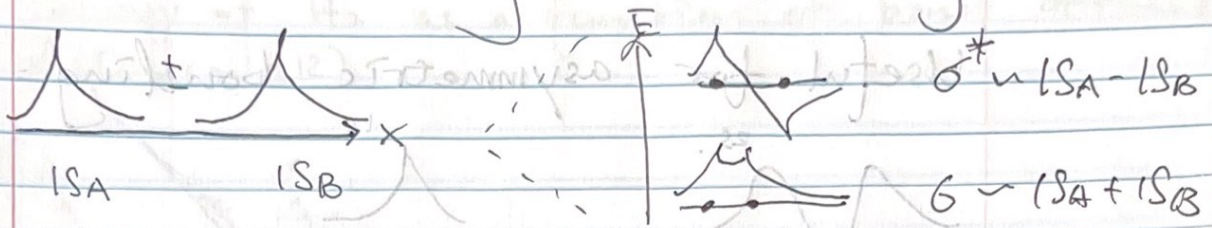


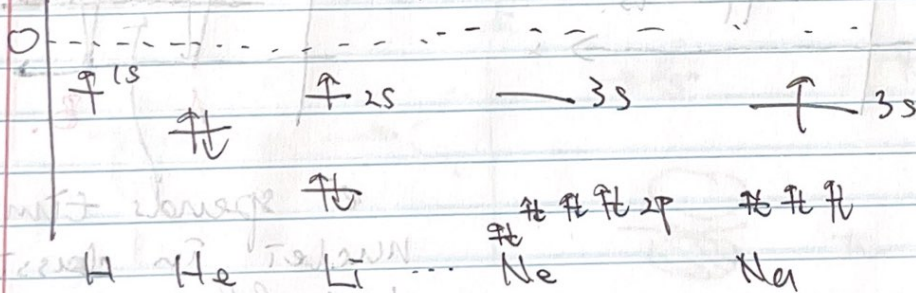
Last time = bonding & antibonding.



H_2^+ H_2

\uparrow $\uparrow\downarrow$
 $E = E_0$ $E = 2 * E_0$

e (orbital energy) Quantum superposition.

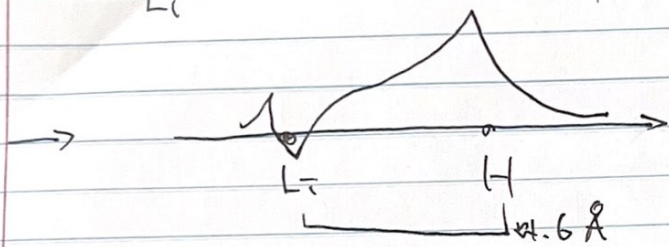
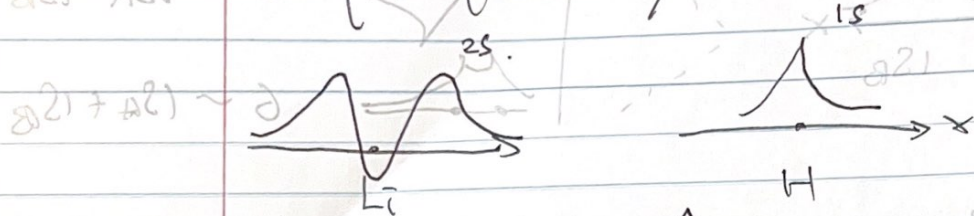


Today: more bonding/antibonding; why CM can't explain bonding.

If two eigenstates have the same (similar) energy, then any linear combination is also an (approx) eigenstate.

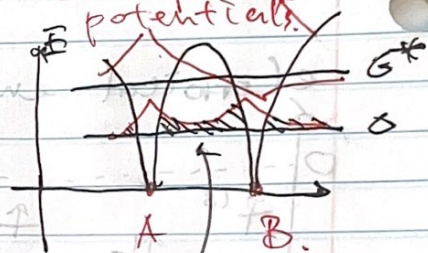
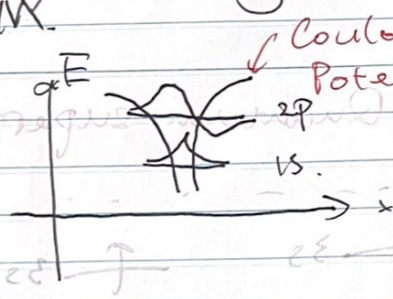
$$\begin{cases} H\psi_A = E\psi_A & \times a \\ H\psi_B = E\psi_B & \times b \end{cases} \Rightarrow H(a\psi_A + b\psi_B) = E(a\psi_A + b\psi_B)$$

Useful for asymmetric bonding:



On 2s (Li)
+ 7.4-1s (H)

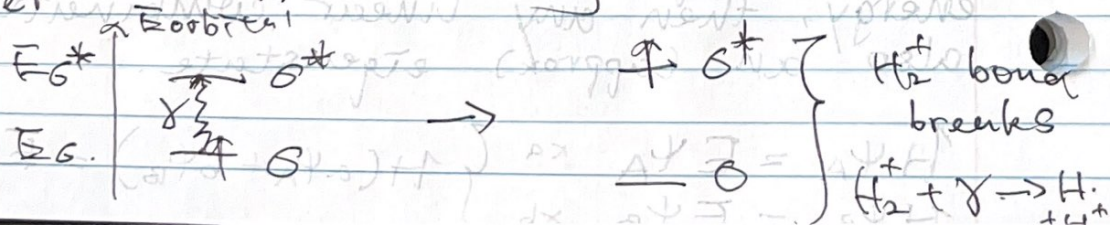
Why bonding is explained by QM, not by CM.



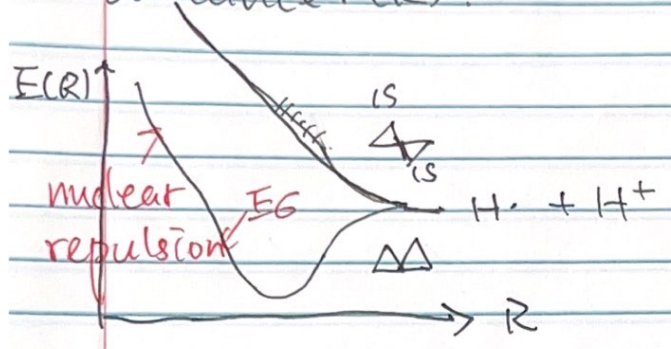
e^- spends time between nuclei in classically forbidden region.

e^- is simultaneously on both sides quantum superposition.

Spectroscopy: exciting the H_2^+ molecules



Energy of H_2^+ as a function of bond distance (R).



* nuclei too far apart = E is high because e^- is not shared

* nuclei too close = E is high because nuclei repel (for many e^- , PEP occur).

P orbital also can make bonds & antibonding

