

$$1) \quad |P_q| = \sqrt{l(l+1)} \hbar$$

$$l = 4$$

$$= \sqrt{20} \hbar$$

$$2) \quad m_l = 1$$

$$z\text{-Component} = 1 \hbar$$

$$3) \quad n = 5$$

$$E = -13.6 / n^2 \quad \text{e.V.}$$

$$= -\frac{13.6}{5^2} = -0.54 \text{ eV}$$

2  
(  
Consider An Example for  
the H-atom

---

Given:  $\Psi_{n,l,m_l} = \Psi_{5,4,1}$

- 1) Magnitude of the orbital Angular Momentum?
- 2) What is the  $z$ -Component of the orbital angular momentum?
- 3) What is the value of the energy?

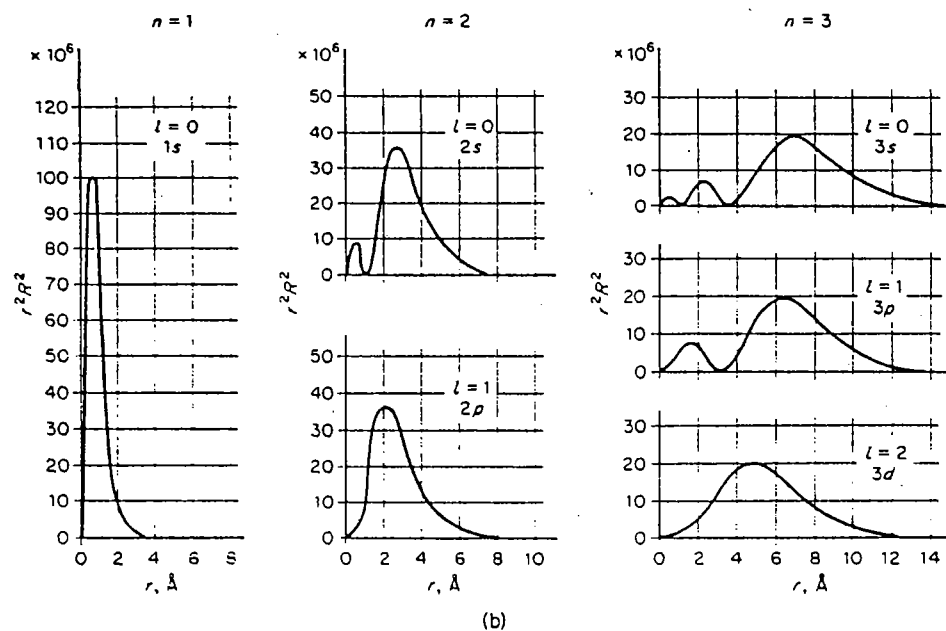
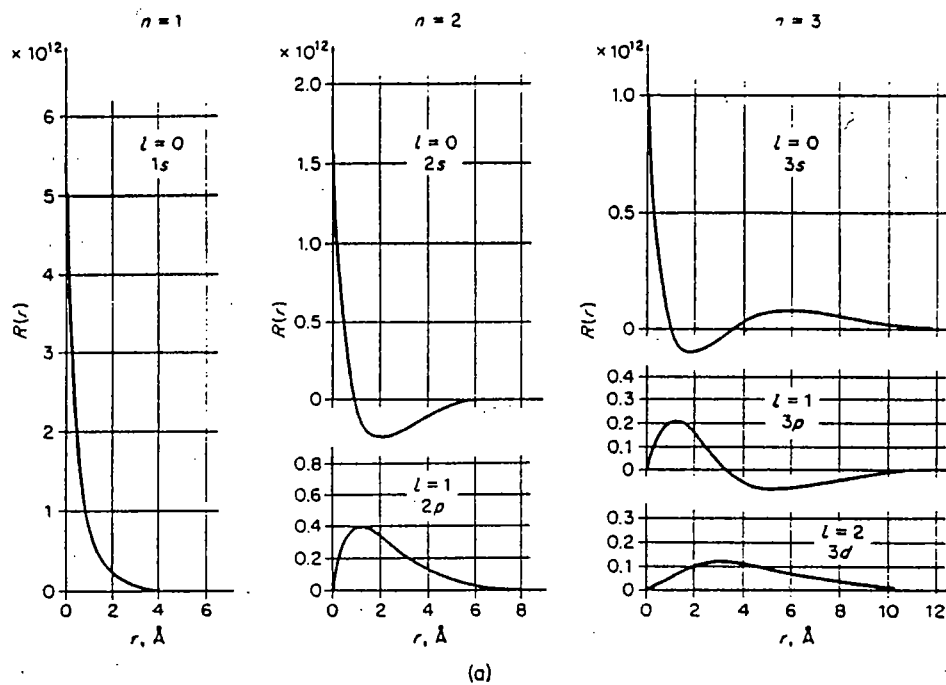


