

## **Lesson Overview**

# **Quantum Mechanics**

**Objective:** The student will be able to define the wave nature of matter and how this definition lead to the location of electrons in an electronic cloud.

### **Lesson Outline:**

**I. The Wave Behavior of Matter**

**II. Quantum Mechanics & Atomic Orbitals**

**III. Representations of Orbitals**

**IV. Quantum Numbers**

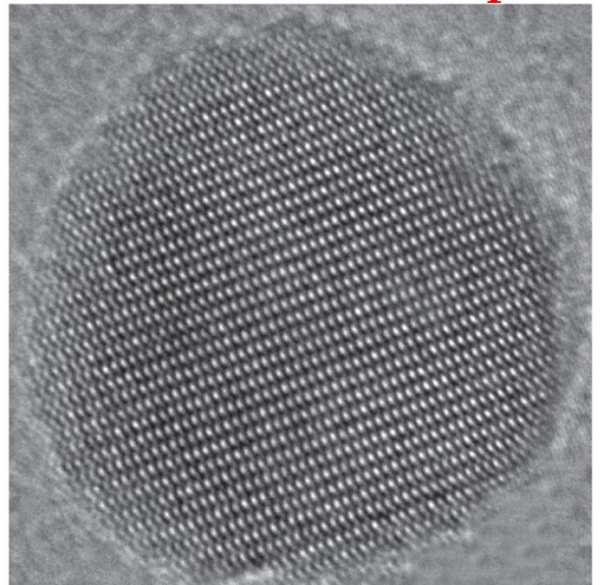
# The Wave Behavior of Matter

Louis de Broglie: Wave-Particle Duality

$$\lambda = \frac{h}{mv}$$

His ideas were confirmed a few years later with experiments in X-ray diffraction.

Electron Microscope



# The Heisenberg Uncertainty Principle

The dual nature of matter places a fundamental limitation on how precisely one can know the location and momentum simultaneously.

$$\Delta x \cdot \Delta m \geq \frac{h}{4\pi}$$

Only important when we look at incredibly small matter (subatomic level)



## Uncertainty Principle Illustration

Calculate the uncertainty in the position,  
given the following:

$$\Delta x \cdot \Delta m \geq \frac{h}{4\pi}$$

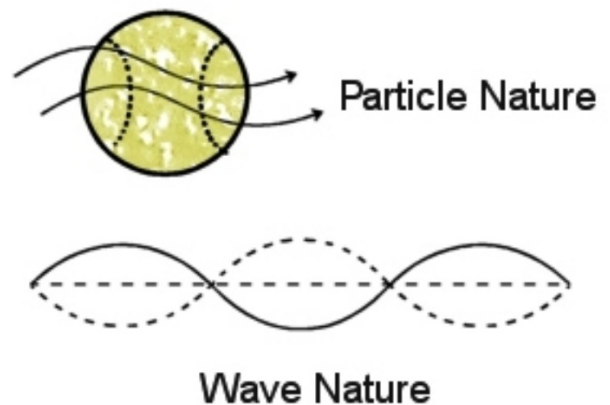
mass of  $e^-$ :  $9.11 \times 10^{-31}$  kg

avg. speed of  $e^-$  in H atom:  $5 \times 10^6$  m/s (with 1% uncertainty)

## Significance of de Broglie & Heisenberg

*"De Broglie's hypothesis and Heisenberg's uncertainty principle set the stage for a new and more broadly applicable theory of atomic structure."*

- Brown, Lemay, Bursten (12 edition)

