

5.111 Lecture Summary #6

Readings for today: Section 1.9 (1.8 in 3rd ed) – Atomic Orbitals.

Read for Lecture #7: Section 1.10 (1.9 in 3rd ed) – Electron Spin, Section 1.11 (1.10 in 3rd ed) – The Electronic Structure of Hydrogen.

Topics: Hydrogen Atom Wavefunctions

I. Wavefunctions (orbitals) for the hydrogen atom ($H\Psi = E\Psi$)

II. Shapes of H-atom wavefunctions: s orbitals

III. Radial probability distributions

ENERGY LEVELS (continued from Lecture #5)

The Rydberg formula can be used to calculate the frequency (and also the E or λ , using $E = h\nu$ or $\lambda = c/\nu$) of light emitted or absorbed by any 1-electron atom or ion.

$$\nu = \frac{Z^2 R_H}{h} \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right) \qquad \nu = \frac{Z^2 R_H}{h} \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right)$$

for $n_i > n_f$

for $n_f > n_i$

$n_f > n_i$ in _____. Electrons absorb energy causing them to go from a lower to a higher E level.

$n_i > n_f$ in _____. Electrons emit energy causing them to go from a higher to a lower E level.

I. WAVEFUNCTIONS (ORBITALS) FOR THE HYDROGEN ATOM

When solving $H\Psi = E\Psi$, the solutions are E_n and $\Psi(r, \theta, \phi)$.

$\Psi(r, \theta, \phi)$ = stationary state wavefunction: time-independent

In solutions for $\Psi(r, \theta, \phi)$, two new quantum numbers appear! A total of 3 quantum numbers are needed to describe a wavefunction in 3D.

1. n = principal quantum number

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

determines binding energy

2. l = angular momentum quantum number

$l =$ _____

l is related to n

largest value of $l = n - 1$

determines angular momentum

3. m = magnetic quantum number

$m =$ _____
 m is related to l
 largest value is $+l$, smallest is $-l$
 determines behavior of atom in magnetic field

To completely describe an orbital, we need to use all three quantum numbers:

$$\Psi_{n/l/m}(r, \theta, \phi)$$

The wavefunction describing the ground state is _____.
 Using the terminology of chemists, the Ψ_{100} orbital is instead called the “___” orbital.

An orbital is (the spatial part) of a wavefunction; **n(shell)** **l(subshell)** **m(orbital)**

$l = 0 \Rightarrow$ ___ orbital $l = 1 \Rightarrow$ ___ orbital $l = 2 \Rightarrow$ ___ orbital $l = 3 \Rightarrow$ ___ orbital

for $l = 1$: $m = 0$ _____ orbital, $m = \pm 1$ states combine to give _____ and _____ orbitals

	State label	wavefunction	orbital	E_n	$E_n[\text{J}]$
$n = 1$ $l = 0$ $m = 0$		ψ_{100}		$-R_H/1^2$	$-2.18 \times 10^{-18} \text{J}$
$n = 2$ $l = 0$ $m = 0$					$-5.45 \times 10^{-19} \text{J}$
$n = 2$ $l = 1$ $m = +1$					$-5.45 \times 10^{-19} \text{J}$
$n = 2$ $l = 1$ $m = 0$	210	ψ_{210}		$-R_H/2^2$	$-5.45 \times 10^{-19} \text{J}$
$n = 2$ $l = 1$ $m = -1$	21-1	ψ_{21-1}		$-R_H/2^2$	$-5.45 \times 10^{-19} \text{J}$

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

- **Degenerate** = having the same energy
- For any principle quantum number, n , there are _____ degenerate orbitals in hydrogen (or any other 1 electron atom).

Energy Level Diagram									
E [J]	9 degenerate states at second excited energy level								
-0.242×10^{-18}	<div><div></div><div>n = 3</div><div>$\ell = 0$</div><div>m = 0</div></div>	<div><div></div><div>3</div><div>$\ell = 1$</div><div>m = ±1</div></div>	<div><div></div><div>3</div><div>$\ell = 1$</div><div>m = 0</div></div>	<div><div></div><div>3</div><div>$\ell = 1$</div><div>m = ±1</div></div>	<div><div></div><div>3</div><div>$\ell = 2$</div><div>±1, ±2</div></div>	<div><div></div><div>3</div><div>$\ell = 2$</div><div>±1, ±2</div></div>	<div><div></div><div>3</div><div>$\ell = 2$</div><div>m = 0</div></div>	<div><div></div><div>3</div><div>$\ell = 2$</div><div>±1, ±2</div></div>	<div><div></div><div>3</div><div>$\ell = 2$</div><div>±1, ±2</div></div>
-0.545×10^{-18}	<div><div></div><div>n = 2</div><div>$\ell = 0$</div><div>m = 0</div></div>	<div><div></div><div>2</div><div>$\ell = 1$</div><div>m = ±1</div></div>	<div><div></div><div>2</div><div>$\ell = 1$</div><div>m = 0</div></div>	<div><div></div><div>2</div><div>$\ell = 1$</div><div>m = ±1</div></div>	4 degenerate states at first excited energy level				
-2.18×10^{-18}	<div><div></div><div>n = 1</div><div>$\ell = 0$</div><div>m = 0</div></div>	1 state at ground energy level 1s state described by ψ_{100} or 1s							

