Chem 103, Section F0F
Unit II - Quantum Theory and Atomic Structure
Lecture 7

- The Quantum mechanical model of the atom

Lecture 7 - Atomic Structure

- Reading in Silberberg
  - Chapter 7, Section 4 *The Qunatum-Mechanical Model of the Atom*

Lecture 7 - Introduction

The discoveries of Planck, Einstein, de Broglie and Heisenberg, showed that matter and energy share common wave-like and particle-like properties

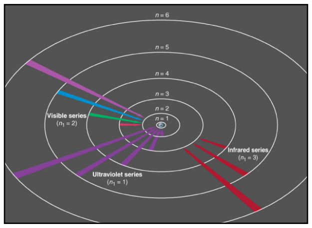
Wave-like Properties	*Particle-like Properties*
Refraction	*Discrete energy values*
Diffraction	*Momentum*
Interference	

- These discoveries lead to the development of a new field of physics called **quantum mechanics**

Lecture 7 - Introduction

Niels Bohr's model of the hydrogen was able to successfully explain the particle-like behavior of light that was emitted from excited hydrogen atoms.

- Unfortunately, his model failed to work with atoms that contained more than one electron.



Lecture 7 - The Quantum Mechanical Model

Quantum mechanics provides a solution to this problem by considering the wave-like properties of the electron in an atom.

- The quantum mechanical model of the atom was first proposed in 1926 Edwin Schrödinger.

$$\mathscr{H}\psi = E\psi$$

- E represents the energy of the electron
- ψ, represents the wave function for the electron with energy E and describes its wave-like properties.
- $\mathscr{H}$ is the Hamiltonian operator, which is applied to ψ and gives the allowed energy states for the electron.

Lecture 7 - The Quantum Mechanical Model

The Hamiltonian operator, $\mathscr{H}$, is a complex function of the electron's potential and kinetic energies:

$$\mathscr{H} = \left[-\frac{h^2}{8\pi^2 m_e}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V\left(x,y,z\right)\right]$$

↑ K.E. ↑ P.E.

- The good news is that you will never in this course be asked to solve Schrödinger's equation.

Lecture 7 - The Quantum Mechanical Model

The solutions to Schrödinger's equation, however, do provide us with very valuable information about the physical and chemical properties of elements and compounds.

- Later we will see how the quantum mechanical model of the atom helps us to understand why the elements are arranged the way they are on the periodic table.

Edwin Schrödinger shared the 1933 Nobel Prize in Physics for his quantum mechanical model of the atom

Lecture 7 - The Quantum Mechanical Model

The wave function, ψ, is also called an **atomic orbital**.

- There is a different wave function for each of the different energy states that an electron can have in an atom

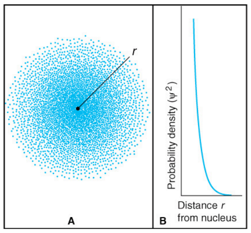
While the wave function, ψ, has no physical meaning, the square of the wave function, ψ^2, is does.

- ψ^2 is called the **probability density** and gives the probability that the electron will be found at a particular location in an atom.
- As shown by Heisenberg's uncertainty principle, we cannot know the exact location in an atom of the electron at any given time
  - the best we can do and calculate a probability of finding it at a particular location.

Lecture 7 - The Quantum Mechanical Model

The probability density functions, ψ^2, which correspond to the allowed energy values for the electron, provides us with valuable 3-dimensional pictures of where we can expect to find the electron in an atom

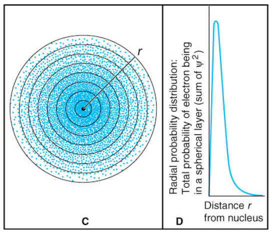
The probability density, ψ^2, as a function of distance from the nucleus.



Lecture 7 - The Quantum Mechanical Model

The radial probability distribution is calculated from the probability density and tells us the probability of finding the electron at a particular distance from the nucleus.

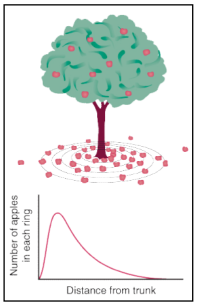
The radial probability distribution is calculated by summing up the volume times ψ^2, as you move out from the nucleus.



Lecture 7 - The Quantum Mechanical Model

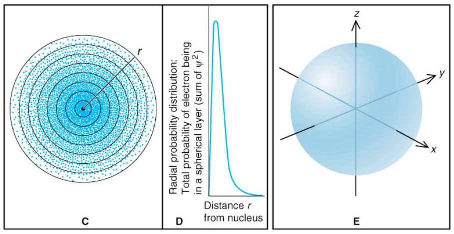
Calculating the radial probability distribution is analogous to collecting apples from the ground under an apple tree.

