UNIT 10: MORE THAN ONE ELECTRON

So far in this course, we have only considered one particle at a time in one dimension. In reality, materials are made up of many electrons and nuclei. For the purposes of this course, we will assume that the electrons do not interact with one another[1]. For concreteness, we will just talk about multiple electrons in this section, although the rules do apply to some other types of particles.

After this unit, you should be able to

- Determine the ground state and excited states of a system of non-interacting electrons using energy level diagrams

Spins

Electrons have an additional internal variable called spin, which we have not covered yet in these notes. Roughly speaking, each electron has a magnetic moment that can either point "up"($\uparrow$) or "down"($\downarrow$). The spin is very quantized, only allowing two outcomes, $\uparrow$ or $\downarrow$ or a superposition of the two.

Filling levels in the non-interacting approximation

Suppose that we have solved for the energy eigenstates of a system. This means that we have a list of states, Ψ_n, and energies E_n, which correspond to solutions of the time-independent Schrödinger equation. For one electron, the ground state (lowest energy state) is given by putting the one electron in the ground state. For two electrons, the ground state is given by putting one electron of each spin $\uparrow$ and $\downarrow$ into the single-particle ground state. Once two electrons are in the lowest energy state, that state is "filled," and the next electron has to go in the next highest level. This procedure is called the *aufbau* principle, which means “building up.”

It’s easiest to understand the *aufbau* procedure using an example. In Fig 1, we put four non-interacting electrons in a harmonic oscillator such that $\hbar\omega = 2$ eV. We mark the electrons with up and down arrows. The total energy of the ground state is $2 \cdot 1 + 2 \cdot 3 = 8$ eV. The states with electrons in them are called occupied states, and the states without electrons in them are called unoccupied states. The lowest excited state is constructed by moving one electron from the highest occupied state to the lowest unoccupied state. The energy of this state is $2 \cdot 1 + 3 + 5 = 10$ eV. That means that this oscillator, if it starts in the ground state, will absorb light at 2 eV. It will also absorb light at many other energies, corresponding to different configurations of the electrons in the states.

[1]The non-interacting approximation turns out to work pretty well for a lot of materials like aluminum, silicon, diamond, gold, and so on. The reason for this is actually not very simple and is the consequence of *emergence*; the electrons **do** interact strongly but the emergent behavior is as if they don’t. The study of this and the emergence of other behaviors is one of the main objectives of an entire subject of physics–condensed matter physics.

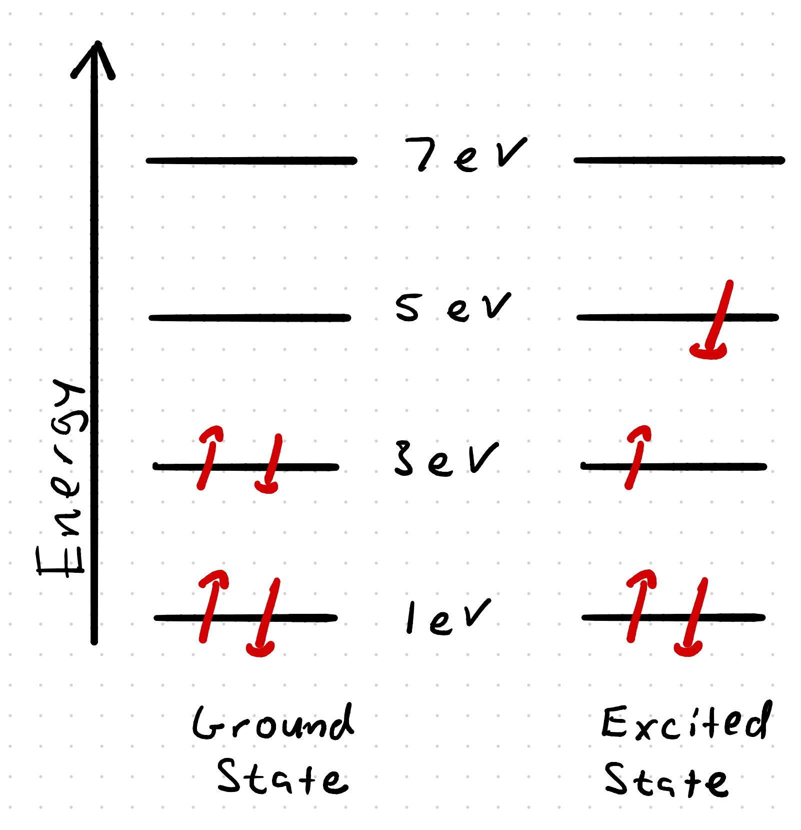

Figure 1: How to construct the ground and first excited state for four electrons in a harmonic oscillator.