II. SHAPES OF H-ATOM WAVEFUNCTIONS: S ORBITALS

THE PHYSICAL INTERPRETATION OF A WAVEFUNCTION

Max Born (German physicist, 1882-1970). The probability of finding a particle (the electron!) in a defined region is proportional to the square of the wavefunction.

$$[\Psi_{n\ell m}(r, \theta, \phi)]^2 = \text{PROBABILITY DENSITY}$$

probability of finding an electron per unit volume at r, θ, ϕ

To consider the shapes of orbitals, let's first rewrite the wavefunction as the product of a radial wavefunction, $R_{n\ell}(r)$, and an angular wavefunction $Y_{\ell m}(\theta, \phi)$

$$\Psi_{n\ell m}(r, \theta, \phi) = \text{_____} \times \text{_____}$$

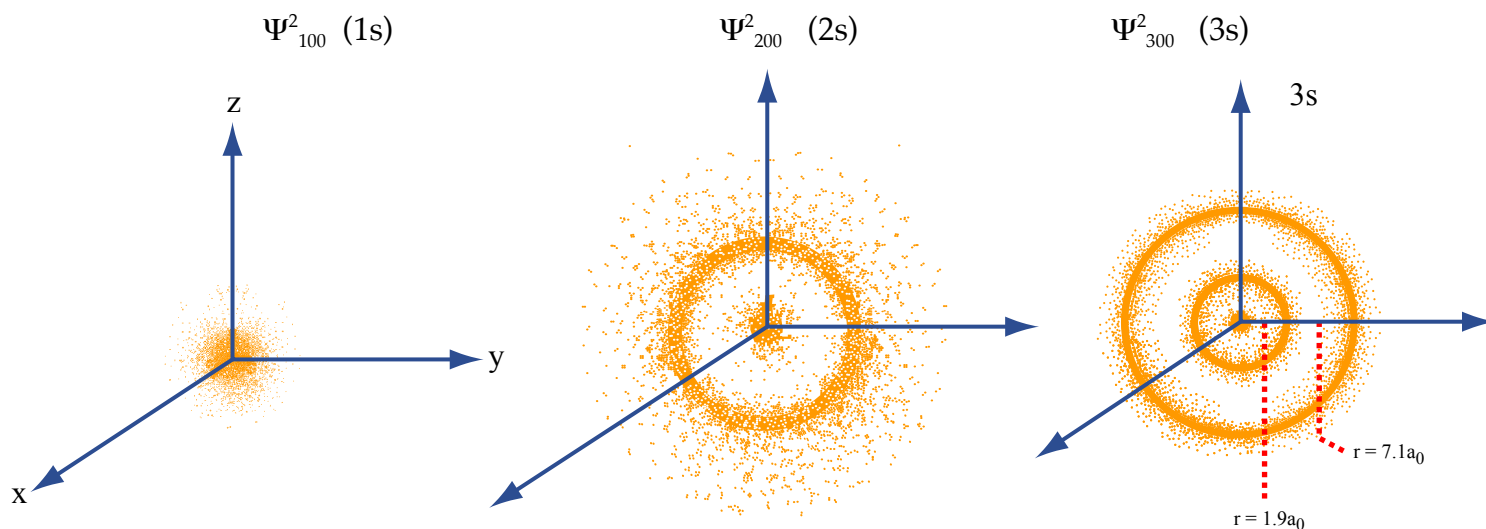
for a ground state H-atom:

$$\Psi_{100}(r, \theta, \phi) = \underbrace{\frac{2e^{-r/a_0}}{a_0^{3/2}}}_{R(r)} \times \underbrace{\left(\frac{1}{4\pi}\right)^{1/2}}_{Y(\theta, \phi)} = \frac{e^{-r/a_0}}{(\pi a_0^3)^{1/2}}$$

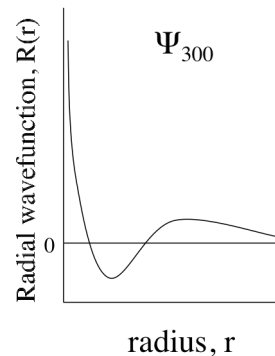
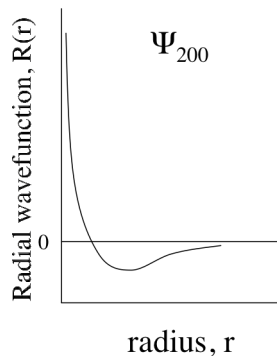
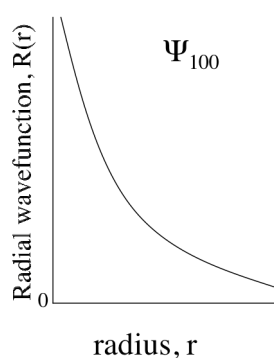
where $a_0 = \text{_____}$ (a constant) = 52.9 pm

- For all s orbitals (1s, 2s, 3s, etc.), the angular wavefunction, Y , is a _____.
- s-orbitals are **spherically symmetrical** – independent of _____ and _____.

