Lecture V Diatomic molecular orbitals (pp. 664-675 Zumdahl)

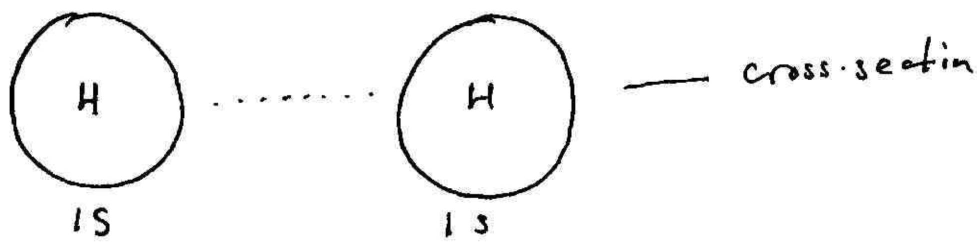
① This week we will turn to diatomic molecular orbital theory. We use 2 ideas from last week

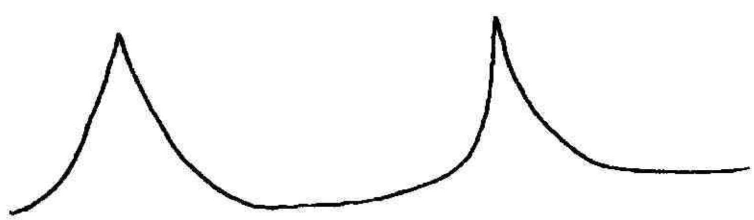
① e^- act a bit like waves

② λ short $\Rightarrow$ E high

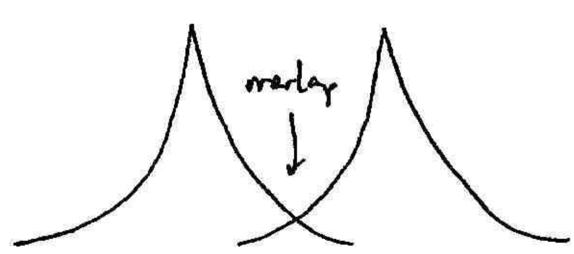
λ long $\Rightarrow$ E low

② Consider H_2.



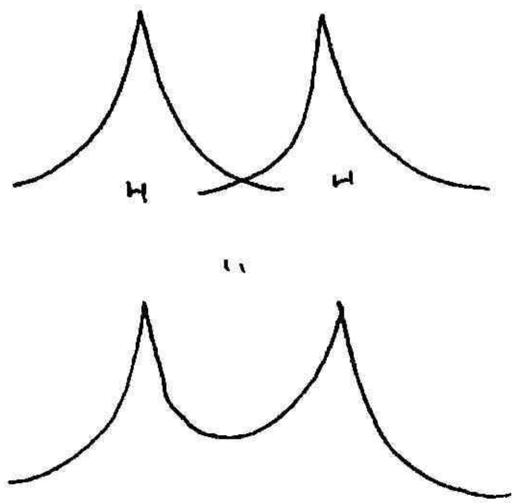


Now bring H's closer to eachother.

