

Chemistry 1B Fall 2016

Sessions 3-4

Chemistry 1B

Fall 2016

sessions lectures 3-4

(537-542, *(543-549), 549-557)

1

quantization of energy

$$E_{\text{photon}} = h\nu$$

absorption and emission spectra of hydrogen atom

$$E_n = -2.178 \times 10^{-18} \text{ J} \left(\frac{Z^2}{n^2} \right) \quad \mathbf{Z=1 \text{ for H atom, } n=1, 2, 3, \dots}$$

$$\frac{1}{\lambda} = \frac{2.178 \times 10^{-18} \text{ J}}{hc} Z^2 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) = 1.0967 \times 10^7 \text{ m}^{-1} Z^2 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

2

wave-particle duality

- diffraction of electrons- (Davisson-Germer Experiment; p. 530)
- De Broglie relationship (p. 528) (HW#1 12.32,12.35)
- What is "meaning" of electron wave??
<http://phys.educ.ksu.edu/vqm/html/doubleslit/index.html>
<http://www.youtube.com/watch?v=DfPeprQ7oGc>
- Wavelengths of "ordinary" objects (p. 528, example 12.2) Silberberg [Table 7.1](#) (HW#1 prob S2)
- Compton Experiment
- Heisenberg uncertainty principle (p. 539) *boing!!* (HW#1 12.49)

3

What to do ??

invent quantum mechanics !!!

4

Solvay Conference 1927



The mid-1920's saw the development of the quantum theory, which had a profound effect on chemistry. Many theories in science are first presented at international meetings. This photograph of well-known scientists was taken at the international Solvay Conference in 1927. Among those present are many whose names are still known today. Front row, left to right: I. Langmuir, M. Planck, M. Curie, H. A. Lorentz, A. Einstein, P. Langevin, C. E. Guye, C. T. R. Wilson, O. W. Richardson. Second row, left to right: P. Debye, M. Knudsen, W. L. Bragg, H. A. Kramers, P. A. M. Dirac, A. H. Compton, L. V. de Broglie, M. Born, N. Bohr. Standing, left to right: A. Piccardi, E. Herzog, P. Ehrenfest, E. Herzog, T. De Donder, E. Schroedinger, E. Verschaffel, W. Pauli, W. Heisenberg, R. H. Fowler, L. Brillouin.

5

'fuel' for quantum mechanics



Werner Heisenberg and Niels Bohr dining in Copenhagen in 1934.

6

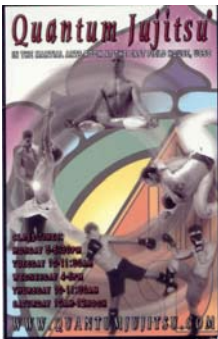
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quantum mechanics: WEIRD



7

Quantum Jujitsu ≠ Quantum Mechanics




8

what quantum mechanics must "include"

- particles have wave-like properties
- some properties, like energy, can only have certain values (energy is quantized)
- the emission or absorption of photons result in the system going from one state to another

9

goals of lectures 3-4



Hydrogen Atom


**the quantum mechanics of the hydrogen atom
(nucleus + electron)**

- what is the quantum mechanical equation that determines the properties of electrons in atoms and molecules?
- what are the "allowed" (stationary) states in which the electron in an hydrogen atom can exist ?
- what will be the energy of an electron in a given state ?
- what are the "probability waves" (orbitals) that describe the where an electron in a given state will be "found"?

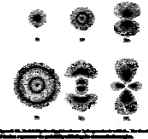
10

Bohr model vs Quantum

- Bohr model got the energies of allowed levels correctly
- However Bohr model assumed electrons traveling around nucleus in orbits of fixed radius (different radii for different n's) and with specific E_n
- This is inconsistent with the wave properties of electron and Heisenberg Uncertainty Principle



electron orbits: no, no




electron orbitals : si, si
(probability waves)

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Schrödinger equation (see pp 540 and 549)

SCHRÖDINGER EQUATION



$$\mathcal{H} \Psi = E \Psi$$

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V \right] \Psi = E \Psi$$



- basic equation of quantum mechanics
- what does it involve ?? (chem 163A)
- what does it tell you ?? Ψ E
- [where can you learn ALL about it in upper division chemistry?](#)

not responsible for pp. (543-549)*, Table 12.1

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hydrogen's electron waves: the three quantum numbers (pp. 550-551)

$$\Psi_{n,\ell,m_\ell} \overbrace{\left(r, \theta, \phi \right)}^{\text{point in space}}$$

n the principal quantum number
 ℓ the angular momentum quantum number
 m_ℓ the magnetic quantum number

