

# ATOMS!

The fact that atoms had a “line spectrum” made it obvious that the energy levels available for electrons in atoms are “discrete,” widely spaced, and we of course understand why... the electrons are bound in the atom, and their probability distributions are 3-dimensional standing waves. A “real” photon is emitted when an electron makes a transition to a lower level:  $|E_i - E_f| = hf = hc/\lambda$ .

## Quantum Description of Hydrogen:

Energies appeared at first to depend only on a principal quantum number  $n$ , so that

$$E_n = -\frac{(m_e k_e^2 e^4)}{(\hbar n)^2} = -\frac{13.6 \text{ eV}}{n^2}.$$

However, there were two other quantum numbers,  $\ell$ , related to the angular momentum of the state, and  $m_\ell$ , related to the  $z$  projection of the angular momentum.

Angular momentum  $\mathbf{L}$  and other such vectors in quantum physics have the property that although their length can be known, no information exists as to their direction, other than their projection along some axis, always taken to be  $z$ . Thus we know  $L = \sqrt{\ell(\ell + 1)}\hbar$  and  $L_z = m_\ell\hbar$ .

The rules: States exist with  $n = 1, 2$ , etc., that is, for any integer up to infinity.

States exist for any  $n$  with  $\ell$  going from 1 to  $(n - 1)$  in steps of 1.

States exist for any  $\ell$  with  $m_\ell$  going from  $-\ell$  to  $\ell$  in steps of 1, so  $(2\ell + 1)$  in all.

Thus for  $n = 2$  there are states with  $\ell = 0$  and  $\ell = 1$  and there are 3 states with  $\ell = 1$ .

The ground state of *any bound, spherically symmetric 3D system* always has  $n = 1, \ell = 0$ .

# ELECTRON SPIN:

A close study of the H spectrum “fine structure” showed that there was another quantum number, called  $m_s$ . An even closer study, revealing “hyper-fine structure,” showed that the atom must be described not by using the classical potential energy  $U = -k_e e^2/r$ , but by breaking the classical field up into virtual photons, as described by relativistic quantum field theory. This was not done successfully until 1947!

Fermions have intrinsic half-integer “spin.” This means  $S = \sqrt{s(s+1)}\hbar$  and  $S_z = m_s\hbar$ .

For the electron,  $s = 1/2$  so  $S = \sqrt{3/2}\hbar$  and  $S_z = \pm(1/2)\hbar$ ,  $m_s = \pm(1/2)$ .

Thus for each  $[n, \ell, m_\ell]$  state, there are actually two additional states, corresponding to the two values of  $m_s$ .

# THE PAULI PRINCIPLE:

Consider two identical particles that can go into two possible states,  $\alpha$  and  $\beta$ . Fermions and bosons behave totally differently. Since we can't tell the difference between particle 1 and particle 2, we must have something like:

$$\psi_{12} = \psi_{\alpha}(1)\psi_{\beta}(2) \pm \psi_{\alpha}(2)\psi_{\beta}(1).$$

For fermions, *the minus sign always occurs*. For bosons, *the plus sign always occurs*. Bosons have integer spin  $s$ , in other words 0, 1, 2, etc. Fermions have half-integer spin,  $1/2$ ,  $3/2$ ,  $5/2$ , etc.

Thus if we try to put two identical fermions in the same state,  $\alpha$ , we *always* get:

$$\psi_{12} = \psi_{\alpha}(1)\psi_{\alpha}(2) - \psi_{\alpha}(2)\psi_{\alpha}(1) = 0.$$

No two identical fermions can be in the same state, with the same set of quantum numbers.

# NOMENCLATURE:

Names for principal quantum number  $n$ :

K,  $n = 1$ ; L,  $n = 2$ ; M,  $n = 3$  and so on...

Names for quantum number  $\ell$  (origins, early days of spectroscopy):

$\ell = 0$ , s;  $\ell = 1$ , p;  $\ell = 2$ , d;  $\ell = 3$ , f, and the rest in alphabetical order.

Atomic facts:

- All atoms are about the same size, within a factor of about 3. The order-of-magnitude atomic radius is  $10^{-8}$  m.
- The ground state energy of an atom with nuclear charge  $Ze$  is roughly

$$E_{1s} = +Z^2 E_{1s,H}, \text{ where } E_{1s,H} \text{ is } -13.6 \text{ eV.}$$

- The binding energy of the weakest-bound electron in an atom varies from roughly 5 to 20 eV for all atoms. An electron is easy to remove if it is the only electron in a “shell.” Metals always have one such electron. On the other hand, atoms that don’t participate in forming molecules have completely filled shells.

- Molecular bonds are generally of the order of an eV.

**Molecules** have bands of closely spaced levels, instead of well-separated energy levels.

**Solids** have bands of energy levels so closely spaced, and so numerous, that for all practical purposes the energies within the bands are continuous.

The basis of all modern electronic technology is the semiconductor. The most widely-used semiconductor is silicon.

## Basic Processes:

- Absorption.
- Spontaneous Emission.
- Stimulated Emission.

Interesting variations:

- Phosphorescence
- Fluorescence

**X-RAYS:** Photons of energies 1000 times the normal several eV of atomic transitions can be produced when a beam of electrons is used to knock electrons out of the most tightly bound (K “shell”) levels of heavy atoms. Since matter is relatively transparent to photons of these energies, they are useful for forming images of the inside of solid objects. However, by the same token, a single X-ray photon can break the bonds of 1000 different molecules, so can cause huge damage at a molecular level.

**LASERS!** Light Amplification by Stimulated Emission of Radiation (at optical wavelengths).