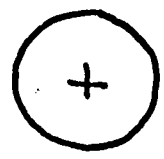
FIG. 12.11 (a) Radial part of wave functions for hydrogen atom; (b) Radial distribution functions — giving probability of finding electrons at a given distance from nucleus. [After G. Herzberg, *Atomic Spectra* (New York, Dover, 1944)].

Consider the Nodal Properties of

$\psi$

$n = 1$

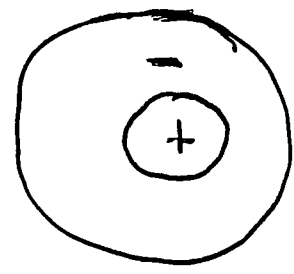
1s



no nodes

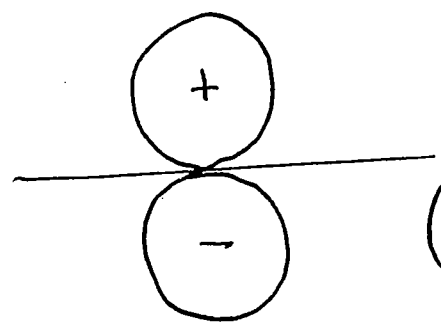
$n = 2$

2s



1 node  
(radial)

2p

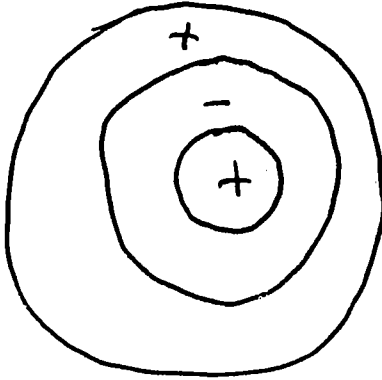


1 node  
(angular planar)

# Radial Nodes (continued)

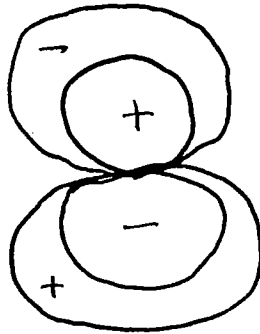
$n = 3$

3s



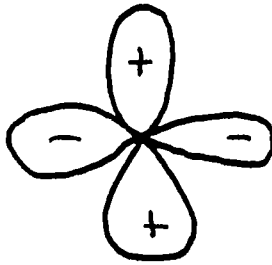
2 nodes  
(radial)

3p



2 nodes  
(1 radial  
1 planar)

3d



2 nodes  
(angular, planar)

Rule: For H-like systems:

ALL states at a given energy level have the same number of nodes =  $n - 1$

# General Rules for the Angular & Radial Nodes

Total # of nodes =  $n-1$

# of angular nodes =  $l$

$\therefore$  number of radial nodes =  $n-l-1$

<u>n</u>	<u>l</u>	<u># Nodes</u>		
		<u>angular</u>	<u>radial</u>	<u>Total</u>
1	0	0	0	0
2	0	0	1	1
2	1	1	0	1
3	0	0	2	2
3	1	1	1	2
3	2	2	0	2

7

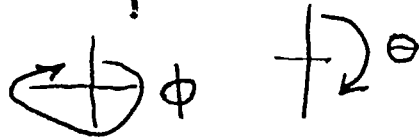
Consider the Probability of Finding an Electron at a Given Location

$$\int P(r) dr = \int |\psi|^2 d\tau \Leftarrow d\text{Volume}$$

The volume element in 3-d,  
polar coordinates

$$d\tau = r^2 dr \sin\theta d\theta d\phi$$

$$P(r) dr = \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} |\psi|^2 r^2 dr \sin\theta d\theta d\phi$$



$$\int_0^{2\pi} \int_0^{\pi} Y_{l,m_l}(\theta, \phi) \sin\theta d\theta d\phi = 1$$