Table 12.1****

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Chemistry 1B -AL
the Hydrogen Atom
Allowed Quantum Numbers

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study guide II, section III (clicker credit)

Learning Algorithms and Workbook 12
Chemistry 1B-AL Fall 2016
Lectures 13-16: The Quantum Mechanics of the Hydrogen Atom and Atomic Orbitals

Read pp. 547-548 and 549-551 (also will not be responsible for the content on pp. 549-550). Answer the QUESTIONS (Q) based on these pages to show your concepts with you.

1. Regarding the "ground state" of the Bohr hydrogen atom:
 a. What feature of the Bohr treatment of the hydrogen atom is correct?

2. What feature is inconsistent with the wave properties of the electron?

3. Although you will have to await the release of QM 1B-AL "Quantum Mechanics and Bohr Spectroscopy" to fully understand and solve the Schrödinger equation that gives the probability of electrons in atoms and molecules, QM1B concepts should have an opportunity with:
 a. What is the name of the famous equation of quantum mechanics that yields the probabilities of the allowed states of electrons in atoms and molecules?

4. When this equation is solved for a particular atom or molecule, how important aspects of the solution for the atom:
 a. the _____ of the allowed states
 b. and the _____ which is related to the _____
 c. of finding the electron or electron probability in space

5. The solution of the Schrödinger equation for the allowed states of the electron in the hydrogen atom are:
 1. characterized by three integer quantum numbers: _____ and _____

Chemistry 1B-AL Fall 2016, Study Guide and Workbook II

2. We expect that these eigenvalues are:
 a. $1, 4, 9, \dots$
 b. for a given l , $1, 2, 3, \dots$
 c. the square of l , $1^2, 2^2, 3^2, \dots$
 d. the square of the difference between l and 0, $1^2 - 0^2, 2^2 - 0^2, 3^2 - 0^2, \dots$
 e. the square of the difference between l and $l-1$, $1^2 - 0^2, 2^2 - 1^2, 3^2 - 2^2, \dots$
 f. the square of the difference between l and $l+1$, $1^2 - 2^2, 2^2 - 3^2, 3^2 - 4^2, \dots$

3. The properties of the allowed orbitals are:
 a. In the hydrogen atom, all orbitals with the same _____ have the same energy. Orbitals with different quantum numbers, but which have the same energy, are called _____ orbitals.
 b. Separation of an electron in orbitals Ψ_{n,ℓ,m_ℓ} associated related to each of the three aspects is:
 1. n
 2. ℓ
 3. m_ℓ
 c. Shapes of the orbitals:
 1. The number and the shape of the radial and angular components of the n is, used to predict patterns in the real and in the imaginary and the volume where the electron and where electron probability is particularly high.
 2. The n and ℓ values correspond with a degree of an orbitals which gives our radial and angular component.
 3. The n and ℓ values correspond with a degree of an orbitals which gives our radial and angular component.
 4. How do the quantum numbers n and ℓ affect the electron density in an orbitals?

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Schrödinger equation (see pp 540 and 549)

SCHRÖDINGER EQUATION

$$\mathcal{H} \Psi = E \Psi$$

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V \right] \Psi = E \Psi$$

- basic equation of quantum mechanics
- what does it involve ??
- what does it tell you ??
- [where can you learn ALL about it in upper division chemistry?](#)

not responsible for pp. (543-549)*, Table 12.1

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hydrogen's electron waves: the three quantum numbers (pp. 550-551)

$$\mathcal{H} \Psi = E \Psi$$

$$\Psi_{n,\ell,m_\ell}$$

wavefunction or orbital that describes allowed states of electron

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hydrogen's electron waves: the three quantum numbers (pp. 550-551)

$$\Psi_{n,\ell,m_\ell} \overbrace{\left(r, \theta, \phi \right)}^{\text{point in space}}$$

n the principal quantum number
 ℓ the angular momentum quantum number
 m_ℓ the magnetic quantum number

