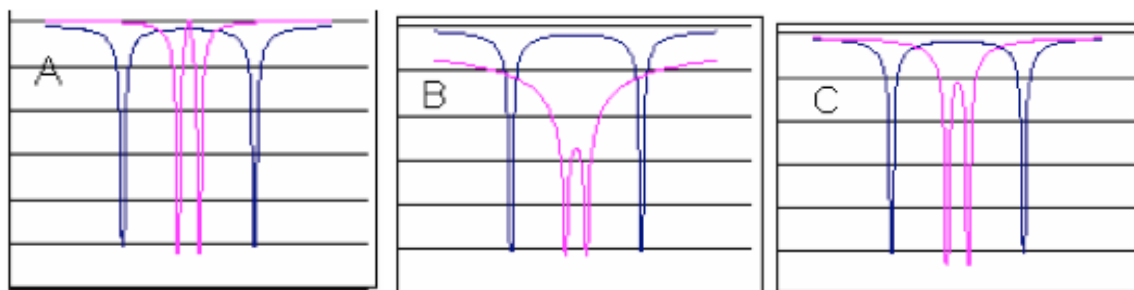
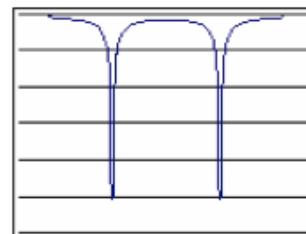


# HW #18

1. In class, we discussed one way to think about the bonding of the  $H_2$  molecule. In this problem we will think more about  $H_2^+$  (two protons and one electron) and  $H_2$  molecules.

Let's begin with  $H_2^+$ , an ionized  $H_2$  molecule (two protons and one electron).

a) If the figure at right represents what the radial distribution of the potential energy of the electron in this system looks like if the 2 protons are far apart, what does the radial distribution of potential energy curve look like if the distance decreases?

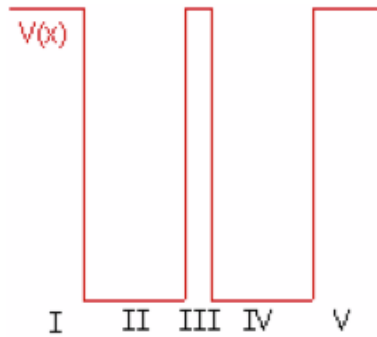


b) Consider the wave functions that are solutions to the  $H_2^+$  system:

- True    False    The bonding orbital places more of the electron density between the two protons than the anti-bonding orbital.
- True    False    The wave function of an electron in the bonding orbital will be tunneling through a potential barrier.
- True    False    The total energy of the  $H_2^+$  system is greater than the energy of an  $H^+$  and an  $H$  atom separated as two distinct atoms.
- True    False    An  $H_2^+$  molecule has a natural separation between the two atoms. No matter what you try to do - push them closer together or pull them further apart - you will have to input energy.

- c) Neutral  $H_2$  has 2 electrons. Into which orbital would this 2<sup>nd</sup> electron go and why?
- i. It would have to go into the anti-bonding orbital because you cannot have more than one electron in each state, but the net effect would be bonding.
  - ii. It would go into the bonding orbital with the other electron because this is the lowest energy state and it is OK to have two identical electrons with same state.
  - iii. It would go into the bonding orbital with the other electron because this is the lowest energy state, but it would have an opposite spin to the electron that is there because you cannot have two identical electrons with same state.

2. Consider an electron that is *bound* ( $E < V$ ) in this 1D system below (which sort of resembles the  $H_2$  system).



a) For each region (I through V): which of the terms below (A through D) would you expect to find in the solutions to Schrodinger's equation for the electron in this potential (you can choose more than one term for each region)?

