

- ... wrap-up Bohr model (refer to 17-JAN lecture materials) H atom Ionization energy, diagram of relative energy levels for H atom.
- Particle in a Box (refer to 17-JAN lecture materials) a simple wave equation and wave-function, boundary conditions, relative energy levels, diagram of relative energy levels,  $\Psi$ , and  $\Psi^2$ , as a function of coordinate  $X$ .
- Schrodinger Wave Equation The text presents the Schrodinger equation from page 21 on. Let's follow its solution (in outline) for H atom (refer to supplemental material).
- Results of the Solution for H atom The equation does account for all aspects of the H atom system, even for the high resolution spectra. Three inter-related integers arise directly and naturally from its solution. They are the quantum numbers  $n, \ell, m_\ell$ . Other features about H atom resulting from solution of the wave equation include:
- radial distribution function* (Table 2-3 and Fig.2-6) show probability of electron density as a function of linear (radial) distance from the nucleus. Notice present of nodes and penetration effects.
  - angular distribution function* (Table 2-2 and Fig. 2-7) show probability of electron density in three-dimensional space as a function of orientation about the nucleus. Notice shapes, labels and trigonometric signs. Recognize that a trigonometric sign DOES NOT represent a charge, it represents the sign of a mathematical function.
  - order of energy levels in H atom (expressed as number values for q.n.  $n$ , and letter equivalents for q.n.  $\ell$ ):

$$1s < 2s = 2p < 3s = 3p = 3d < 4s = 4p = 4d = 4f < 5s \dots$$

Results of the solution for polyelectronic atoms polyelectronic atoms are those containing two or more electrons, in other words, all atoms beyond hydrogen. The wave equation can not be solved explicitly for polyelectronic cases, but very dependable methods of approximation have been developed which match experimental measurements of energy levels to a high degree of reliability. So we now use PC software programs to calculate the energies and properties of polyelectronic atoms, and even molecules.

An additional quantum number is met in polyelectron cases. It has the symbol  $S$  and represents electron spin. Spin quantum number  $S$  has only one value,  $S = 1/2$ , but also has an associated projection,  $m_s$  having two values  $\pm 1/2$ .


symbol	values	names
$S$	$1/2$	spin quantum number, <i>spin angular momentum q.n.</i>
$m_s$	$\pm 1/2$	<i>projection of spin angular momentum</i>

$m_s = +1/2$  is often represented as an up-arrow  $\uparrow$  and  
 $m_s = -1/2$  as a down-arrow  $\downarrow$

- a. order of energy levels in polyelectronic atoms is different from that of H atom, b/c two or more electrons interact (repulsively) whereas in H atom that's not a possibility. The order of polyelectronic energy levels (in general) is as follows :

$$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < 5d^1 < 4f < 5d < 6p \dots$$

Note that electrons will enter the 4s before the third shell is filled b/c the 4s subshell is slightly lower in energy than the 3d subshell. Similarly for the 5s which is lower in energy than the 4d, and for the 6s which is lower in energy than the 5d and 4f. (Fig. 2-11)

- b. Each individual electron in a polyelectronic atom/ion can be specified by a unique set of values for the four quantum numbers  $n, \ell, m_\ell, m_s$ . This is a restatement of the Paul Exclusion Principle, "no two electron can have the same set of values for quantum numbers  $n, \ell, m_\ell, m_s$ ". (text p. 33).
- c. Electrons reside in orbitals, and orbitals are represented by quantum number  $m_\ell$ . There are as many orbitals in a given subshell as there are numeric values for  $m_\ell$ . So all  $s$  subshells (specified by  $\ell = 0$ ) will only have ONE orbital (specified by  $m_\ell = 0$ ),  $p$  subshells ( $\ell = 1$ ) will have THREE orbitals ( $m_\ell = +1, 0, -1$ ),  $d$  subshells will have FIVE orbitals, and  $f$  subshells will have SEVEN.
- d. Electrons reside in orbitals, and each orbital can accommodate TWO electrons, but only when they have opposite spins. If one electron is present in an orbital and has the condition of  $m_s = +1/2$ , then a second electron may also occupy that same orbital, but only if it has the condition  $m_s = -1/2$ . In such a situation the two electrons are said to be **spin paired**, and a corresponding diagram shows a base-line (to represent the orbital) and two arrows (one pointing up, the other down, to represent the two electrons) as shown above.
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- e. When an electron enters a subshell with several orbitals of same energy (for example,  $p$  subshells have three orbitals of same energy,  $m_\ell = +1, 0, -1$ ), and if other electrons are initially present, then double-occupancy and spin-pairing occurs only after all orbitals are half-occupied. This is a restatement of Hund's rule. (text p. 33)
- f. Electrons reside in orbitals and each orbital can accommodate TWO electrons. Consequently, the **maximum** number of electrons *per subshell* is TWO for  $s$  subshells, SIX for  $p$  subshells, TEN for  $d$  subshells, and FOURTEEN for  $f$  subshells.
- g. The periodic table is a master guide to the ordering of energy levels in atoms, and is therefore a master guide to the assignment of electrons in atoms according to the proper shell, subshell, and orbitals involved. Note the appearance of four sections in the periodic table. One section has a width of TWO elements, another of SIX elements, another of TEN elements, and a final one of FOURTEEN elements. These widths are not accidental. Each section contains elements whose last electrons are being added to  $s, p, d,$  and  $f$  subshells respectively. The representation of electrons in atoms according to shell and subshell is called an *electronic configuration*. Electronic configurations are "read" from the periodic table.