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rules for allowed quantum numbers

principal quantum number
 n

$n = 1, 2, 3, \dots, \infty$

positive, non-zero, integers

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rules for allowed quantum numbers

angular momentum quantum number
 l

for given value of n

$l = 0, 1, 2, \dots, (n-1)$

zero and positive integers < n

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rules for allowed quantum numbers

angular momentum quantum number
 l

designations of orbitals with various values of l

l			
0	→ s orbital	sharp	<i>'from spectroscopy'</i>
1	→ p orbital	principal	
2	→ d orbital	diffuse	
3	→ f orbital	fundamental	
⋮	⋮		
⋮	⋮		

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for example n=3

What values of l are allowed for orbitals with principal quantum number $n=3$?

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rules for allowed quantum numbers

magnetic quantum number
 m_l

for given value of l

allowed m_l are positive and negative integers
from $-l$ to $+l$ including 0

$m_l = -l, -l+1, \dots, -1, 0, +1, +2, \dots, +l$

or $m_l = 0, \pm 1, \pm 2, \dots, \pm l$

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for example 2p and 3f orbitals

what are the possible 2p orbitals?

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for example how many 3p orbitals ??

how many 3p orbitals ?

$3p$
 $n=3$ $l=1$ $m_l = -1, 0, 1$
3 different 3p components

how many orbitals with $n=3$?

study guide & learning objectives II

v. thus for $n=3$ there would be _____ different orbitals.

12

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Zumdahl Tables 12.2 and 12.3

TABLE 12.2 The Angular Momentum Quantum Numbers and Corresponding Letter Symbols

Value	Letter Used
0	s
1	p
2	d
3	f
4	g

TABLE 12.3 Quantum Numbers for the First Four Levels of Orbitals in the Hydrogen Atom

n	l	Orbital Designation	m_l	Number of Orbitals
1	0	1s	0	1
2	0	2s	0	1
2	1	2p	-1, 0, +1	3
3	0	3s	0	1
3	1	3p	-1, 0, 1	3
3	2	3d	-2, -1, 0, 1, 2	5
4	0	4s	0	1
4	1	4p	-1, 0, 1	3
4	2	4d	-2, -1, 0, 1, 2	5
4	3	4f	-3, -2, -1, 0, 1, 2, 3	7

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learning objectives II (and clickey-click)

III. The solutions of the Schrödinger equation for the allowed states of the electron in the hydrogen atom are:

1. characterized by three integer quantum numbers _____, _____ and _____

Chemistry 1B-AL Fall 2016, Study Guide and Worksheet II

2. the values that these integers can take are:

i. $n =$ _____

ii. for a given n $l =$ _____

iii. for a given l $m_l =$ _____

iv. the "names" for different values of l are $l=0$ _____, $l=1$ _____, $l=2$ _____, $l=3$ _____

v. thus for $n=3$ there would be _____ different orbitals.

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quantum mechanics of the hydrogen atom
(the electron waves in H atom and their physical meaning)

- quantum numbers of "allowed" orbitals
[table 12.2 and 12.3](#)
- energies and 'sizes' of orbitals
- orbitals and the electron density diagram
 - orbital (wavefunction, Ψ) [Ψ can have relative sign, \pm values]
 - electron density (probability, Ψ^2) [$\Psi^2 \geq 0$]
 - radial probability distribution ($4\pi r^2 \Psi^2$)
[Fig 12-16 & 12-17](#) [handout figures](#)

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CHEM 1B-AL video 2
is
finis

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Wednesday, 4 October !!!

iClicker-Check-Up exercise 2
Study Guide 2 I-III

How's your CHEM1B-AL health?

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Chemistry 1B Fall 2016 Sessions 3-4

quantum mechanics of the hydrogen atom
(the electron waves in H atom and their physical meaning)

- quantum numbers of “allowed” orbitals
[table 12.2 and 12.3](#) →
- orbitals and the electron density diagram
 - orbital (wavefunction, Ψ) [Ψ can have relative sign, \pm values]
 - electron density (probability, Ψ^2) [$\Psi^2 \geq 0$]
 - radial probability distribution ($4\pi r^2 \Psi^2$)