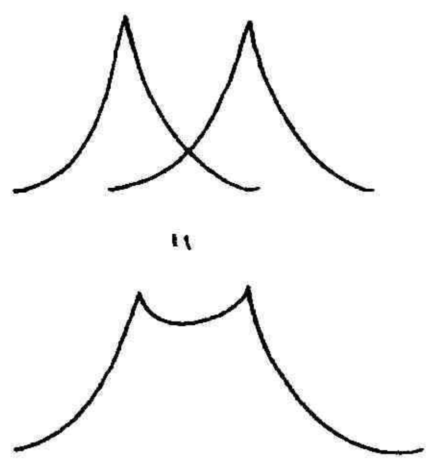


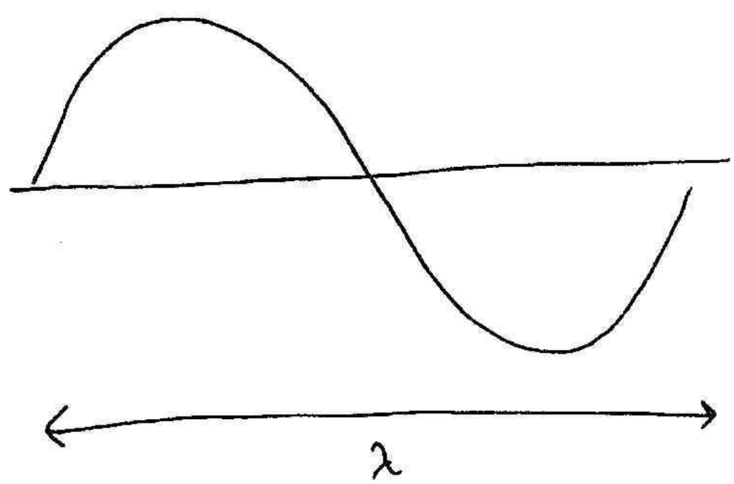
When waves overlap their heights add together.

③



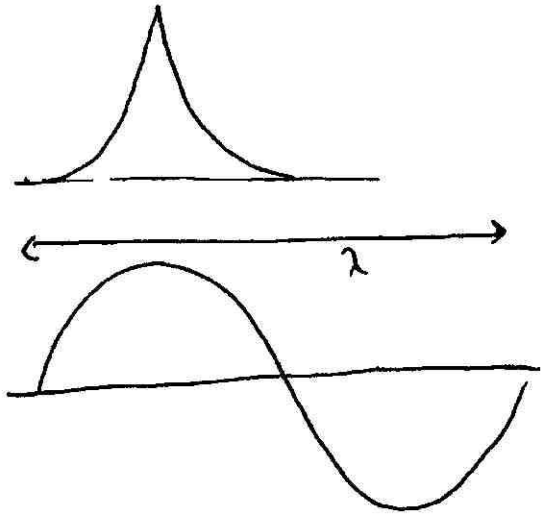
& even closer we find





By bringing the H's closer together how have we changed λ?

④ Single H



Compare to bottom picture of p. V.2. Has λ increased or decreased.

⑤ λ increases in H_2 vs. H. ∴ $E(e^- \text{ in } H_2)$ decrease vs. $E(e^- \text{ in } H)$.

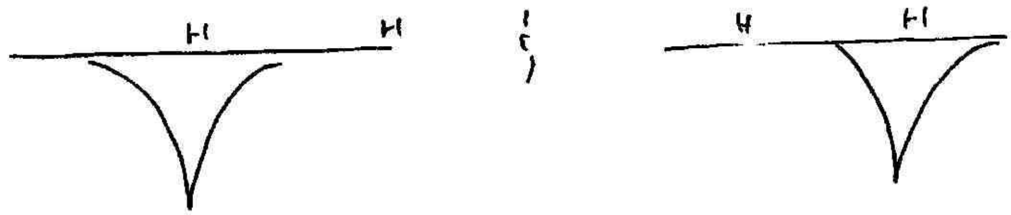
∴ The energy of H_2 is <u>less</u> than the energy of 2 H's.

⑥ We call this difference in energy the bond energy.

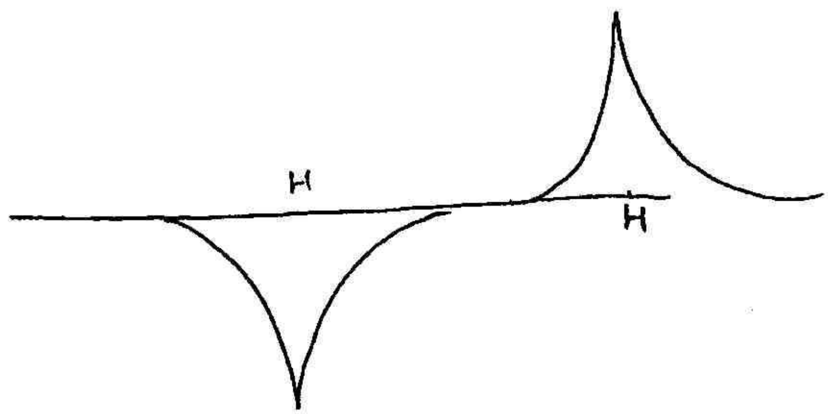
The chemical bond in H_2 is caused by decreasing the energy of the electron orbitals.