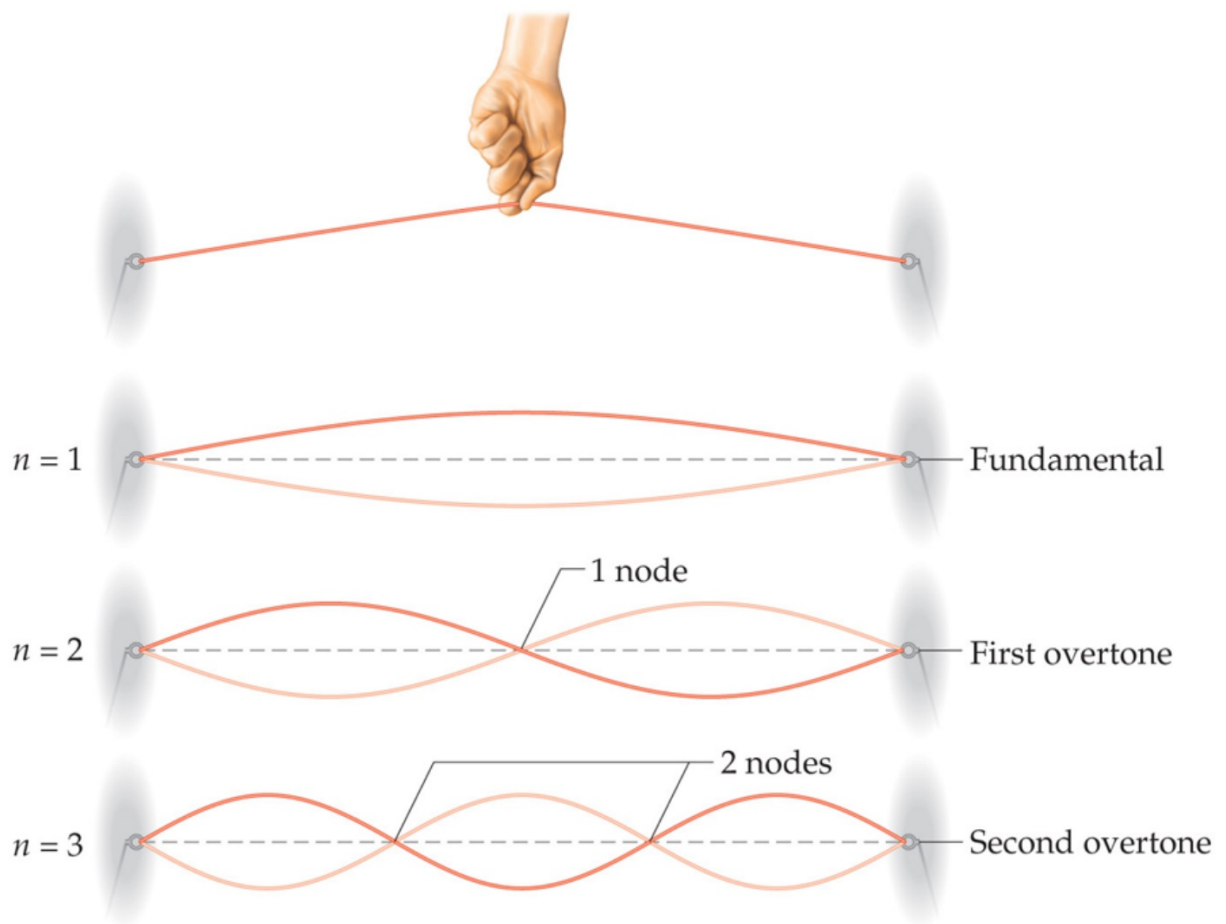


# Quantum Mechanics & Atomic Orbitals

## - Schrödinger and Equation

$$\frac{\delta^2\psi}{\delta x^2} + \frac{\delta^2\psi}{\delta y^2} + \frac{\delta^2\psi}{\delta z^2} + \frac{8\pi^2m}{h^2} (E - V)\psi = 0$$

- incorporates both the wave-like and particle-like behaviors of the electron.
- treated the electron in Hydrogen as a plucked guitar string.



**An electron is like a plucked guitar string.**

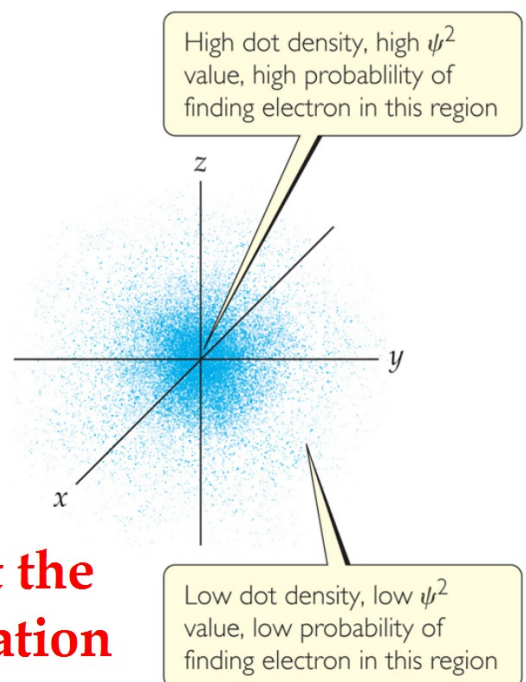


# The Schrödinger Equation

Solving the equation leads to a series of mathematical functions called wave functions that describe the electron in the atom.

The actual solution of the value  $\psi$  has no significance, it is the square of the wave function,  $\psi^2$ , that has meaning.

