Atomic Considerations

ELEC 424

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Modern Physics

- Interest in atomic scale physics grew
- Newtonian Physics adequately defines in a "common sense" manner matter in motion we observe daily
- Quantum Mechanics are needed to describe behavior of atomic scale particles and may seem to defy "common sense", only because we observe atomic interactions only indirectly.

Late 1800's

- Light is observed to diffract into interference patterns when shone through slits…must be wave-like.
- BUT when light strikes certain metal surfaces the energy of the electrons ejected depend on the frequency of the exciting light, not the amount…making light seem to be particle-like.
- Electrons diffract when shone through slits…wave-like.
- BUT we always thought of electrons as particles.

Early 1900's

- In 1911, Rutherford establishes that atoms are composed of a solid core surrounded by a much larger shell of electrons.

  - Classical EM and mechanical theory - orbits should erode as energy is radiated, causing the atoms to collapse.

- Radiated spectra from heated bodies and from hydrogen atoms could not be explained classically.

- Electron interaction with magnetic fields was observed to be weirdly constrained.

So…

- 1901 - Plank proposed atomic processes occur in "Quanta". Properly predicts blackbody radiation.
- 1905 – Einstein explained photelectrics using the particle nature of light (and won a Nobel Prize).
- 1913 – Bohr explained the spectra of the Hydrogen atom assuming "quantized" orbits.
- 1922 – Compton demonstrated photon/electron interaction.
- 1924 – Pauli postulated his exclusion principle
- 1925 – deBroglie described the wave-particle duality.
- 1926 – Schrodinger described wave-based QM
- 1927 – Hisenberg described matrix mechanics-based QM and defines limits of certainty.

Photelectric Effect

Light particles??

h = Planck's constant
(6.63×10^{-34} J-s)
v = Frequency

Light

$E = hv$

Electron

Metal

(a)

E_m

Slope = h

v

$-q\Phi$

(b)
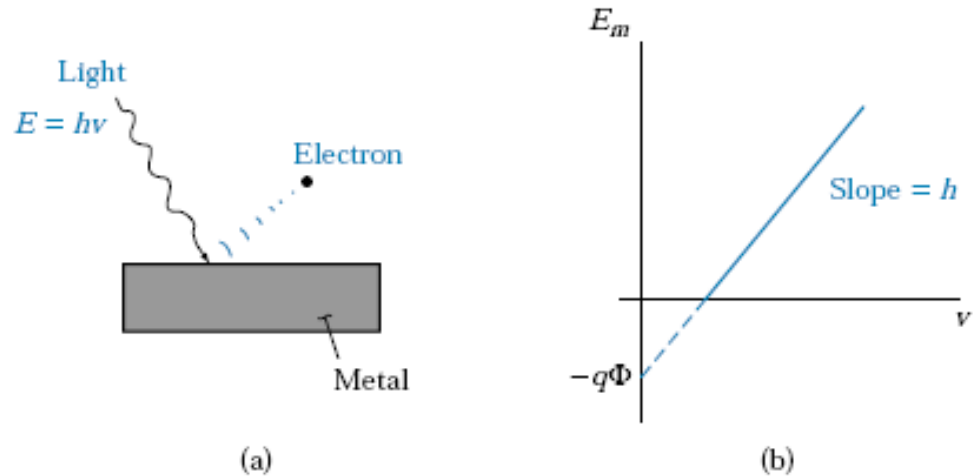
A simple experiment with a variable resistor and a voltage source determine the emitted particle energy. A voltage applied to the collecting plate was adjusted to just stop emissions at varying frequencies of light. The resulting plot of energy vs. frequency is a straight line (y=mx+b) with the y-intercept of $-q\Phi$ being the work function of the metal. This irrefutably tied the frequency of light waves to Planck's "quanta" … and won Albert Einstein a Nobel prize.

Dispersion Relationship

How frequency relates to wavelength

> Light waves can be thought of as localized packets of energy, called *photons,* of energy $E=h\nu$.

> Electrons can be though of with wave characteristics, such as wavelength of $\lambda=h/p=h/mv$.

