A) Write the expression for the appropriate hybrid orbitals.
(B) Write the Heitler London wavefunction using the constructed hybrid orbital for the two bonds,
(C) Predict if the overlap integral for the 1s orbital of H with the 2px orbital or with the hybrid orbital will be greater.

A) The two sp hybrid orbitals of Be:

$$\phi_a = \frac{1}{\sqrt{2}}(\phi_{2s} + \phi_{2p_x})$$

$$\phi_b = \frac{1}{\sqrt{2}}(\phi_{2s} - \phi_{2p_x})$$

(B) $H_B - Be - H_A$

consider $Be - H_A$ bond.

sp - hybrid orbital of Be (ϕ_a) and 1s orbital or H_A (ϕ_{1s_A}) are involved.

$$\therefore \quad \psi_1 = \phi_a(1)\,\phi_{1s_A}(2)$$

$$\psi_2 = \phi_a(2)\,\phi_{1s_A}(1)$$

Heitler - London wavefunction:

$$\psi = c_1\psi_1 + c_2\psi_2$$

$$= c_1\,\phi_a(1)\,\phi_{1s_A}(2) + c_2\,\phi_a(2)\,\phi_{1s_A}(1)$$

similarly you can construct for $H_B - Be$ bond with ϕ_b and ϕ_{1s_B}.

(C) Overlap integral will be greater for 1s orbital of H with sp - hybrid orbital of Be.