⑦ <u>Advisory</u>: The actual situation is unfortunately much more complicated. I finally have worked it out for myself & I believe the story I am telling you is correct. But Chem. 216 is not the right place to go into this story. Let's leave it like this. What seems to be true is <u>really</u> true (after a bit of thought).

⑧ At the same time each H wave function is also:

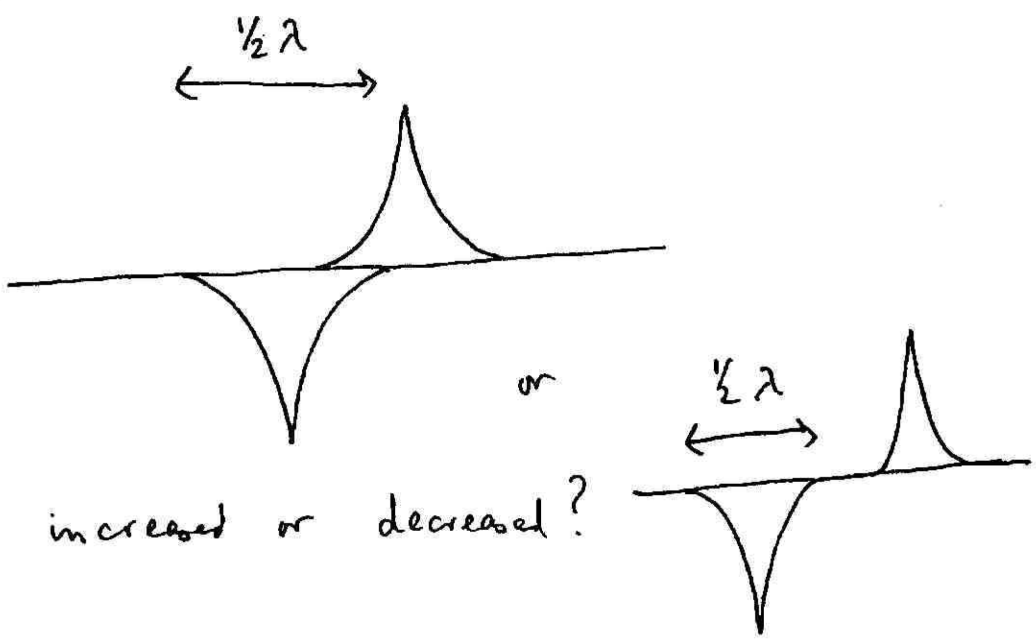


⑨ We can add:



As we bring these two wave to eachother we can add (linearly combine) these wave together.