The radial probability distribution for the apples is obtained by collecting the apples in each ring into a separate box, and then counting the apples in each box



Lecture 7 - The Quantum Mechanical Model

The surface of an atomic orbital is often represented by the surface within which there is a 90% chance of finding the electron.



- This is the way we will be picturing at the atomic orbitals.

Lecture 7 - The Quantum Mechanical Model

The spherical atomic orbital described so far is the **ground state** orbital in the hydrogen atom.

- When the hydrogen atom is excited, the electron can transfer to a higher energy state, which will have a different wave function (atomic orbital).

Each different atomic orbital is characterized by a set of numbers called **quantum numbers**.

- These numbers determine the *size*, *shape* and *orientation* of the orbitals.
- We will see that not all of the possible orbitals are spherical

Lecture 7 - The Quantum Mechanical Model

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Lecture 7 - The Quantum Mechanical Model

There are four types of quantum numbers, we will focus first on three of these:

- *n*, is the **principal quantum number** and is related to the *size* of the orbital.
  - It is a positive integer, 1, 2, 3, …
- *l*, is the **angular momentum quantum number** and is related to the *shape* of the orbital.
  - It has an integer that runs from 0 to (*n*-1), where *n* is the corresponding principal quantum number.
- m_l, is the **magnetic quantum number** and is related to the *orientation* of the orbital.
  - It is an integer that runs from -*l* to +*l*, where *l* is the corresponding angular momentum quantum number.

Lecture 7 - The Quantum Mechanical Model

For the first three principal quantum numbers, n, Table 7.2 shows the possible values for the *l* and m_l quantum numbers.

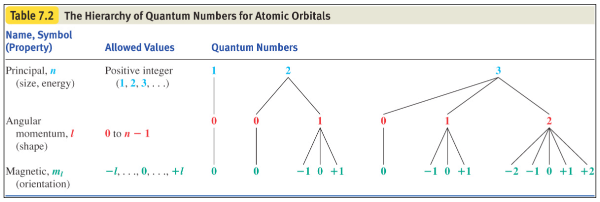


Table 7.2 The Hierarchy of Quantum Numbers for Atomic Orbitals

Name, Symbol (Property)	Allowed Values	Quantum Numbers					
Principal, *n* (size, energy)	Positive integer (1, 2, 3, . . .)	1	2		3		
Angular momentum, *l* (shape)	0 to $n - 1$	0	0	1	0	1	2
Magnetic, m_l (orientation)	$-l, \ldots, 0, \ldots, +l$	0	0	−1 0 +1	0	−1 0 +1	−2 −1 0 +1 +2

Lecture 7 - Question 1

Which of the following lists gives all possible values for the magnetic quantum number, m_l, when *l* = 2?

A) 0

B) 0, 1

C) -1, 0, 1

D) -2, 1, 0, 1, 2

Lecture 7 - The Quantum Mechanical Model

Other terminology related to the quantum numbers:

- The principal quantum number, *n*, designates the **energy level** or **shell** that an electron is in.
- The angular momentum quantum number, *l*, designates the **sublevel** or **subshell** that an electron is in.
  - Letters are used to represent these sublevels:

l = 0, *s*
l = 1, *p*
l = 2, *d*
l = 3, *f*
l = 4, *g*

- For example, the sublevel with the quantum numbers *n* = 2 and *l* = 1, is called the *2p* sublevel.

Lecture 7 - The Quantum Mechanical Model

Each sublevel can have one or more orbitals, depending on the m_l quantum number.

- Each set of allowed values for n, l, and m_l, designates a specific atomic orbital.

See sample problem 7.7

Lecture 7 - Question 2

What are the n, l, and possible m_l values for the orbitals in the *2p* sublevel?

A) $n = 2$, $l = 1$, $m_l = -1, 0, 1$ (3 orbitals)

B) $n = 1$, $l = 1$, $m_l = -1, 0, 1$ (3 orbitals)

C) $n = 2$, $l = 1$, $m_l = 0, 1$ (2 orbitals)

D) $n = 5$, $l = 3$, $m_l = -3, 2, -1, 0, 1, 2, 3$ (7 orbitals)

E) $n = 5$, $l = 4$, $m_l = -4, -3, 2, -1, 0, 1, 2, 3, 4$ (9 orbitals)

Lecture 7 - Question 2

What are the n, l, and possible m_l values for the orbitals in the *5f* sublevel?