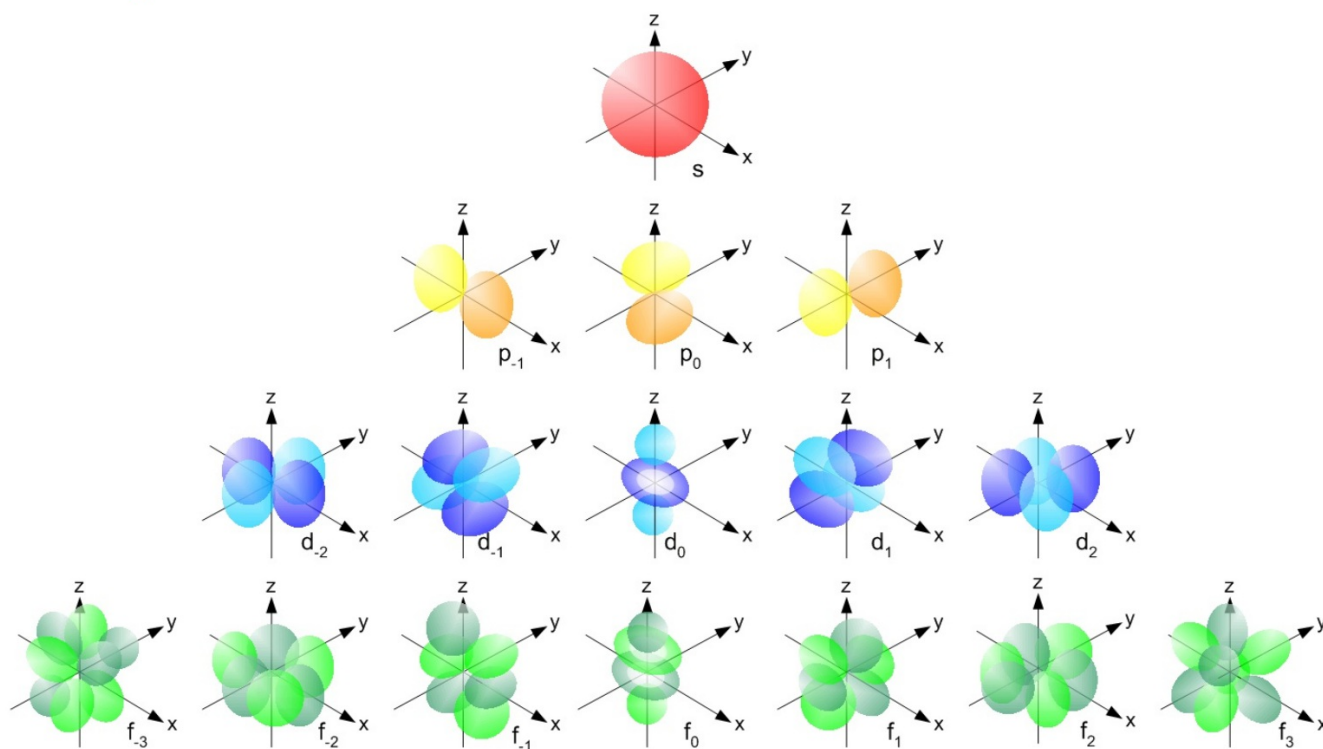
$\psi^2$  represents the probability that the electron will be found in that location