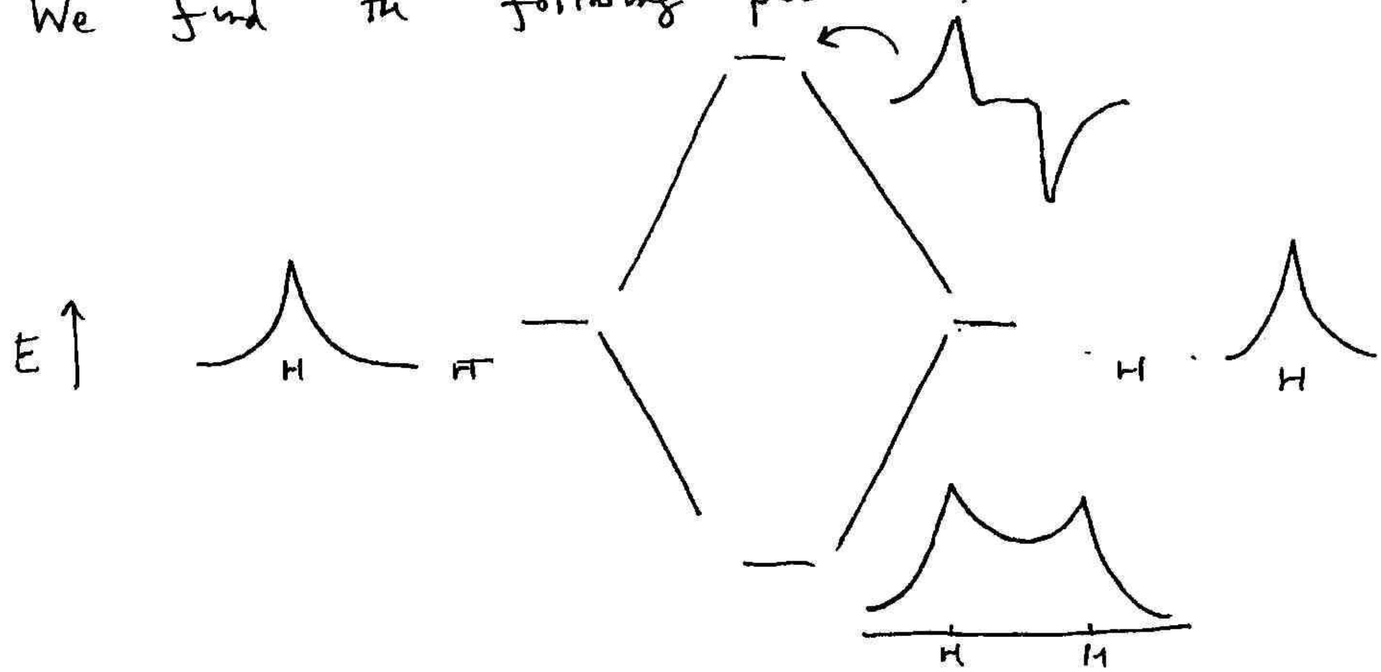
We get.



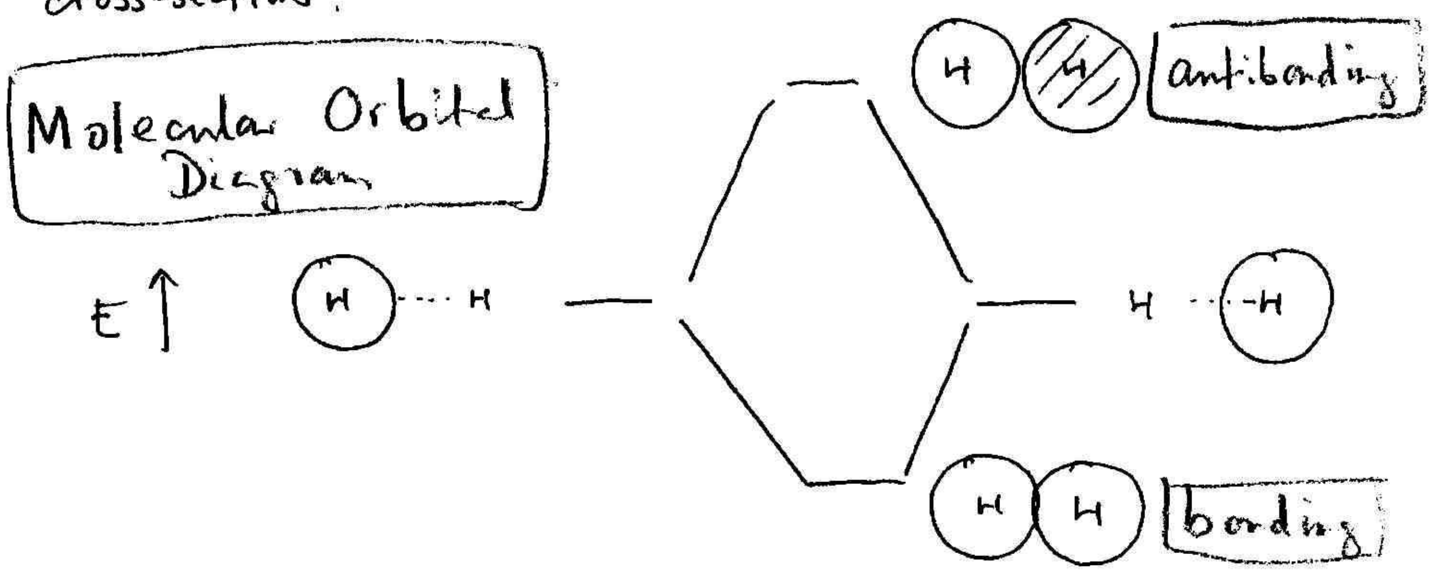
Has λ increased or decreased?