[Fig 12-16 & 12-17](#) handout figures
→

- orbital identification [team activity](#) Friday, 7 October

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energies of hydrogen orbitals

$$E_n = -\frac{me^4}{8\epsilon_0^2 h^2} \frac{Z^2}{n^2} = -\left(2.178 \times 10^{-18} \text{ J}\right) \frac{Z^2}{n^2}$$

for H atom, $Z=1$

- in hydrogen atom, energy only depends on n quantum number
[Fig. 12.23](#) →
- the ‘size’ of the orbital is approximated by
 $r_{\text{avg}} \equiv \bar{r} \approx a_0 \frac{n^2}{Z} = (5.29 \times 10^{-11} \text{ m}) \frac{n^2}{Z}$
(where a_0 is a constant, the Bohr radius)

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segue/review

1. Ψ_{n,ℓ,m_ℓ} possible allowed states \Leftrightarrow waves for an electron in H atom
2. Allowed values of n, ℓ, m_ℓ
3. $E_n = -\left(2.178 \times 10^{-18} \text{ J}\right) \frac{Z^2}{n^2}$ $Z=1$ for H atom
states of given n but various ℓ, m_ℓ have same energy (are degenerate)
4. Shapes of orbitals, $\Psi, \Psi^2, 4\pi r^2 \Psi^2$
 $n - \ell - 1$ radial (spherical) nodes ℓ angular (planar) nodes
5. use $r_{\text{BOHR}} \approx r_{\text{avg}} \equiv \bar{r} \approx \frac{n^2}{Z} a_0 = (5.29 \times 10^{-11} \text{ m}) \frac{n^2}{Z}$
 $r_{\text{most probable}} = a_0$
[actually: $\bar{r} = \frac{n^2}{Z} a_0 \left\{ 1 + \frac{1}{2} \left(1 - \frac{\ell(\ell+1)}{n^2} \right) \right\}$]

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shapes of orbitals nodal surfaces (identifying orbitals)

radial and angular “nodes” of atomic orbitals

radial node: a spherical shell (of radius r) where $\Psi=0$ (and $\Psi^2=0$);
 Ψ has different sign on opposite sides of radial node

angular node: a surface (plane) where $\Psi=0$ (and $\Psi^2=0$);
 Ψ has different sign on opposite sides of angular node

d’ rules !!

an orbital with quantum numbers n, ℓ, m_ℓ will have

- $n - \ell - 1$ radial nodes
- ℓ angular nodes
- $n - 1$ total nodes
- and $2\ell + 1$ components in different orientations
(from the different possible m_ℓ values)

“hold your horses” 34

shapes of orbitals

- radial and angular “nodes”
- s-orbitals [Fig. 12.18](#) →
- p-orbitals [Fig. 12.19 & 12.20](#) →
- d-orbitals [Fig. 12.21](#) →
- orbital pics in [handouts](#) →

[WWW orbital viewers](#) →

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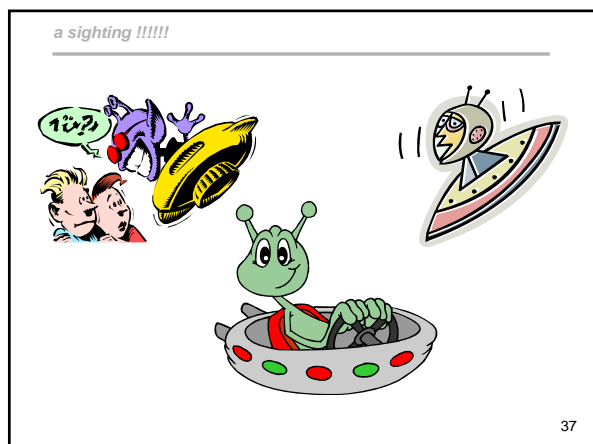
properties associated with n, ℓ, m_ℓ (HW#2 Prob x)

- n
 - energy
 - radial and total nodes
 - average distance from the nucleus
- ℓ
 - angular velocity (angular momentum)
 - shape (angular nodal planes)
- m_ℓ
 - orientation of orbital

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Chemistry 1B Fall 2016

Sessions 3-4



no not aliens !!! just d-orbital electrons

news and views

Electrons seen in orbit

Colin J. Humphreys

The classic textbook shape of electron orbitals has now been directly observed. As well as confirming the established theory, this work may be a first step to understanding high-temperature superconductivity.

