LECTURE # 16, Mon., 11-7

→ GENERAL OBSERVATIONS (on radial prob. densities)

1) average distance $\bar{r}$ (see ⊗) "jumps" (increases) from n = 1 (1s) to n = 2 (2s, 2p) to n = 3 (3s, 3p and 3d [not shown])

SEE FIGURE, NEXT PAGE

2) s electrons "penetrate" better, i.e., get closer to the nucleus, than p electrons [and, similarly, it turns out that p's penetrate better than d's....]

THUS

$$Z_{eff}(ns) > Z_{eff}(np) > Z_{eff}(nd)$$

and, since

$$E_{n\ell}^{\text{many-e atom}} \approx -\frac{\left(Z_{eff}(n\ell)\right)^2}{n^2} R,$$

it follows that

$$E_{ns} < E_{np} < E_{nd}$$

WE'RE GOING TO USE THIS IDEA TO UNDERSTAND THE ELECTRONIC STRUCTURE OF MANY-ELECTRON ATOMS

→ The "BUILDING UP" ("AUF BAU") PRINCIPLE

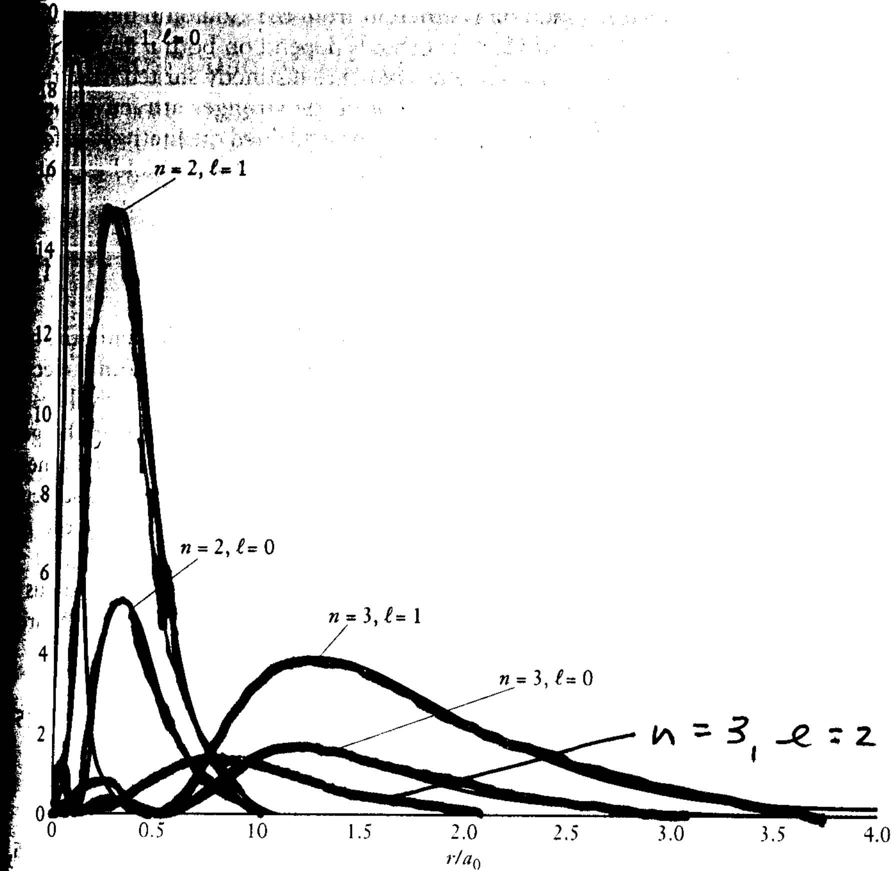

FIGURE 15.34 The shell structure of an argon atom calculated by Hartree's method. The fact that the radial probability for all orbitals with the same value of n have maxima very near one another suggests that the electrons can be viewed in "shells" made up of these orbitals.

→ FIRST NEED TO INTRODUCE THE FINAL (4th!) "QUANTUM NUMBER" FOR EACH ELECTRON

n + ℓ + m + ... SPIN QUANTUM #

$m_s = +\frac{1}{2}$ or $-\frac{1}{2}$

"up" "down"

COMES FROM (Stern-Gerlach) EXPERIMENT (Fig. 15.33, p. 543), in which ground-state H-atoms (i.e., with electrons in $n=1$, $\ell=0$, $m=0$ state) are "split" deflected up and down in a magnetic field gradient

→ PAULI EXCLUSION PRINCIPLE imposes a limit on how many e's can be found in the same n, ℓ, m orbital, since it excludes the possibility of any two e's having all their four quantum #'s the same

→ FINAL "RULE"/GUIDELINE

* When placing e's into equal-energy orbitals, e.g., $2p_x$, $2p_y$, $2p_z$, avoid doubling up e's in same n, ℓ, m orbital as long as possible (and keep e's "parallel" -- same m_s -- as long as possible)

ENERGIES ARE LOWER IN THIS WAY