(10) λ has decreased $\therefore$ E has increased.

We find the following picture.

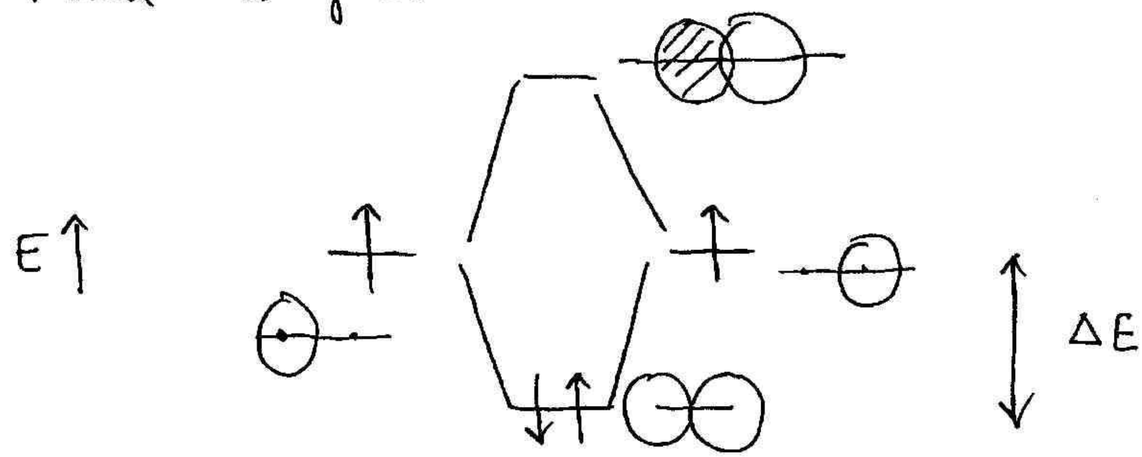


(11) or drawing H 1s orbitals as spheres (not as cross-sections):



We recall Pauli's exclusion principle: Only one e^- can be in a given orbital (now a molecular orbital) at a time. We recall we have $m_s = +\frac{1}{2}$, represented as $\uparrow$ & $m_s = -\frac{1}{2}$, represented as $\downarrow$.

⑫ Final diagram



∴ bonding energy of $H_2 = 2\Delta E$.

Excercise (II.1) He also has a 1s orbital, but it has two electrons in this orbital (one ↑ the other ↓). Using the diagram above estimate the bonding energy of He_2. Does He exist as a diatomic molecule or as a monoatomic atom?