> *The Dispersion Relationship is the relationship between frequency and wavelength, and is different for different objects. For photons $\lambda=c/v$, but not for electrons, as will be discussed in chapter 3.*

Atomic Spectra
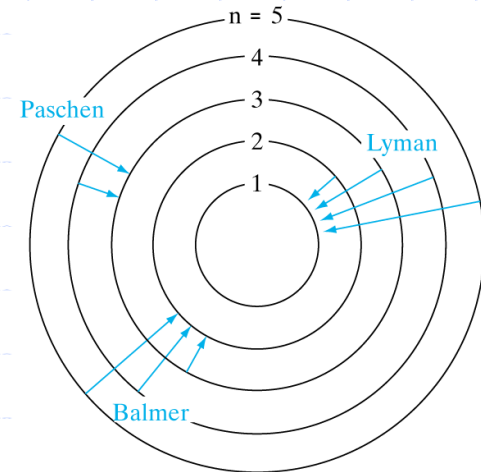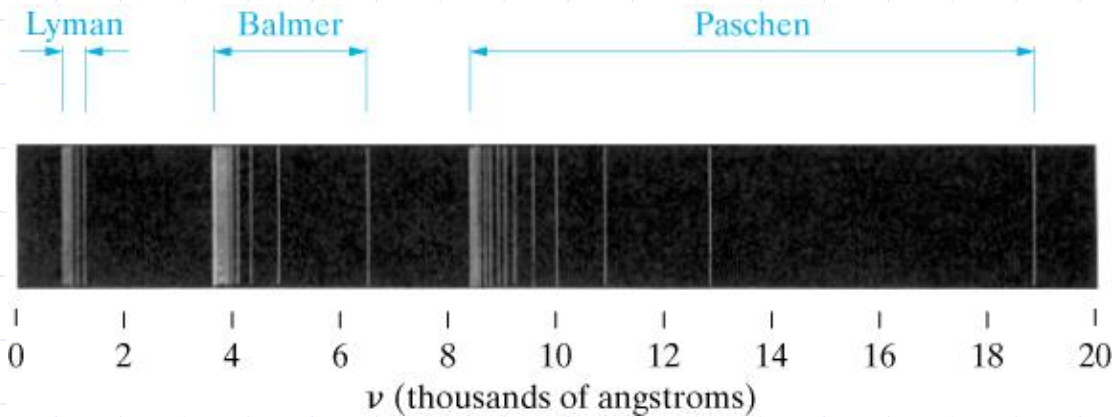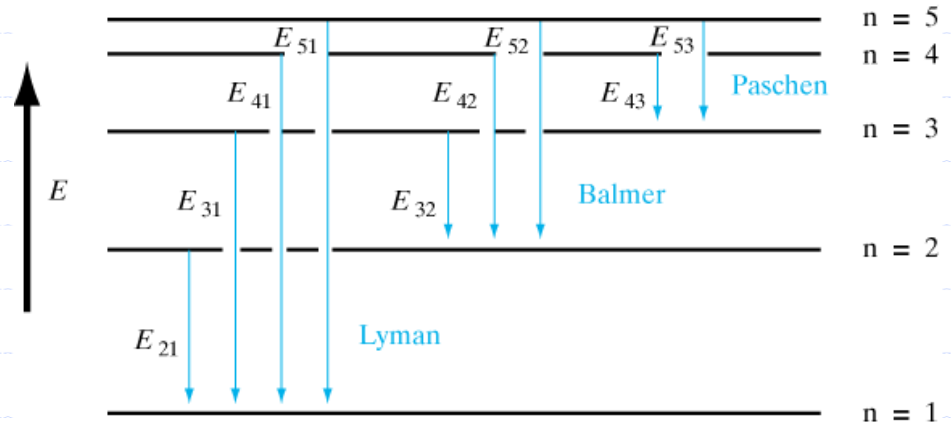*Analysis of light emissions from atoms*

$$v = cR(1 - \frac{1}{n^2}), n = 2,3,4$$

$$v = cR(\frac{1}{4} - \frac{1}{n^2}), n = 3,4,5$$

$$v = cR(\frac{1}{9} - \frac{1}{n^2}), n = 4,5,6$$

Lyman
Balmer
Paschen

R=Rydberg constant=109,678/cm

Bohr's Atom

Postulates
1. Orbits are stable
2. Electrons can change orbits
3. Angular momentum of each orbit is an integral multiple of Planck's constant divided by 2π.

