The p-orbitals

$$\Psi_{nlm_l}(r,\theta,\phi) = R_{nl}(r)\, Y_{lm_l}(\theta,\phi)$$

$$\Psi_{210} = R_{21}(r)\, Y_{10}(\theta,\phi)$$

$$R_{21}(r) = \left(\frac{Z}{a_0}\right)^{3/2} e^{-\rho/2}\, \rho_n\, \frac{1}{2\sqrt{6}}$$

$$Y_{10}(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$\Psi_{210} = \left(\frac{Z}{a_0}\right)^{3/2} e^{-\frac{2Zr}{na_0}\cdot\frac{1}{2}}\ \frac{2Zr}{na_0}\,\frac{1}{2\sqrt{6}}\ \sqrt{\frac{3}{4\pi}}\cos\theta$$

$Z=1$
$n=2$

$$\Psi_{210} = \sqrt{\frac{3}{4\pi}}\cdot\frac{1}{2\sqrt{6}}\left(\frac{1}{a_0}\right)^{3/2} e^{-\frac{r}{2a_0}}\ \frac{r}{a_0}\cos\theta$$

$$\Psi_{210} = \underbrace{\sqrt{\frac{3}{4\pi}}\cdot\frac{1}{2\sqrt{6}}\left(\frac{1}{a_0}\right)^{3/2}\left(\frac{1}{a_0}\right)}_{\text{constant }(C)}\ r\cos\theta\, e^{-r/2a_0}$$

$$\Psi_{210} = C\cdot r\cos\theta\cdot f(r)$$

$$\Psi_{210} = C\, z\, f(r) \Rightarrow \underline{p_z \text{ orbital}}$$

$$\Psi_{211} = R_{21}(r)\, Y_{11}(\theta, \phi)$$

$$= R_{21}(r) \sqrt{\frac{3}{8\pi}} \sin\theta\, e^{i\phi}$$

$Z=1$, $n=2$ $\rightarrow$

$$= (\text{constant})\, r \sin\theta\, e^{i\phi}\, e^{-r/2a_0}$$

$$\Psi_{21-1} = (\text{constant})\, r \sin\theta\, e^{-i\phi}\, e^{-r/2a_0}$$

$$\Psi_{211} + \Psi_{21-1}$$

$$= (\text{constant})\, \underset{\downarrow \, e^{-r/2a_0}}{f(r)}\, r \sin\theta\, 2\cos\phi$$

$$= 2(\text{constant})\, f(r)\, \underbrace{r \sin\theta \cos\phi}_{x}$$

$$= 2(\text{constant})\, x\, f(r) \quad \Rightarrow \quad \underline{\underline{p_x \text{ orbital}}}$$

$$\Psi = \Psi_1 + \Psi_2$$

$$\left.\begin{aligned} H\Psi_1 &= E_1 \Psi_1 \\ H\Psi_2 &= E_2 \Psi_2 \end{aligned}\right\} \rightarrow E_1 = E_2$$

(degenerate)

$$H\Psi = H(\Psi_1 + \Psi_2)$$

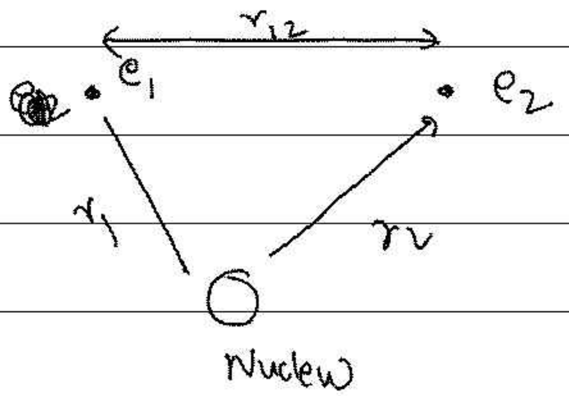
$$H\Psi = H\Psi_1 + H\Psi_2$$

$$H\Psi = E_1\Psi_1 + E_2\Psi_2$$

$$H\Psi = E(\Psi_1 + \Psi_2)$$

$$\Psi(r,\theta,\phi) \Rightarrow \langle r \rangle, \left\langle \frac{1}{r} \right\rangle, \ldots$$

<u>Helium Atom</u>



$$\hat{H} = -\frac{\hbar^2}{2m_e}\nabla_1^2 - \frac{\hbar^2}{2m_e}\nabla_2^2$$

$$- \frac{Ze^2}{4\pi\varepsilon_0 r_1} - \frac{Ze^2}{4\pi\varepsilon_0 r_2}$$

$$+ \frac{e^2}{4\pi\varepsilon_0 r_{12}}$$

e-e repulsion term!

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \frac{e^2}{4\pi\varepsilon_0 r_{12}}$$

$$\hat{H}_1 = -\frac{\hbar^2}{2m_e}\nabla_1^2 - \frac{Ze^2}{4\pi\varepsilon_0 r_1}$$

$$\hat{H}_2 = -\frac{\hbar^2}{2m_e}\nabla_2^2 - \frac{Ze^2}{4\pi\varepsilon_0 r_2}$$

$$\hat{H} = \hat{H}_1 + \hat{H}_2 \quad \text{(ignored e-e repulsion)}$$

$$\hat{H}\,\psi(r_1, r_2) = \hat{H}\,\psi(r_1)\,\psi(r_2)$$

$$\hat{H} = \hat{H}_1 + \hat{H}_2$$

$H_1 \psi(r_1) = E_1 \psi(r_1)$

$$\begin{aligned}
(\hat{H}_1 + \hat{H}_2)\,\psi(r_1, r_2) &= (\hat{H}_1 + \hat{H}_2)\,\psi(r_1)\,\psi(r_2) \\
&\cancel{= \hat{H}_1 \psi(r_1) + \hat{H}_2 \psi(r_2)\,\psi(r_1)} \\
&= \hat{H}_1 \psi(r_1)\psi(r_2) + \hat{H}_2 \psi(r_1)\psi(r_2) \\
&= E_1 \psi(r_1)\psi(r_2) + E_2 \psi(r_1)\psi(r_2) \\
&= (E_1 + E_2)\,\psi(r_1)\,\psi(r_2)
\end{aligned}$$

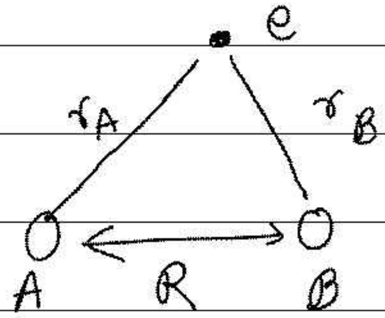
$$E_1 = -13.6\,\frac{Z^2}{n^2} = -13.6 \cdot \frac{2^2}{1^2}$$

$$E_1 = -54.4\text{ eV}$$

$$E = E_1 + E_2 = 2E_1 = -108.8\text{ eV}$$

$$E_{exp} = \sim 79.2\text{ eV}$$

Diatomic molecule (H_2^+)



$$\hat{H} = -\frac{\hbar^2}{2m_A}\nabla_A^2 - \frac{\hbar^2}{2M_B}\nabla_B^2$$

$$- \frac{\hbar^2}{2m_e}\nabla_e^2$$

$$- \frac{Ze^2}{4\pi\varepsilon_0 r_A} - \frac{Ze^2}{4\pi\varepsilon_0 r_B}$$

$$+ \frac{(\ )}{4\pi\varepsilon_0 R}$$