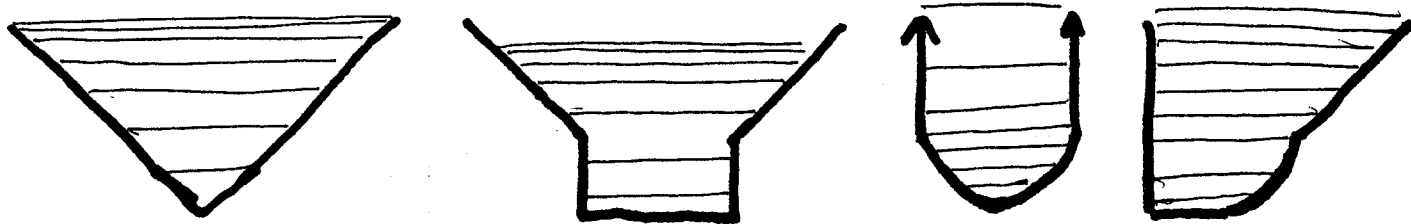
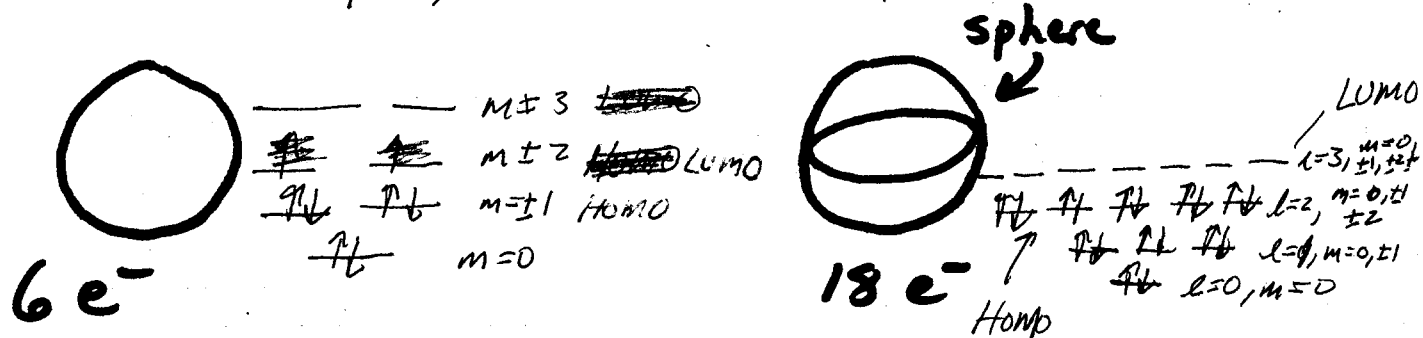


Answers Recitation Exercises *Answers*

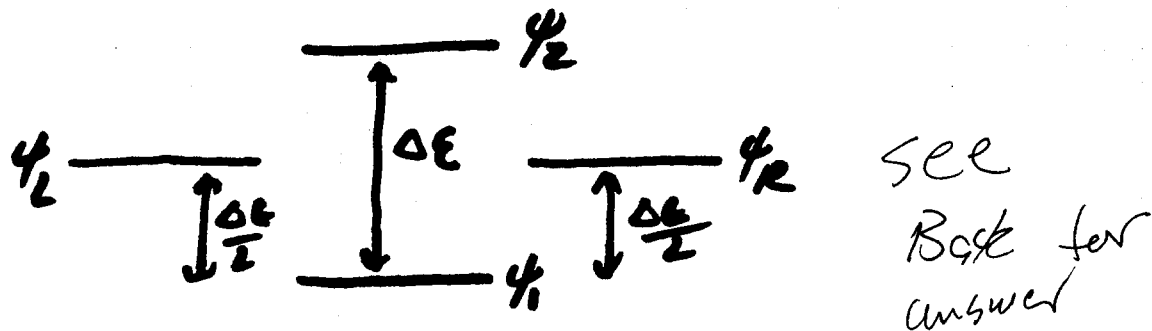
Qualitatively sketch the behavior of the energy levels for the following Potentials



Qualitatively sketch the energy level diagram for the following systems. Identify the HOMO and LUMO



The "left" and "right" states get their name because one often draws them as



- 1) Show that ψ_L and ψ_R are not eigenfunctions of \hat{H}_{T2S}
- 2) Show that the energy of ψ_L and ψ_R is $\frac{\Delta E}{2}$. Since they are not eigenfunctions one must find the average energy $\langle E \rangle = \langle \hat{H}_{T2S} \rangle$

$$1) \quad \psi_L = \frac{1}{\sqrt{2}} \psi_1 + \frac{1}{\sqrt{2}} \psi_2$$

$$\hat{H} \psi_L = \frac{\epsilon_1}{\sqrt{2}} \psi_1 + \frac{\epsilon_2}{\sqrt{2}} \psi_2 \quad \text{not eigenfunction}$$

$$\psi_R = \frac{1}{\sqrt{2}} \psi_1 - \frac{1}{\sqrt{2}} \psi_2$$

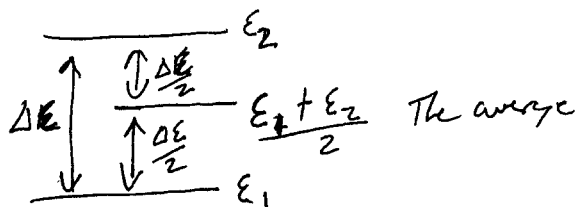
$$\hat{H} \psi_R = \frac{\epsilon_1}{\sqrt{2}} \psi_1 - \frac{\epsilon_2}{\sqrt{2}} \psi_2 \quad \text{not eigenfunction}$$

$$2) \quad \langle E \rangle = \langle H \rangle = \int \psi_L^* H \psi_L d\Omega$$

$$= \int \left(\frac{1}{\sqrt{2}} \psi_1^* + \frac{1}{\sqrt{2}} \psi_2^* \right) \left(\frac{\epsilon_1}{\sqrt{2}} \psi_1 + \frac{\epsilon_2}{\sqrt{2}} \psi_2 \right) d\Omega$$

$$= \frac{\epsilon_1}{2} \int \psi_1^* \psi_1 d\Omega + \frac{\epsilon_2}{2} \int \psi_2^* \psi_2 d\Omega + \frac{\epsilon_1}{2} \int \psi_1^* \psi_2 d\Omega + \frac{\epsilon_2}{2} \int \psi_2^* \psi_1 d\Omega$$

$$= \frac{\epsilon_1}{2} + \frac{\epsilon_2}{2} = \frac{\epsilon_1 + \epsilon_2}{2} \quad \text{the average energy}$$



Similarly for ψ_R