Coulombic attractive force must equal centrifugal force

Orbit radii are constrained as momentum can only exist as integer multiples of $\hbar$

Bohr's atom was OK for hydrogen, but misses some subtleties, and falls short on more complicated atoms....hence QM!
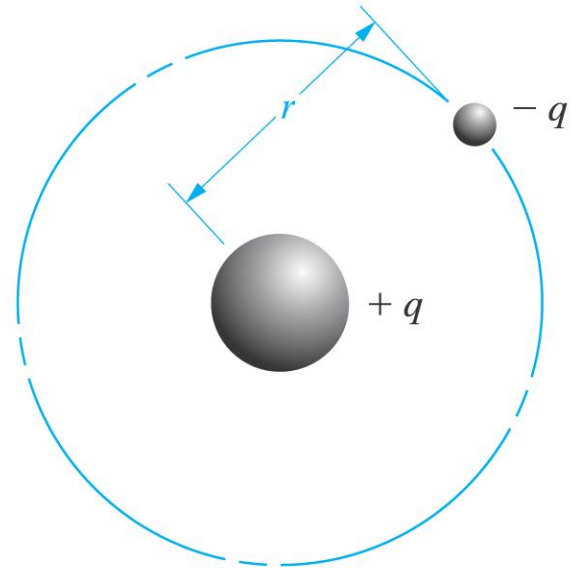
$$-\frac{q}{Kr^2} = -\frac{mv^2}{r}$$

$$K = 4\pi\varepsilon_0$$
$$p_\theta = mvr = n\hbar$$
$$\hbar = h/2\pi$$

Schrodinger and Hisenberg

1926 – Schrodinger describes wave-based QM
- Each particle can be described as a wave function, ψ (Psi)
- Classical variables are mapped to quantum operators (p 42).
- The probability of finding a particle is expressible by its wave function and volume of interest.

1927 – Hisenberg describes matrix mechanics-based QM and defines limits of certainty.
- Cannot know position and momentum precisely.
- Cannot know energy and time precisely.
- Limit to either certainty product is $\hbar$
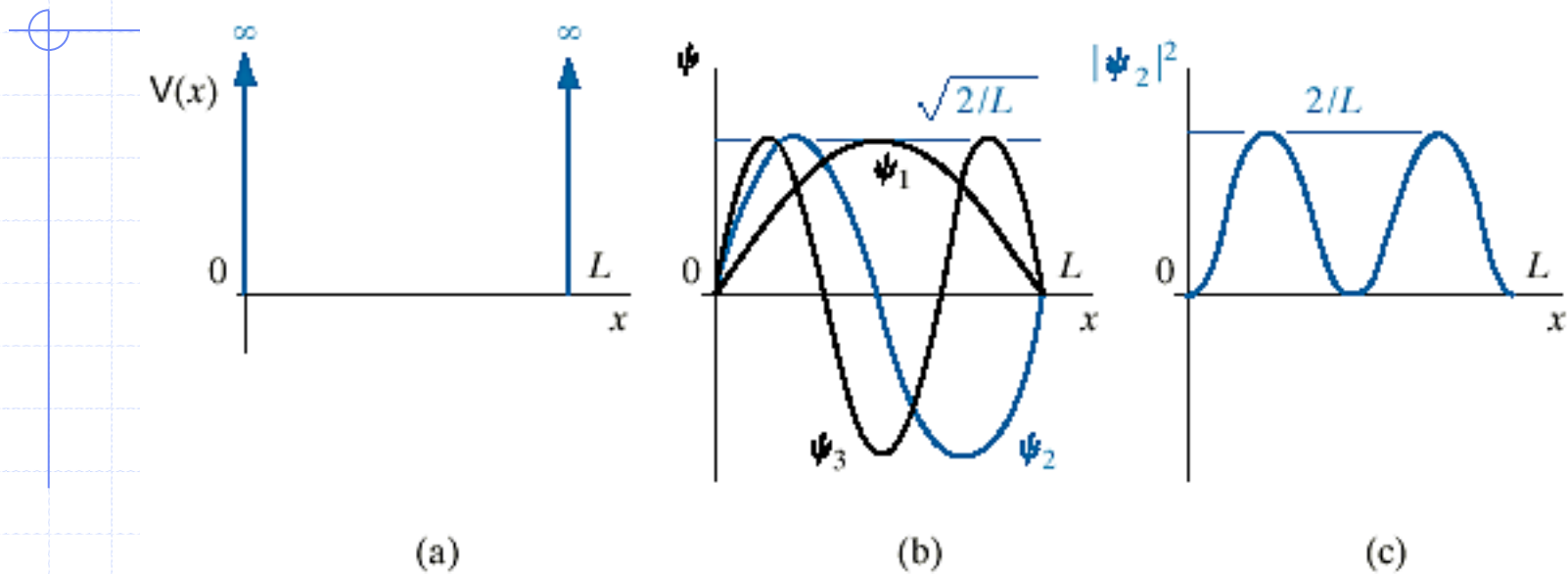
Figure 2—5
The problem of a particle in a potential well: (a) potential energy diagram;
(b) wave functions in the first three quantum states; (c) probability density
distribution for the second state.