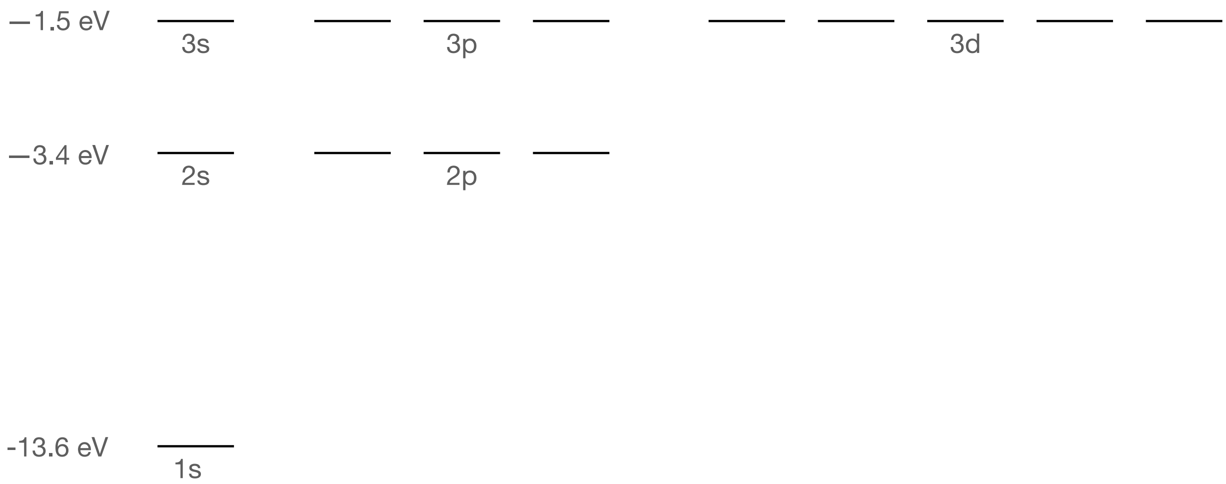

Figure 2: Energy level diagram for a hydrogen atom.

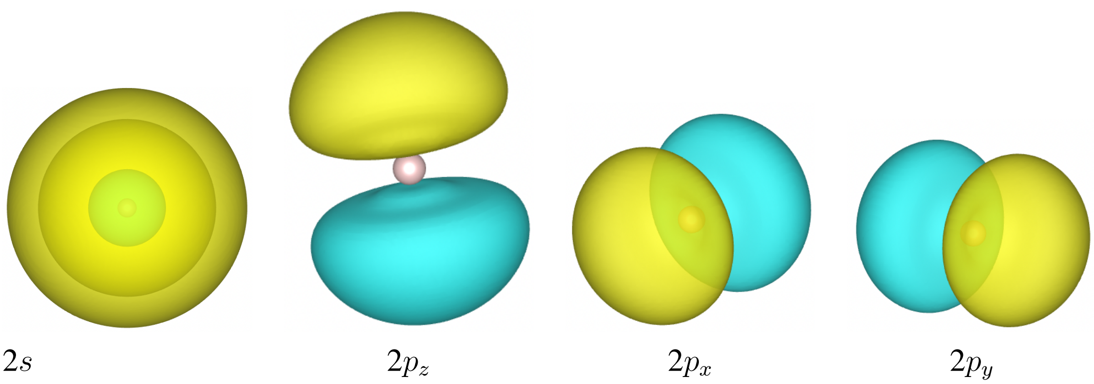

Figure 3: Images of the four states at the -3.4 eV energy level for hydrogen.

The hydrogen atom

We now know enough to understand the periodic table and some basic chemistry, such as chemical bonds from a quantum mechanical perspective. The first three energy levels of the simplest atom, hydrogen, are shown in Fig 2. Each energy level has a different number of energy eigenstates with the same energy. For example, the energy level at -13.6 eV has only one state associated with it, while the energy level at -3.4 eV has four states. The states are labeled using terms that you may be familiar with from chemistry. The general formula for energy levels in the hydrogen atom is

$$E_n = -\frac{13.6}{n^2}\,\text{eV}. \tag{1}$$

Renders of some of the energy eigenstates are presented in Fig 3. These energies and wave functions are determined by solving the Schrödinger equation in three dimensions, which one can do by hand in more advanced quantum mechanics courses.[2]

[2] Something to look forward to!

We use the labels to indicate which state the electron is in. For example, atomic hydrogen which starts in the ground state can absorb light of the following energies, among others:

Transition	Energy (eV)
$1s \rightarrow 2p$	10.2 eV
$1s \rightarrow 3p$	12.1 eV

The periodic table from quantum mechanics

The energy levels of multi-electron atoms are qualitatively very similar to those of hydrogen.[3] To find the ground state of the atom, we fill the states starting from the bottom of Fig 2, proceeding left, remembering to fill them with two electrons per *state*.

Atom	Number of electrons/protons	Ground state
H	1	$1s^1$
He	2	$1s^2$
Li	3	$1s^2 2s^1$
Be	4	$1s^2 2s^2$
B	5	$1s^2 2s^2 2p^1$
C	6	$1s^2 2s^2 2p^2$
N	7	$1s^2 2s^2 2p^3$
O	8	$1s^2 2s^2 2p^4$
F	9	$1s^2 2s^2 2p^5$
Ne	10	$1s^2 2s^2 2p^6$

The structure of the energy levels of atoms tells us why some atoms behave very similarly to others. For example, He and Ne are both called noble gases. Both of them have completely filled energy levels; all states at that energy are filled. This results in the non-reactivity of those atoms. On the other hand, atoms like nitrogen, oxygen, and hydrogen have unfilled levels, which leads to them forming molecules like N_2, O_2, and H_2.

[3] This is true until you get up to potassium (K), which has 19 electrons.