Lecture 11: From atoms to molecules

Lecture 10 review:

$x, y, z \rightarrow r, \theta, \varphi$

3 coordinates, 3 q #'s.

n ↑ 1, 2, 3 ... ; l ↑ 0, 1, ..., n-1 ; m_l ↑ -l, ..., l

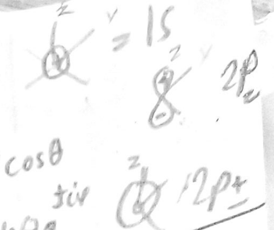
$\psi_{n,l,m_l} \propto e^{-\frac{r}{na_0}}$ $\quad a_0 = \frac{4\pi\varepsilon_0 \hbar^2}{m_e e^2}$

$E_n = -\frac{R_y}{n^2}, \quad R_y = \frac{m_e e^4}{8\varepsilon_0^2 h^3 c} \approx 1300\ J/mol$

$\psi_{1,0,0} \propto e^{-\frac{r}{a_0}}$

$\psi_{2,1,0} \propto e^{-\frac{r}{2a_0}} \cos\theta$

$\psi_{2,1,\pm1} \propto e^{-\frac{r}{2a_0}} \sin\theta\, e^{\pm i\varphi}$



- If two wavefunctions ψ_A and ψ_B for the same particle have the same energy, any linear combination ψ_C (e.g. $\psi_C = \psi_A + \psi_B$ or $\psi_C = \psi_A - \psi_B$) is also a solution of the Schrödinger equation.
- Proof (by postulate 2):

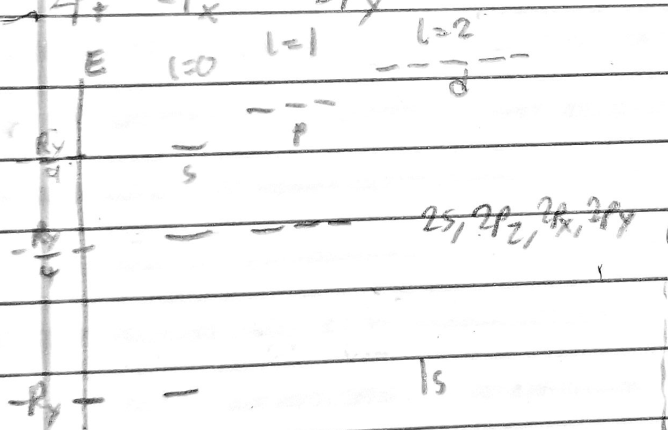
same E + same particle

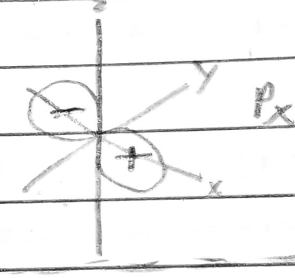
$$\left.\begin{array}{l}\hat{H}\psi_A = E\psi_A \\ \hat{H}\psi_B = E\psi_B\end{array}\right\} \xrightarrow{+} \hat{H}(\psi_A + \psi_B) = E(\psi_A + \psi_B) \rightarrow \hat{H}\psi_C = E\psi_C$$

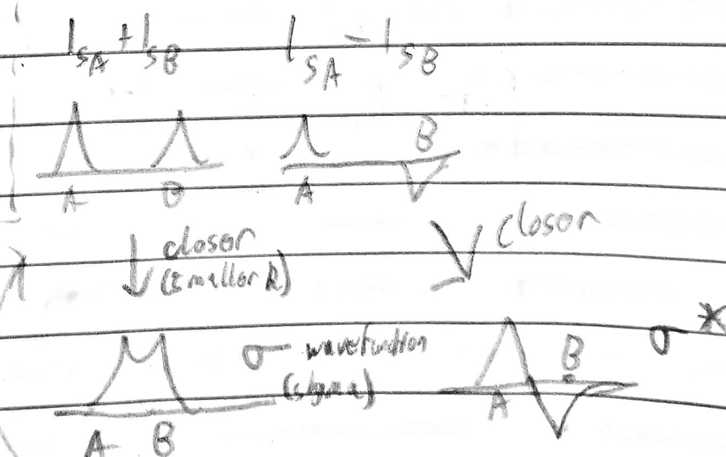
- $2p_+ + 2p_- \sim r e^{-\frac{r}{2a_0}} \sin\theta \left(e^{i\varphi} + e^{-i\varphi}\right) = r e^{-\frac{r}{2a_0}} \sin\theta\left(\overbrace{\cos\varphi + i\sin\varphi}^{} + \cos\varphi - i\sin\varphi\right)$

$= 2r e^{-\frac{r}{2a_0}} \sin\theta \cos\varphi$

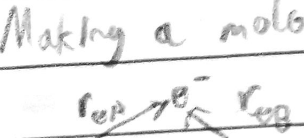
- $2p_+ - 2p_x \sim 2p_y$







- Making a molecule: H_2^+



- If the e^- has the same E in all these cases, then we can combine them.