$$P(r) dr = 4\pi r^2 \left| R \right|^2 dr$$

Next page

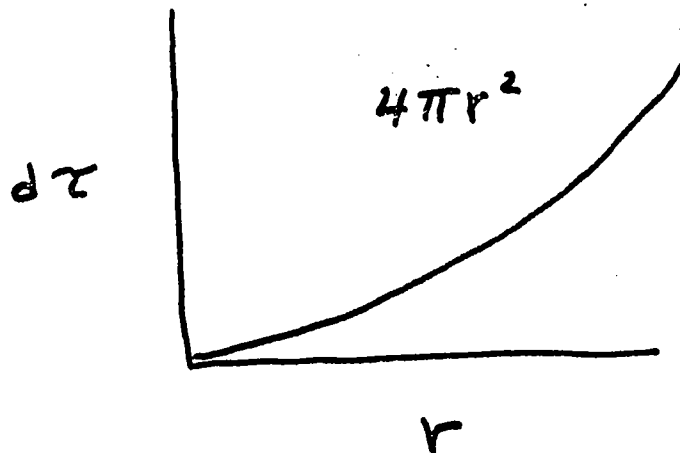
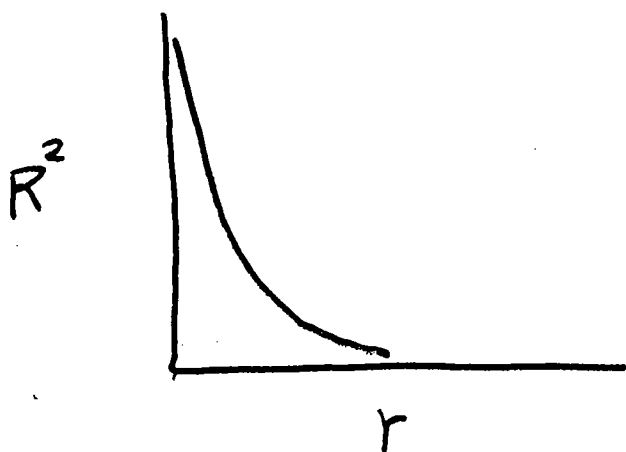
Consider

$$\iiint \underbrace{r^2 dr \sin \theta d\theta d\phi}$$

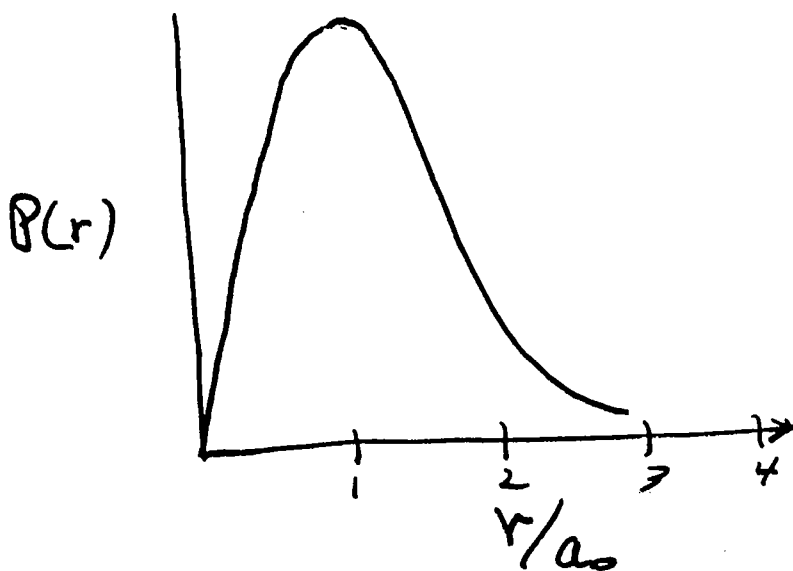
$$\underbrace{\int_0^{2\pi} d\phi}_{2\pi} \underbrace{\int_0^{\pi} \sin \theta d\theta r^2 dr}_2$$