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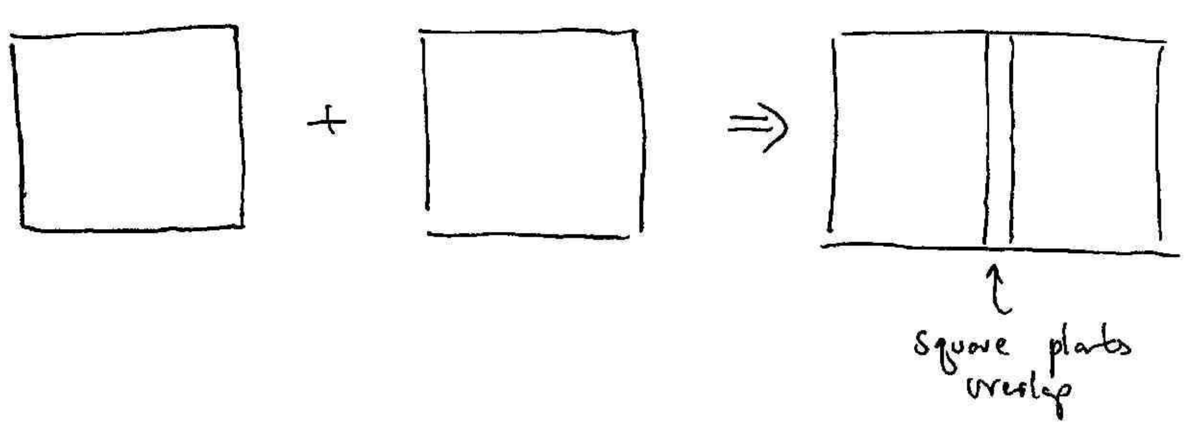
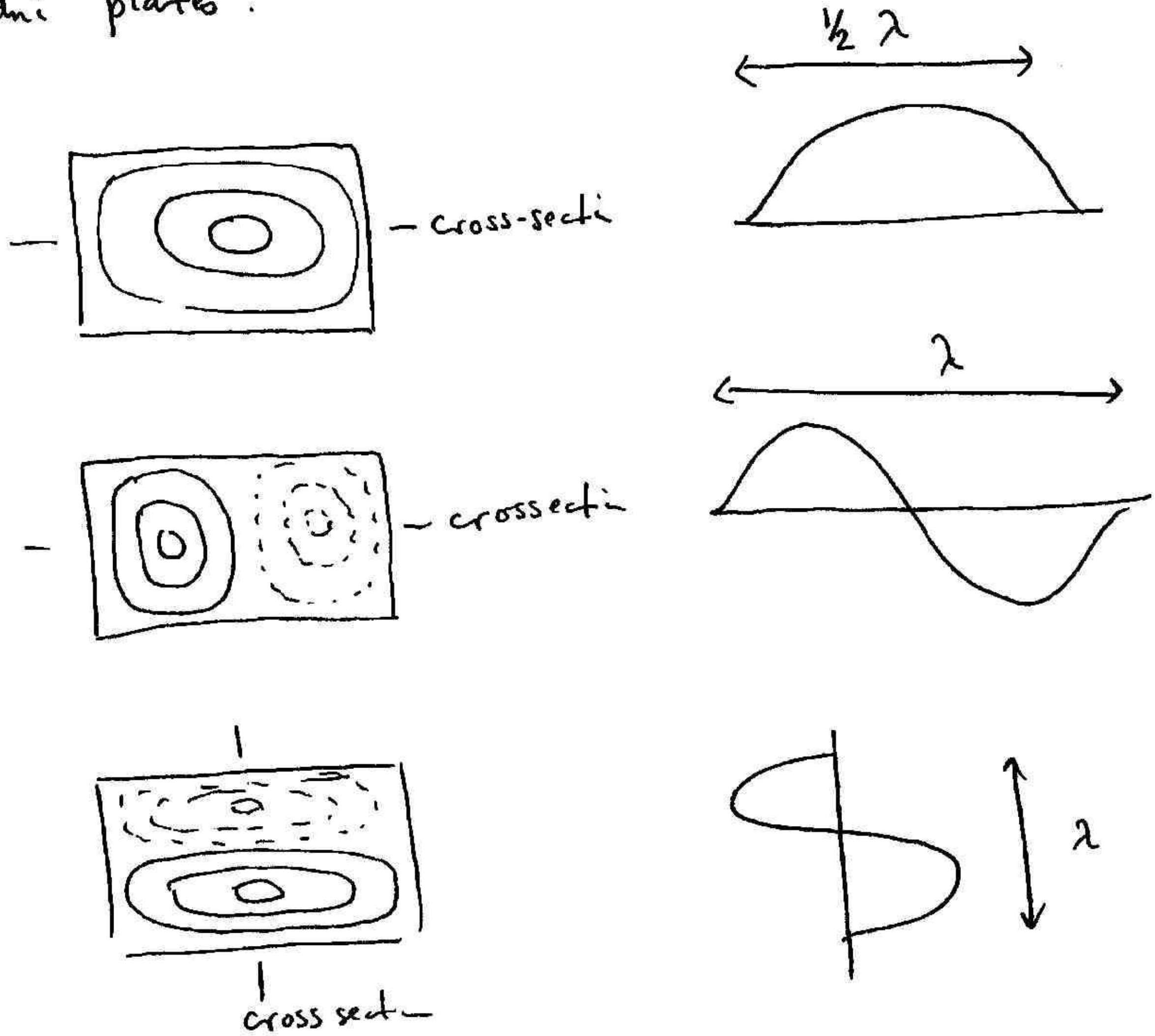
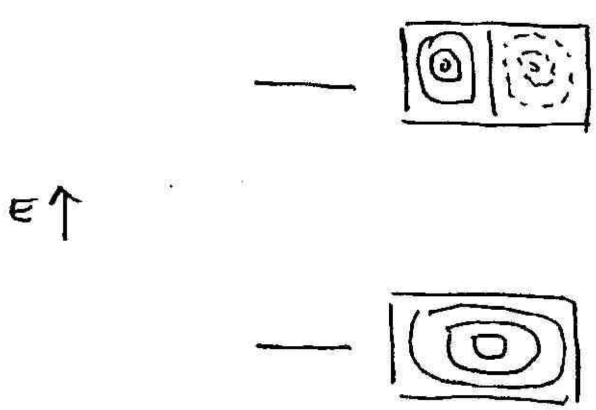
⑬ Let's see what Chladni plates has to tell us. Consider two square plates which are then joined together as a rectangular plate.