Figure 2—6

Quantum mechanical tunneling: (a) potential barrier of height V 0 and
thickness W; (b) probability density for an electron with energy E < V 0,
indicating a non-zero value of the wave function beyond the barrier.

Figure 2—7
The spherical coordinate system.

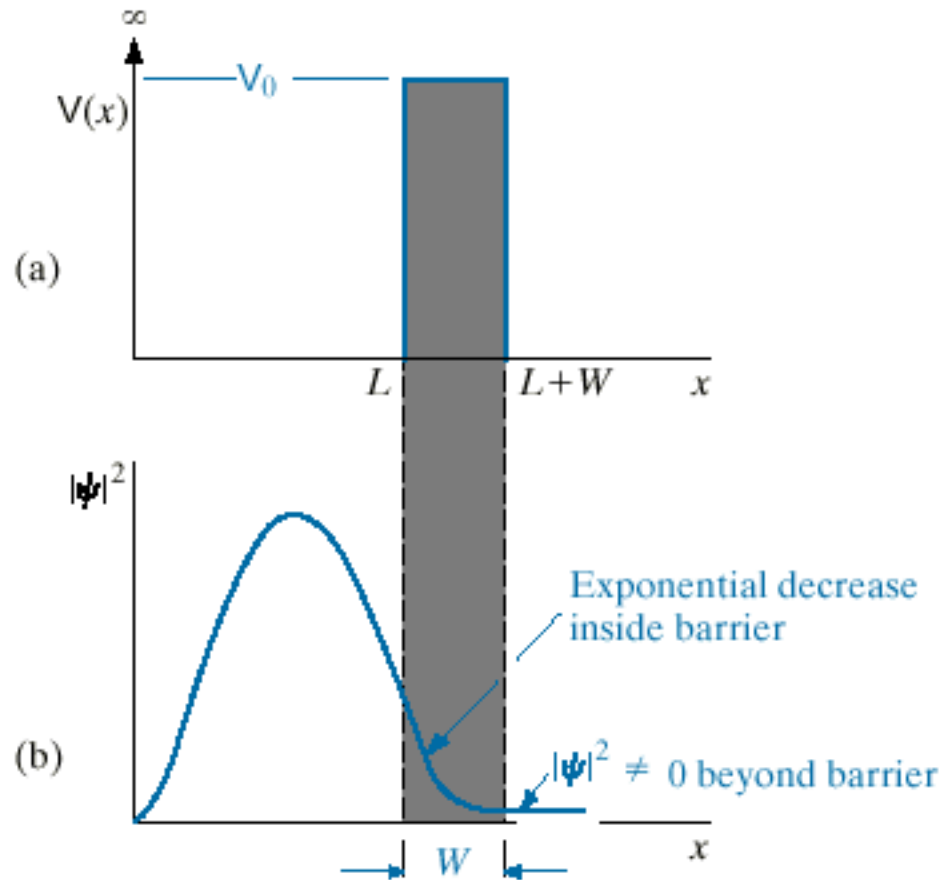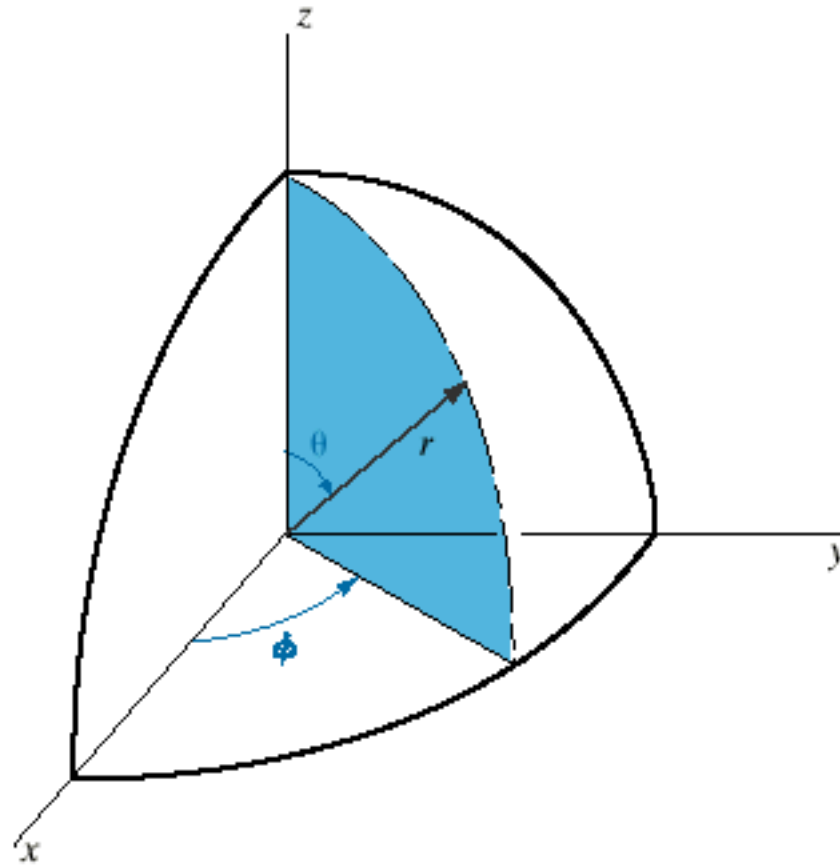| n	l	m	s/ℏ	Allowable states in subshell	Allowable states in complete shell
1	0	0	$\pm\frac{1}{2}$	2	2
2	0	0	$\pm\frac{1}{2}$	2	8
	1	-1	$\pm\frac{1}{2}$		
		0	$\pm\frac{1}{2}$	6	
		1	$\pm\frac{1}{2}$		
3	0	0	$\pm\frac{1}{2}$	2	18
	1	-1	$\pm\frac{1}{2}$		
		0	$\pm\frac{1}{2}$	6	
		1	$\pm\frac{1}{2}$		
	2	-2	$\pm\frac{1}{2}$		
		-1	$\pm\frac{1}{2}$		
		0	$\pm\frac{1}{2}$	10	
		1	$\pm\frac{1}{2}$		
		2	$\pm\frac{1}{2}$		