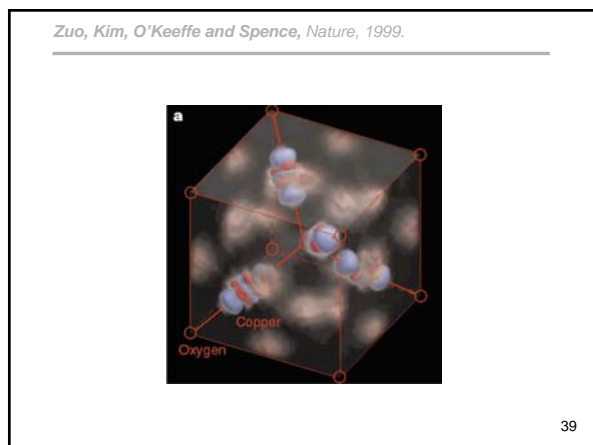
The world famous bingo drums player, Richard Feynman, who also won the Nobel Prize for Physics, once asked the following question: if you had only one sense in which to pass on to the next generation the most important scientific knowledge we possess, what would that sentence be? Feynman's own answer was "everything is made of atoms." But what is their size and shape? the next generation might reply, "and how do they stick together?"

orange. But in reality, many atoms are not spherical and the shape of atoms critically affects how they bond together."

On page 49 of this issue, Zuo *et al.* use a combination of electron and X-ray diffraction to study the shape and bonding of oranges — in this case, copper atoms in copper oxide. For the first time the striking shape of some of the electron orbitals is revealed experimentally. These methods could be used to determine bonding in high-temperature superconductors.

single electron at a distance r from the nucleus is attracted to the nuclear charge Z^+ by a potential $V = -Z^+/r$. Solving the quantum-mechanical Schrödinger equation for this potential tells us which electron states are allowed. Because V has spherical symmetry about the nucleus, the simplest solutions also have spherical symmetry. The lowest energy state, or ground state, is called the 1s orbital. So, the hydrogen atom in its ground state may be visualized as being a spherical charge dis-

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WHEW !!!

end of lectures 3-4

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the sign \pm of Ψ

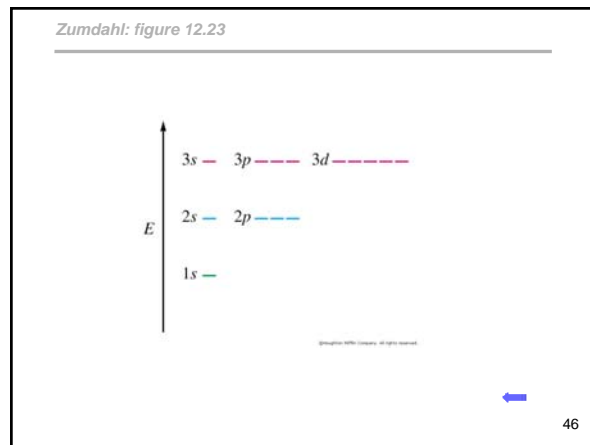
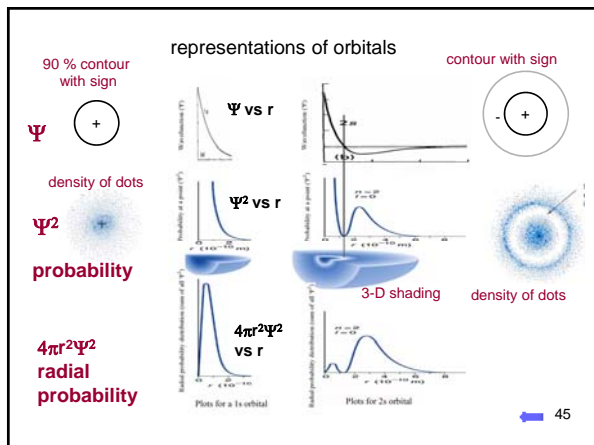
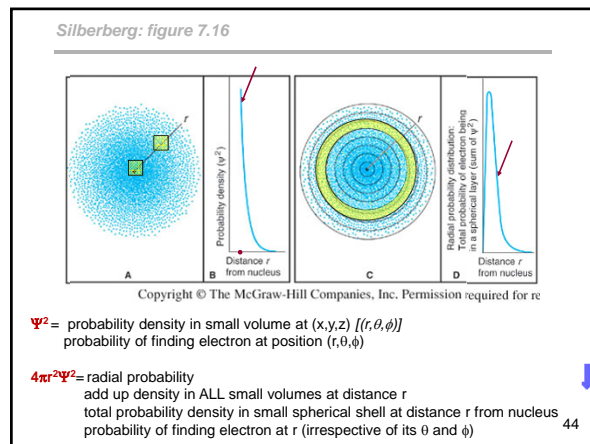
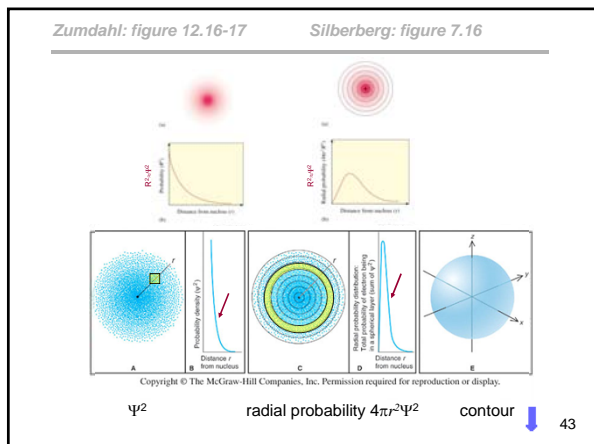
http://www.ch.ic.ac.uk/vchemlib/course/mo_theory/