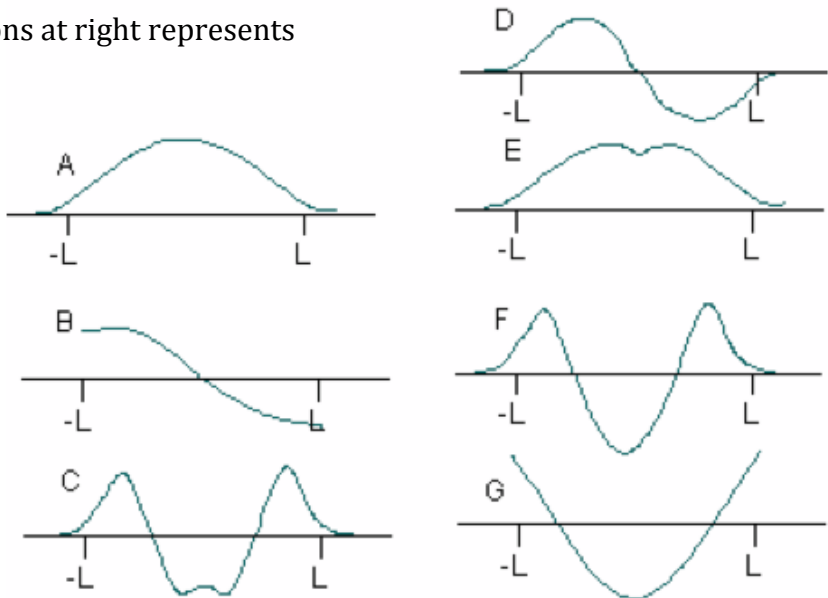
- |                        |             |
|------------------------|-------------|
| A: $A \exp(\alpha x)$  | Region I:   |
| B: $B \exp(-\alpha x)$ | Region II:  |
| C: $C \exp(ikx)$       | Region III: |
| D: $D \exp(-ikx)$      | Region IV:  |
|                        | Region V:   |

b) Which one of the wave functions at right represents the solution for the

i) ground state?

ii) first-excited state?

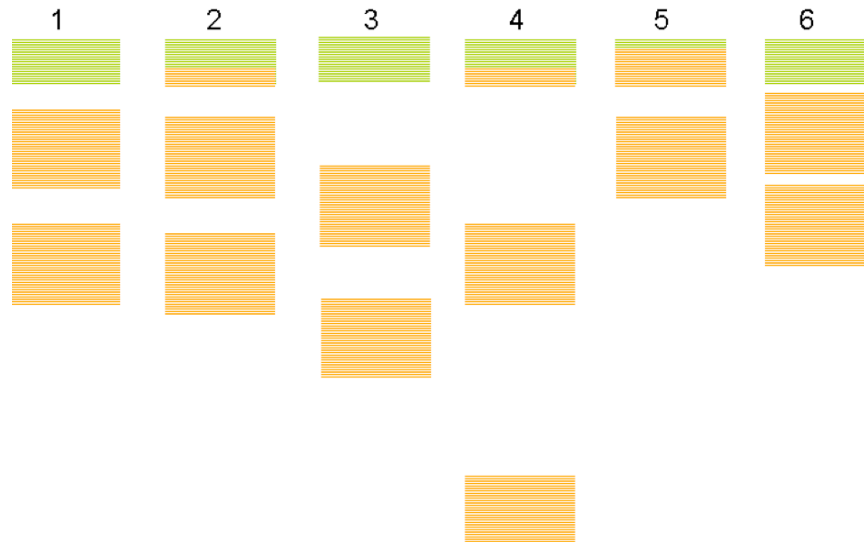
iii) second excited state?



c) True False      The probability of finding the electron between the two wells is higher for the ground state than for the 1<sup>st</sup> excited state.

3. Describe qualitatively what happens (in terms of the electron wave functions) when you bring together a bunch of copper atoms to form a solid block of copper, how this affects the allowed energy levels for copper, and how the electrons are filled in these energy levels. (You should write a full paragraph. You can include a sketch to make your explanation clearer).

4. a) Below are some depictions of different materials where the narrow orange lines represent a virtual continuum of filled energy levels and the narrow green lines represent empty electron energy levels, identify each material as conducting or non-conducting:



b) Of the non-conductors, rank them in order of most semi-conductor like to most insulator like:

c) True or false:

- True    False    In order for electrons to move as in a current, there must be empty energy levels *just* above for them to move into and then flow.
- True    False    Without any outside intervention, a piece of semi-conductor will always act as a conductor.
- True    False    Without any outside intervention, a piece of doped semi-conductor will always act as a conductor.
- True    False    Exposing a semiconductor to light or heat reduces the band gap.
- True    False    An insulator has a very small band gap.
- True    False    Any material with a partially filled band will conduct.
- True    False    Electrons are not allowed in the band gap.
- True    False    A semiconductor becomes conducting when exposed to light or heat.

d) Explain how and why exposing a semi-conductor to heat or light can change its conductivity.

e) When you put a glass bowl in a microwave oven and heat it up, why doesn't it become a good conductor like a hot semiconductor and start reflecting the microwaves in the same way the conducting walls of the oven do?