Table 2.1

Quantum numbers to **n** = 3 and allowable states for the electron in a hydrogen atom: The first four columns show the various combinations of quantum numbers allowed by the selection rules of Eq. (2–46); the last two columns indicate the number of allowed states (combinations of **n**, *l*, **m**, and **s**) for each *l* (subshell) and **n** (shell, or Bohr orbit).

		$n = 1$ $l = 0$	2 0 1	3 0 1 2	4 0 1	
		$1s$	$2s$ $2p$	$3s$ $3p$ $3d$	$4s$ $4p$	
Atomic number (Z)	**Element**		**Number of electrons**			**Shorthand notation**
1	H	1				$1s^1$
2	He	2				$1s^2$
3	Li		1			$1s^2\,2s^1$
4	Be		2			$1s^2\,2s^2$
5	B		2 1			$1s^2\,2s^2\quad 2p^1$
6	C	helium core,	2 2			$1s^2\,2s^2\quad 2p^2$
7	N	2 electrons	2 3			$1s^2\,2s^2\quad 2p^3$
8	O		2 4			$1s^2\,2s^2\quad 2p^4$
9	F		2 5			$1s^2\,2s^2\quad 2p^5$
10	Ne		2 6			$1s^2\,2s^2\quad 2p^6$
11	Na			1		[Ne] $3s^1$
12	Mg			2		$3s^2$
13	Al			2 1		$3s^2\,3p^1$
14	Si	neon core,		2 2		$3s^2\,3p^2$
15	P	10 electrons		2 3		$3s^2\,3p^3$
16	S			2 4		$3s^2\,3p^4$
17	Cl			2 5		$3s^2\,3p^5$
18	Ar			2 6		$3s^2\,3p^6$
19	K				1	[Ar] $4s^1$
20	Ca				2	$4s^2$
21	Sc			1	2	$3d^1\;4s^2$
22	Ti			2	2	$3d^2\;4s^2$
23	V			3	2	$3d^3\;4s^2$
24	Cr			5	1	$3d^5\;4s^1$
25	Mn			5	2	$3d^5\;4s^2$
26	Fe			6	2	$3d^6\;4s^2$
27	Co	argon core,		7	2	$3d^7\;4s^2$
28	Ni	18 electrons		8	2	$3d^8\;4s^2$
29	Cu			10	1	$3d^{10}\,4s^1$
30	Zn			10	2	$3d^{10}\,4s^2$
31	Ga			10	2 1	$3d^{10}\,4s^2\,4p^1$
32	Ge			10	2 2	$3d^{10}\,4s^2\,4p^2$
33	As			10	2 3	$3d^{10}\,4s^2\,4p^3$
34	Se			10	2 4	$3d^{10}\,4s^2\,4p^4$
35	Br			10	2 5	$3d^{10}\,4s^2\,4p^5$
36	Kr			10	2 6	$3d^{10}\,4s^2\,4p^6$