$$4\pi r^2 dr$$

Consider 1s Electrons



Product



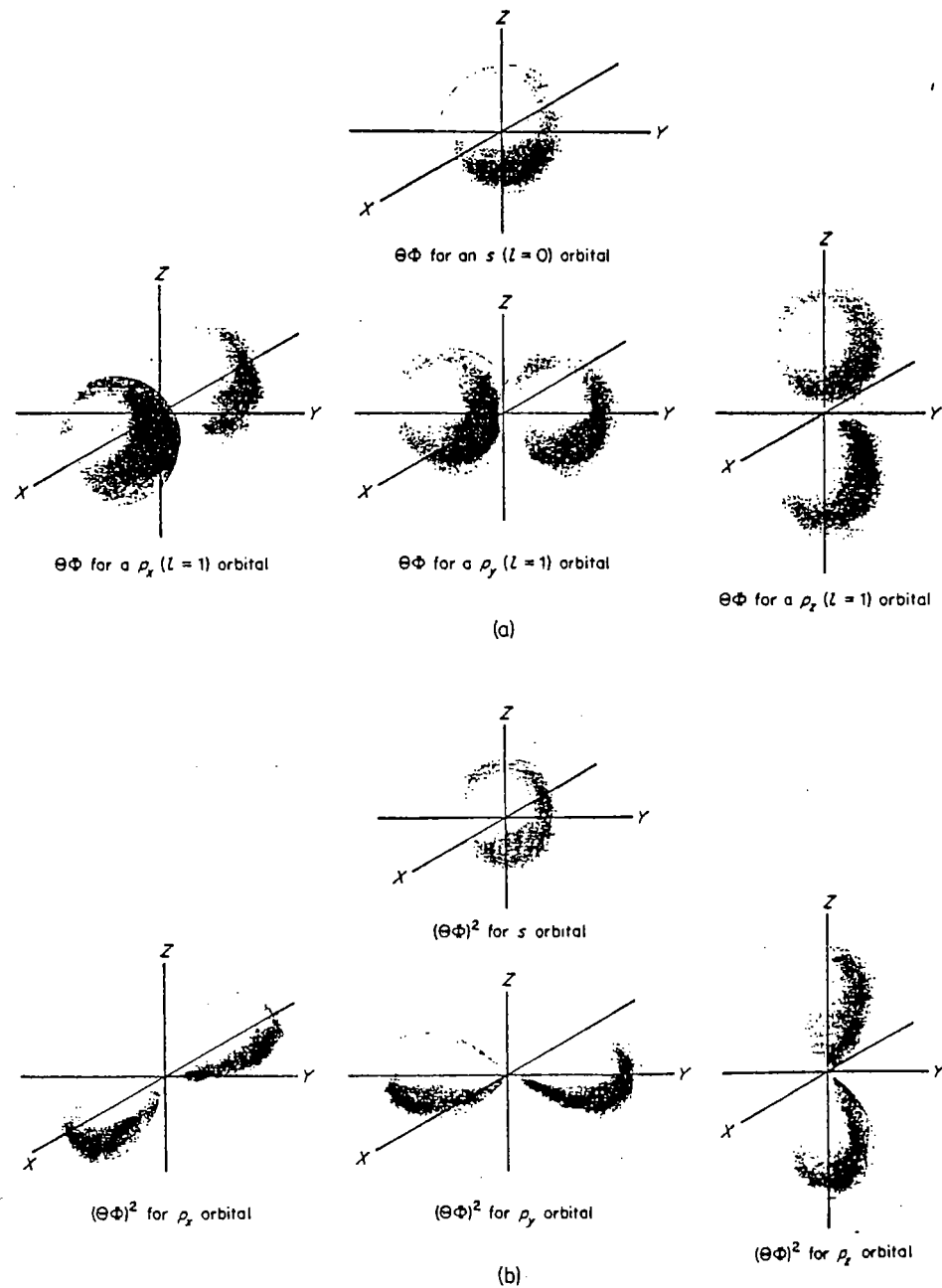


FIG. 12.19 Polar graphs: (a) the absolute values of  $\Theta\Phi$ , the angular part of the hydrogen-atom wave functions for  $l = 0$  (s) and  $l = 1$  (p) orbitals; (b)  $(\Theta\Phi)^2$  which is proportional to the electron densities.

