Readings for today: Section 1.9 – Atomic Orbitals. Section 1.10 – Electron Spin, Section 1.11 – The Electronic Structure of Hydrogen. (Same sections in 4th ed.)
Read for Lecture #7: Section 1.12 – Orbital Energies (of many-electron atoms), Section 1.13 – The Building-Up Principle. (Same sections in 4th and 5th ed.)

Topics:  
I. Wavefunctions (Orbitals) for the Hydrogen Atom  
II. Shape and Size of S and P Orbitals  
III. Electron Spin and the Pauli Exclusion Principle

I. WAVEFUNCTIONS (ORBITALS) FOR THE HYDROGEN ATOM
Solving the Schrödinger Equation provides values for $E_n$ and $\Psi(r, \theta, \phi)$.

A total of 3 quantum numbers are needed to describe a wavefunction in 3D.

1. $n = \text{principal quantum number}$  
   $n =$ ____________________________  
   determines binding energy (energy level or shell)

2. $l = \text{angular momentum quantum number}$  
   $l =$ ____________________________  
   $l$ is related to $n$, determines angular momentum, describes subshell, shape of orbital  
   largest value of $l = n - 1$

3. $m = \text{magnetic quantum number}$  
   $m =$ ____________________________  
   $m$ is related to $l$, determines behavior in magnetic field, describes the specific orbital

To describe an orbital, we need to use all three quantum numbers:  
$\Psi_{nlm}(r, \theta, \phi)$

The wavefunction describing the ground state is ______________.

Using the terminology of chemists:

The $\Psi_{100}$ orbital is instead called the _____ orbital.

$n$ designates the shell or energy level (1,2,3...)  
$l$ designates the subshell (shape of orbital) (s, p, d, f...)  
$m$ designates orbital orientation (specific orbital) (pₓ, pᵧ, pᵦ...)

$\ell = 0 \Rightarrow$ ____ orbital $\ell = 1 \Rightarrow$ ____ orbital $\ell = 2 \Rightarrow$ ____ orbital $\ell = 3 \Rightarrow$ ____ orbital

for $\ell = 1$: $m = 0$ is $p_z$ orbital, $m = \pm 1$ are the $p_x$ and $p_y$ orbitals
<table>
<thead>
<tr>
<th>n = 1</th>
<th>State label</th>
<th>wavefunction</th>
<th>orbital</th>
<th>H atom E_n</th>
<th>H atom E_n[J]</th>
</tr>
</thead>
<tbody>
<tr>
<td>ℓ = 0</td>
<td>ψ_{100}</td>
<td></td>
<td></td>
<td>–2.18 × 10^{-18}J</td>
<td></td>
</tr>
<tr>
<td>m = 0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>n = 2</td>
<td>ψ_{200}</td>
<td></td>
<td></td>
<td>–5.45 × 10^{-19}J</td>
<td></td>
</tr>
<tr>
<td>ℓ = 0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>m = 0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ℓ = 1</td>
<td>ψ_{211}</td>
<td></td>
<td></td>
<td>–5.45 × 10^{-19}J</td>
<td></td>
</tr>
<tr>
<td>m = +1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>n = 2</td>
<td>210ψ_{210}</td>
<td></td>
<td>–R_H/2</td>
<td>–5.45 × 10^{-19}J</td>
<td></td>
</tr>
<tr>
<td>ℓ = 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>m = 0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ℓ = 1</td>
<td>21-1ψ_{21-1}</td>
<td></td>
<td>–R_H/2</td>
<td>–5.45 × 10^{-19}J</td>
<td></td>
</tr>
<tr>
<td>m = -1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

What is the corresponding orbital for a 5,1,0 state?

For a hydrogen atom, orbitals with the same n value have the same energy: E = -R_H/n^2.

\[\text{having the same energy}\]

For any principle quantum number, n, there are \underline{degenerate} orbitals in hydrogen (or any other 1 electron atom).

\[\text{IN THEIR OWN WORDS}\]

MIT graduate student Benjamin Ofori-Okai discusses how energy levels relate to research in nanoscale MRI (magnetic resonance imaging), a technique that allows 3-D imaging of biological molecules, such as proteins, and viruses.
THE PHYSICAL INTERPRETATION OF A WAVEFUNCTION
The probability of finding a particle (the electron!) in a defined region is proportional to the square of the wavefunction.

\[ |\Psi_{nlm}(r,\theta,\phi)|^2 = \text{PROBABILITY DENSITY} = \] 

probability of finding an electron per unit volume at \( r, \theta, \phi \)

IIA. SHAPE OF S ORBITAL
To consider the shapes of orbitals, we can rewrite the wavefunction \( \Psi_{nlm} \) as the product of a radial wavefunction, \( R_{nl}(r) \), and an angular wavefunction \( Y_{lm}(\theta,\phi) \)

\[
\Psi_{nlm}(r,\theta,\phi) = R_{nl}(r) \times Y_{lm}(\theta,\phi)
\]