Table 2.2

Electronic configurations for atoms in the ground state.

Valence
Orbits

Inner
Orbits

Valence
Electron

First
Excitation
Orbit

Core
Electrons

Nucleus
+14

(a)

Ionization or Zero Energy Level

Distance

0

Energy

3p

First Excitation Level
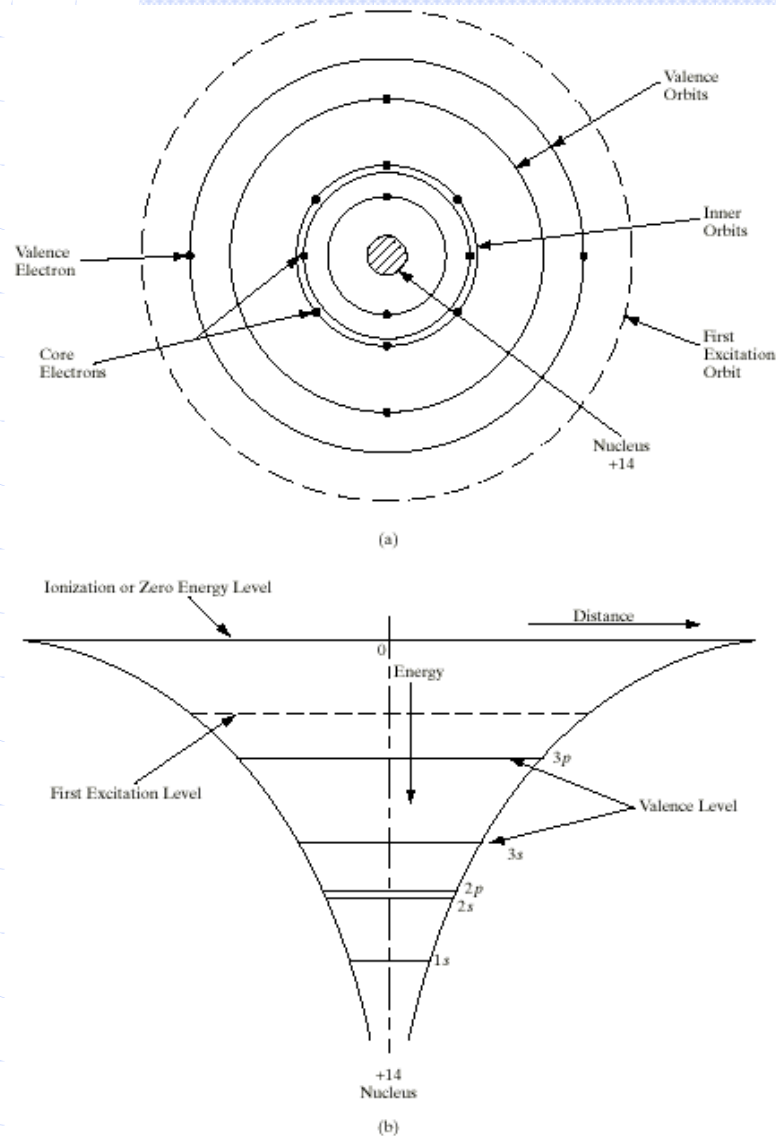
Valence Level

3s

2p
2s

1s

+14
Nucleus

(b)