- Ψ , the orbital or wave function, can have differing signs \pm in differing spatial regions; but Ψ^2 , the probability of finding an electron at a position, is always **positive**
- In going between + and - regions there will be a place where $\Psi=0$. This is a **node** of the orbital.
- Does the \pm of Ψ indicate regions of + charge and - charge? **NO !!! Repeat after me:**

The + or - regions of Ψ DO NOT correspond to regions of positive and negative charge, but just to the relative sign of the wavefunction !!

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Zumdahl Tables 12.2 and 12.3

TABLE 12.2 The Angular Momentum Quantum Numbers and Corresponding Letter Symbols

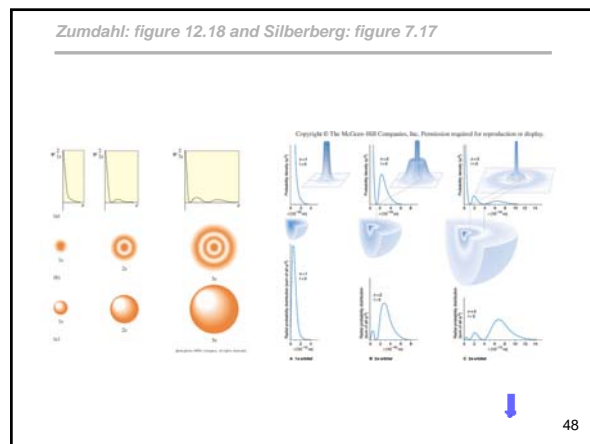
Value	Letter Used
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TABLE 12.3 Quantum Numbers for the First Four Levels of Orbitals in the Hydrogen Atom