<table>
<thead>
<tr>
<th>(a) radial wave functions</th>
<th>(b) angular wave functions</th>
</tr>
</thead>
<tbody>
<tr>
<td>( n )</td>
<td>( l )</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>( \frac{1}{2\sqrt{6}} \left( \frac{Z}{a_0} \right)^{\frac{3}{2}} \left( \frac{Zr}{a_0} \right) e^{-\frac{Zr}{2a_0}} )</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
</tr>
</tbody>
</table>

where \( a_0 = \) (a constant) = 52.9 pm

for a ground state H-atom:

\[
\Psi_{100}(r,\theta,\phi) = 2e^{-r/a_0} \times \left( \frac{1}{4\pi} \right)^{1/2} = e^{-r/a_0} \frac{1}{\left( \pi a_0 \right)^{3/2}}
\]

For all s orbitals (1s, 2s, 3s, etc.), the angular wavefunction, \( Y \), is a .

s orbitals are spherically symmetrical – independent of and .

There are three common plots used to help us visualize an s orbital: (1) Probability density \( \Psi^2 \) plot of s orbitals in which density of dots represents probability density; (2) Wavefunction plotted again \( r \) (distance from nucleus); (3) Radial probability distribution as a function of radius.
RADIAL PROBABILITY DISTRIBUTION (RPD) reports on the probability of finding an electron in a spherical shell of thickness $dr$ at a distance $r$ from origin. Maximum probability or most probable value of $r$ is denoted $r_{mp}$.

$r_{mp}$ for a 1s H atom = $a_0 = 52.9$ pm = $0.529 \times 10^{-10}$ m = $0.529 \AA$

$a_0$ = Bohr radius

**NODE:** A value for $r$, $\theta$, or $\phi$ for which $\Psi$ (and $\Psi^2$) = ______.

**RADIAL NODE:** A value for _____ for which $\Psi$ (and $\Psi^2$) = 0. In other words, a radial node is a distance from the radius for which there is no probability of finding an electron.
To calculate the number of radical nodes $n - 1 - l$

1s: $1 - 1 - 0 = 0$ radial nodes

2s: ______________ radial nodes

3s: ______________ radial nodes

4p: ______________ radial nodes

IIB. THE SHAPE OF P ORBITALS

- Unlike s orbitals, p orbitals have $\theta, \phi$ dependence.
- P orbitals ___________ spherically symmetrical.
- P orbitals consist of two lobes (of opposite sign) separated by a ___________ plane on which $\Psi = 0$ (and $\Psi^2 = 0$).
- There is zero probability of finding a p-electron in a nodal plane. Thus, there is _______ probability of finding a p-electron at the nucleus.

Probability density maps of p orbitals:

Nodal planes: xy yz xz

Nodal planes (planes that have no electron density) arise from angular nodes in the wavefunction.

ANGULAR NODE: A value for ______________ at which $\Psi$ (and $\Psi^2$) = 0.

In general, an orbital has: $n - 1$ total nodes

_________ angular nodes

_________ radial nodes

2s: __________ total nodes, _________ angular nodes, _________ radial nodes

2p: __________ total nodes, _________ angular nodes, _________ radial nodes

3d: __________ total nodes, _________ angular nodes, _________ radial nodes
IIIC. ORBITAL SIZE

As n increases (from 1 to 2 to 3), the orbital $r_{mp}$ “size” ______________.

As l increases (from s to p to d) for a given n, the orbital $r_{mp}$ “size” ______________.

Only electrons in s states have a substantial probability of being very close to nucleus. This means that although the “size” (also called the boundary surface) of s orbitals is larger than p or d orbitals, s-electrons are the __________ shielded.

III. ELECTRON SPIN: THE FOURTH QUANTUM NUMBER

A fourth quantum number describes the spin of an electron within an orbital: the spin magnetic quantum number, ______

There is no classical analogy to spin.

- An electron can have two spin states:
  
  $m_s = ______$ (spin up) or $m_s = ______$ (spin down).

- $m_s$ completes the description of an ______________ and is NOT dependent on the orbital.
So we can describe a given orbital using three quantum numbers \((n, l, m_l)\) and a given electron using 4 quantum numbers \((n, l, m_l, m_s)\).

\[
\Psi_{n/m_l}
\]
describes an \[\ ]
\[
\Psi_{n/m_l/m_s}
\]
describes an \[\ ]

**PAULI EXCLUSION PRINCIPLE**

No two electrons can be in the same orbital and have the same spin.
No two electrons in the same atom can have the same _____ quantum numbers.

\[
\begin{array}{cccc}
1s^2 & 2s^2 & 2p_x^2 & 2p_y^2 & 2p_z^2 \\
\end{array}
\]
Ne

Within each orbital, electrons are paired (one spin up and one spin down).
One orbital can hold no more than two electrons.