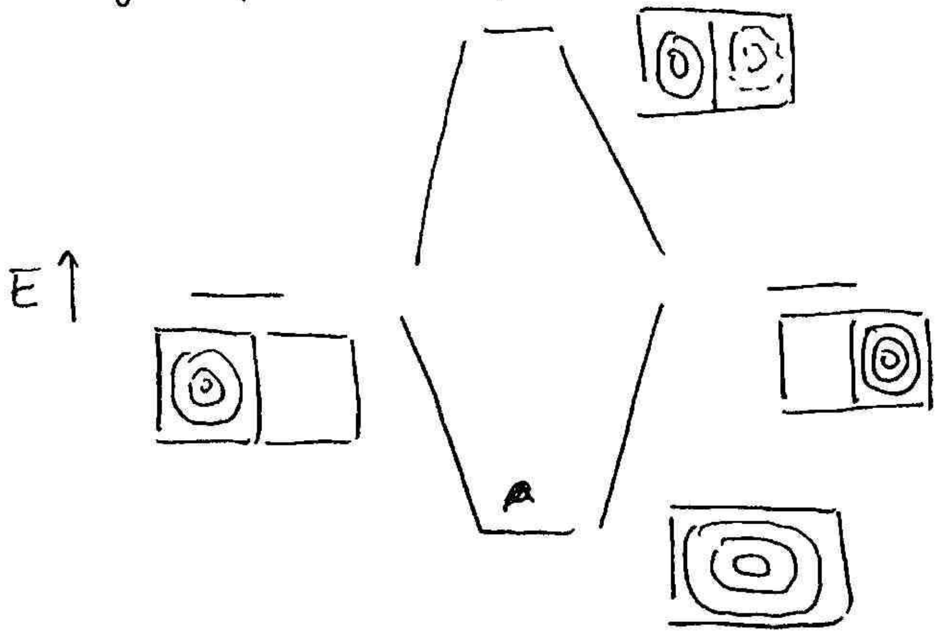
(13) Lowest frequency (energy) modes of the rectangular Chladni plates.



∴ two lowest energies



Comparing these to the original square plates (note the square plates overlap a bit)



It is (except for the Pauli exclusion principle) the same diagram as for H_2 !