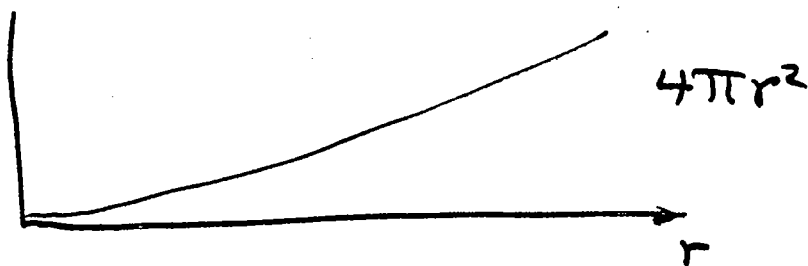
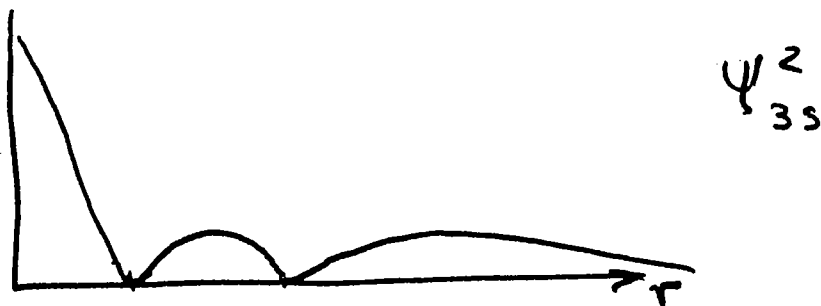
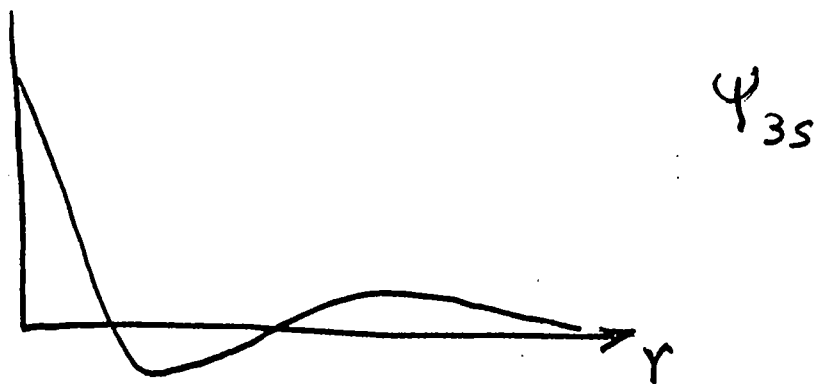
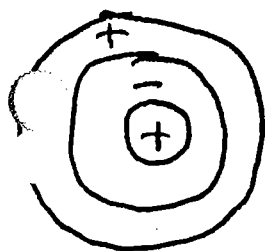
Consider 3s Electrons

11

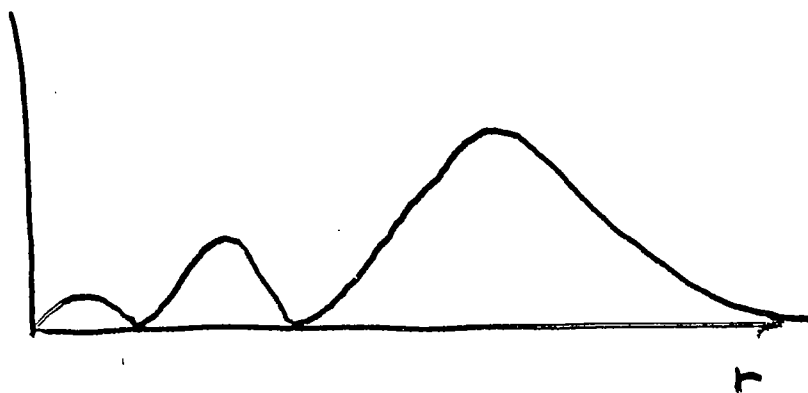
$$n = 3$$

$$l = 0$$

$\therefore$  2 radial nodes



$$4\pi r^2 \psi_{3s}^2$$



most electronic charge lies outside the 2nd radial node

# The General Idea of Selection Rules

12

$$\Delta E = h\nu$$

frequency of a given transition given by energy difference between two levels

Photon : possesses intrinsic spin angular momentum corresponding to  $s = 1$

Suppose atom in d-orbital :

then a photon emitted :

System cannot drop to s-orbital

$$l = 2 \not\rightarrow l = 0$$

Likewise :  $s \not\rightarrow s$

not allowed

Some transitions allowed / some forbidden

Selection Rules: tell us what is allowed.

---

Case: 1-electron atom

$$\Delta n = \text{any integer}$$

$$\Delta l = \pm 1$$

$$[\Delta m_l = 0 \text{ or } \pm 1]$$