Figure 2—8
Electronic structure and energy levels in a Si atom: (a) The orbital model of a Si atom
showing the 10 core electrons (n = 1 and 2), and the 4 valence electrons (n = 3); (b)
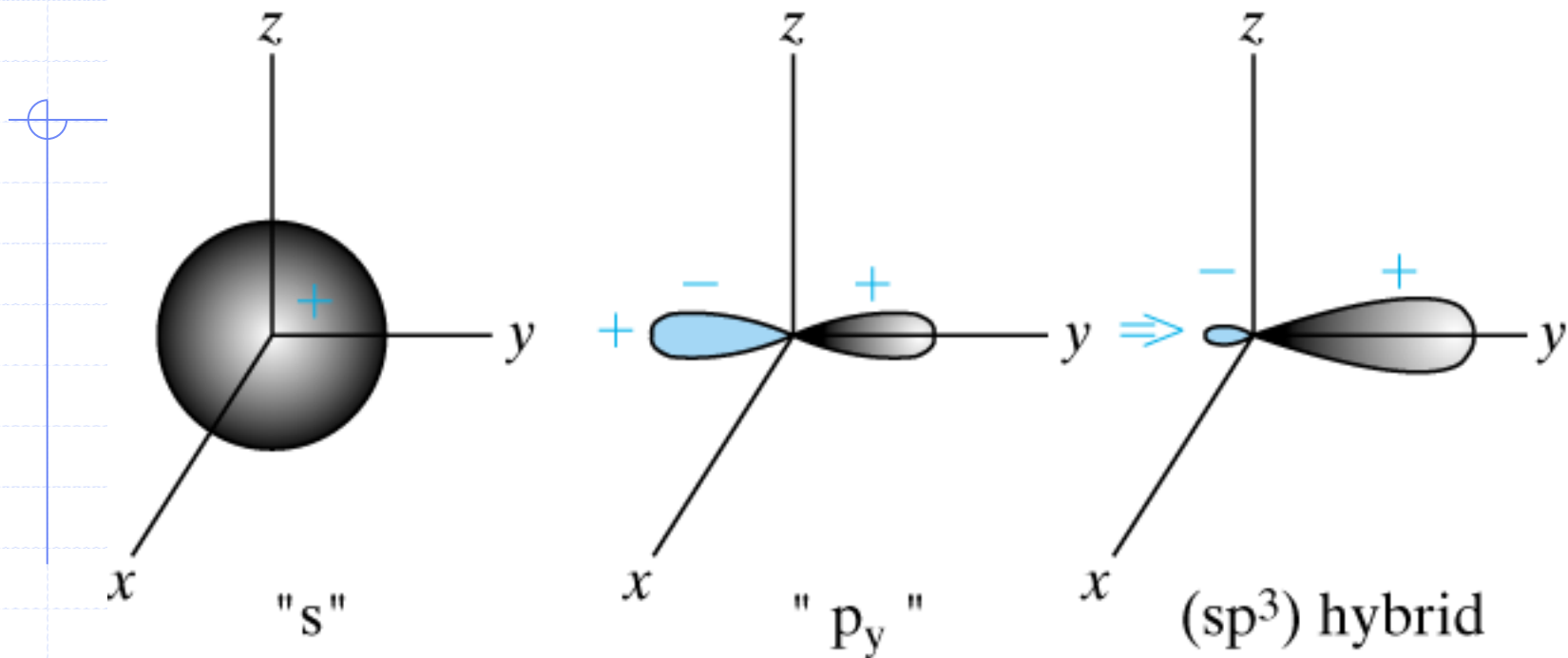energy levels in the coulombic potential of the nucleus are also shown schematically.

Figure 2—9

Orbitals in a Si atom: The spherically symmetric " s" type wave functions or orbitals are positive everywhere, while the three mutually perpendicular "p" type orbitals (p x , p y , p z) are dumbbell shaped and have a positive lobe and a negative lobe. The four sp 3 "hybridized" orbitals, only one of which is shown here, point symmetrically in space and lead to the diamond lattice in Si.

Homework Due 6/2/15

- Point A is at an electrostatic potential of +1V relative to point B in a vacuum. An electron initially at rest at B moves to A. What energy (expressed in Joules and in eV) does the electron have at A? What is its velocity in m/s?