Probability density plot of s orbitals: density of dots represent probability density



Figures by MIT OpenCourseWare.



NODE: A value for r , θ , or ϕ for which Ψ (and Ψ^2) = _____. In general, an orbital has $n - 1$ nodes.

RADIAL NODE: A value for _____ for which Ψ (and Ψ^2) = 0. In other words, a radial node is a distance from the radius for which there is no probability of finding an electron.

In general, an orbital has $n - 1 - l$ radial nodes.

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

2s: _____ - _____ - _____ = _____ radial nodes

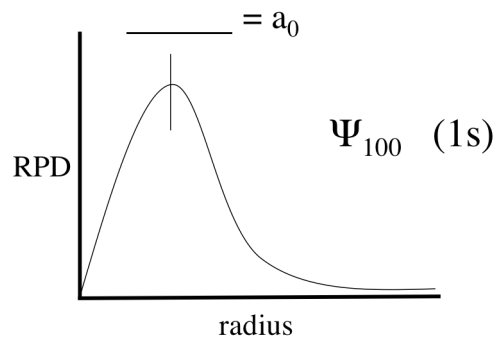
3s: _____ - _____ - _____ = _____ radial nodes

III. RADIAL PROBABILITY DISTRIBUTION

Probability of finding an electron in a spherical shell of thickness dr at a distance r from origin.

Radial Probability Distribution (for s orbitals ONLY) = $4\pi r^2 \Psi^2 dr$

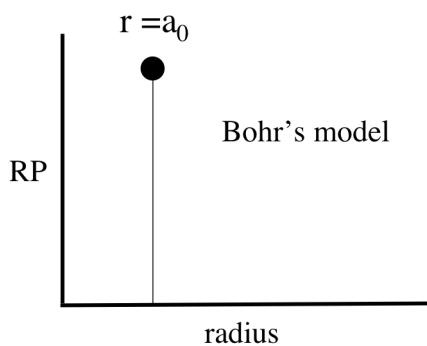
We can plot the radial probability distribution as a function of radius.
Radial probability distribution for a hydrogen 1s orbital:



Maximum probability or most probable value of r is denoted r_{mp} .

$$r_{mp} \text{ for a 1s H atom} = a_0 = 0.529 \times 10^{-10} \text{ m} = 0.529 \text{ \AA} \quad a_0 \equiv \text{BOHR radius}$$

1913 Niels Bohr (Danish scientist) predicted quantized levels for H atom prior to

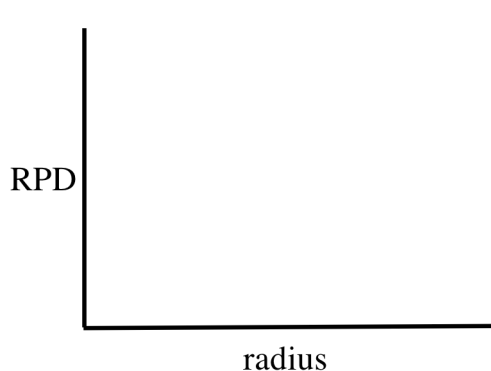


QM development, with the electron in well-defined circular orbits.

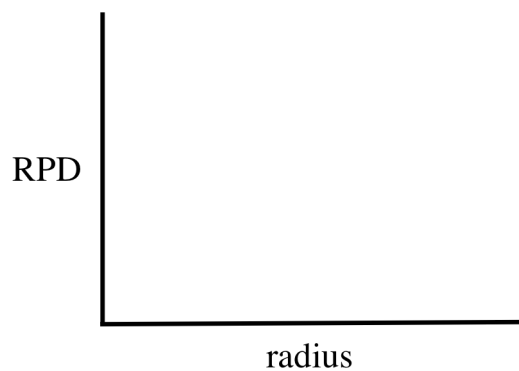
This was still a purely particle picture of the e^- .

But, an electron does not have well-defined orbits! The best we can do is to find the probability of finding e^- at some position r .

Knowing only probability is one of main consequences of Quantum Mechanics. Unlike CM, QM is non-deterministic. The uncertainty principle forbids us from knowing r exactly.



Ψ_{200} (2s)



Ψ_{300} (3s)

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