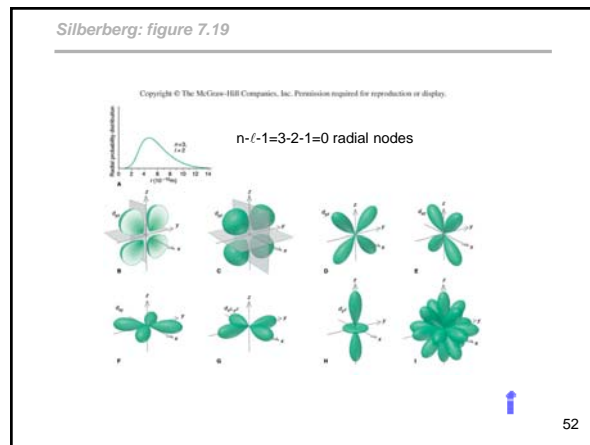
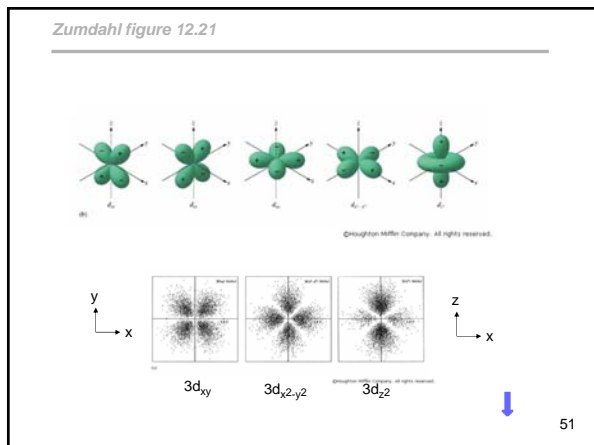
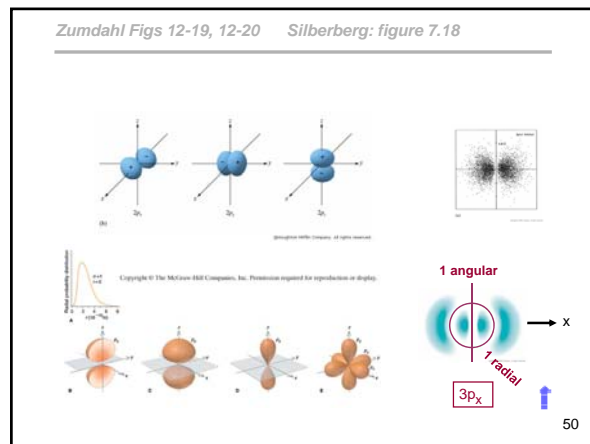
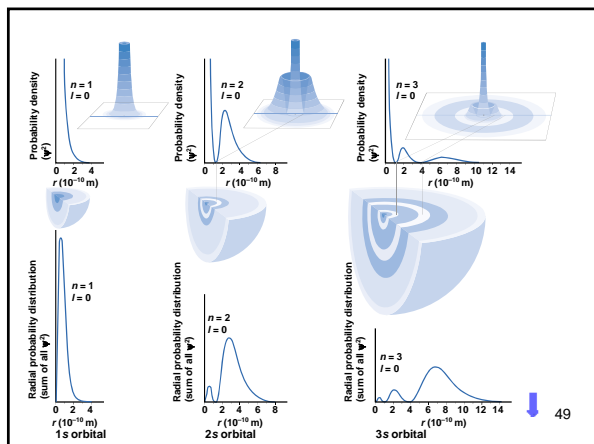
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2	0	2s	0	1
2	1	2p	-1, 0, +1	3
3	0	3s	0	1
3	1	3p	-1, 0, +1	3
3	2	3d	-2, -1, 0, +1, +2	5
4	0	4s	0	1
4	1	4p	-1, 0, +1	3
4	2	4d	-2, -1, 0, +1, +2	5
4	3	4f	-3, -2, -1, 0, +1, +2, +3	7

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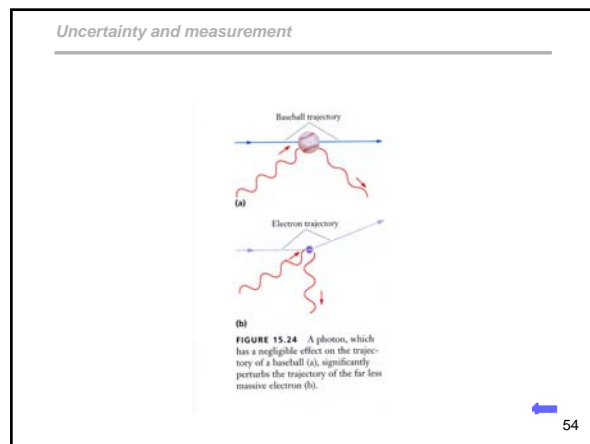
Silberberg Table 7.1

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note mass in g, need to use kg for $mv\lambda=h$
(l correct in table)

Substance	Mass (g)	Speed (m/s)	λ (m)
Slow electron	9×10^{-28}	1.0	7×10^{-4}
Fast electron	9×10^{-28}	5.9×10^6	1×10^{-10}
Alpha particle	6.6×10^{-24}	1.5×10^7	7×10^{-15}
One-gram mass	1.0	0.01	7×10^{-29}
Baseball	142	25.0	2×10^{-34}
Earth	6.0×10^{27}	3.0×10^4	4×10^{-63}

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