A) $n = 2$, $l = 1$, $m_l = -1, 0, 1$ (3 orbitals)

B) $n = 1$, $l = 1$, $m_l = -1, 0, 1$ (3 orbitals)

C) $n = 2$, $l = 1$, $m_l = 0, 1$ (2 orbitals)

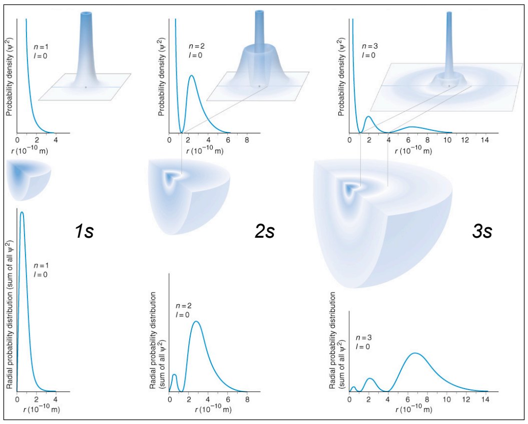
D) $n = 5$, $l = 3$, $m_l = -3, 2, -1, 0, 1, 2, 3$ (7 orbitals)

E) $n = 5$, $l = 4$, $m_l = -4, -3, 2, -1, 0, 1, 2, 3, 4$ (9 orbitals)

Lecture 7 - The Quantum Mechanical Model

The shape of an orbital is determined by its angular momentum quantum number, l:

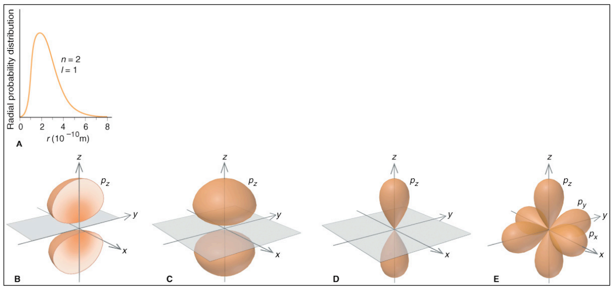
- The *s* orbitals ($l = 0$) are *spherical*
  - As n increases, the number of nodes, where the probability density distribution is 0, is equal to (n-1)
  - And the radius where the electron is most likely to be found extents further from the nucleus.



Lecture 7 - The Quantum Mechanical Model

The shape of an orbital is determined by the angular momentum quantum number, l:

- The *p* orbitals ($l = 1$) are dumbbell shaped
  - There are three possible orientations, one for each of the corresponding m_l quantum numbers (m_l = -1, 0, 1)
  - The three *p* orbitals are named p_x, p_y, and p_z.
  - Each *p* orbital has a single node plane.



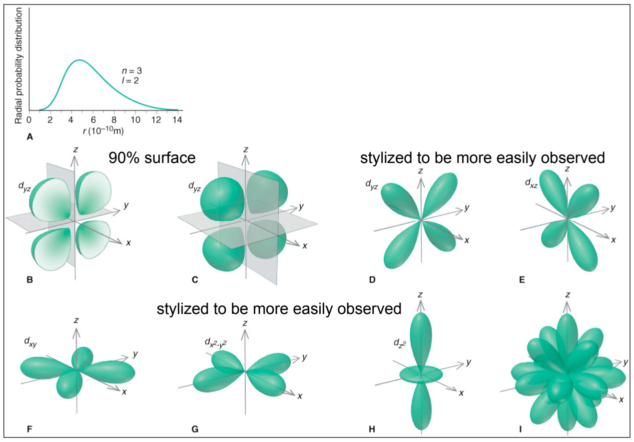
90% surface

stylized to be more easily observed

Lecture 7 - The Quantum Mechanical Model

The shape of an orbital is determined by the angular momentum quantum number, *l*:

- The *d* orbitals ($l = 2$) have a couple of different shapes.
  - There are five possible orientations, one for each of the corresponding m_l quantum numbers (m_l = -2, -1, 0, 1, 2)
  - The five *d* orbitals are named d_{yz}, d_{xz}, d_{xy}, $d_{x^2\text{-}y^2}$, and d_{z^2}.
  - Each *d* orbital has two node surfaces.



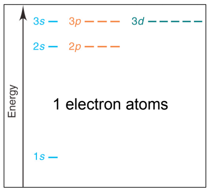
Lecture 7 - The Quantum Mechanical Model

So far we have still been talking about the hydrogen atom with only 1 electron.

- Later we will see that the quantum mechanical model of the atom also works for atoms with more than one electron.

Lecture 7 - The Quantum Mechanical Model

For atoms with only 1 electrons, the energy of the sublevels depends only on the principal quantum number, *n*.



- Later we will see that for atoms with more than one electron, the energy of the sublevels depends on both the *n* and the *l* quantum numbers.

Unit II - Up Next

Unit II - The Elements and the Structure of Their Atoms

- More on the periodic table
- Some characteristics of atoms that have more than 1 electron
- The quantum mechanical model of the atom and the periodic table
- The periodic trends observed for three key properties of the elements
- How the electronic structure of the elements affects their chemical reactivity.

The End