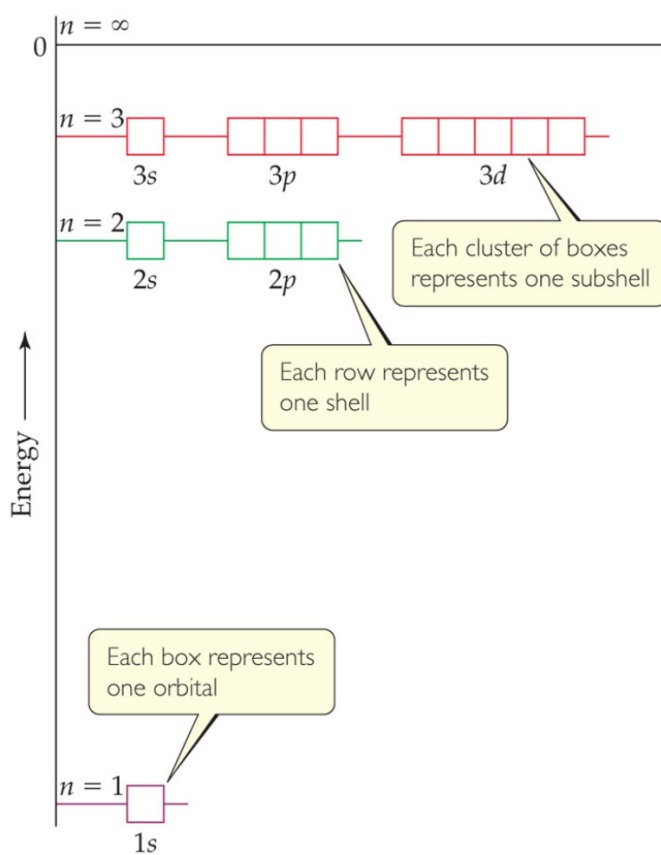


# Orbitals and their Shapes

The solution to Schrödinger's equation for the hydrogen atom yields a set of wave functions called orbitals.



# Orbital Diagrams

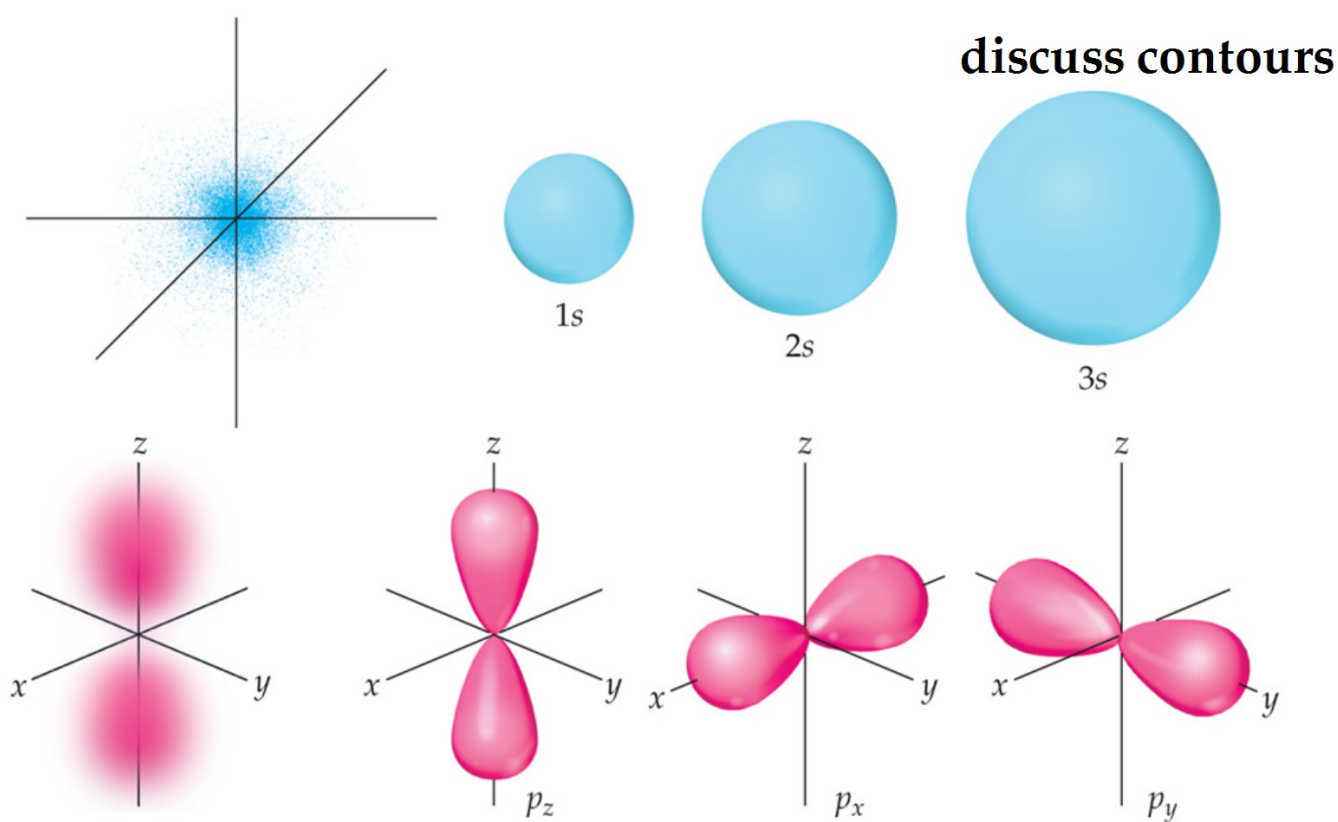


$n = 1$  shell has one orbital

$n = 2$  shell has two subshells composed of four orbitals

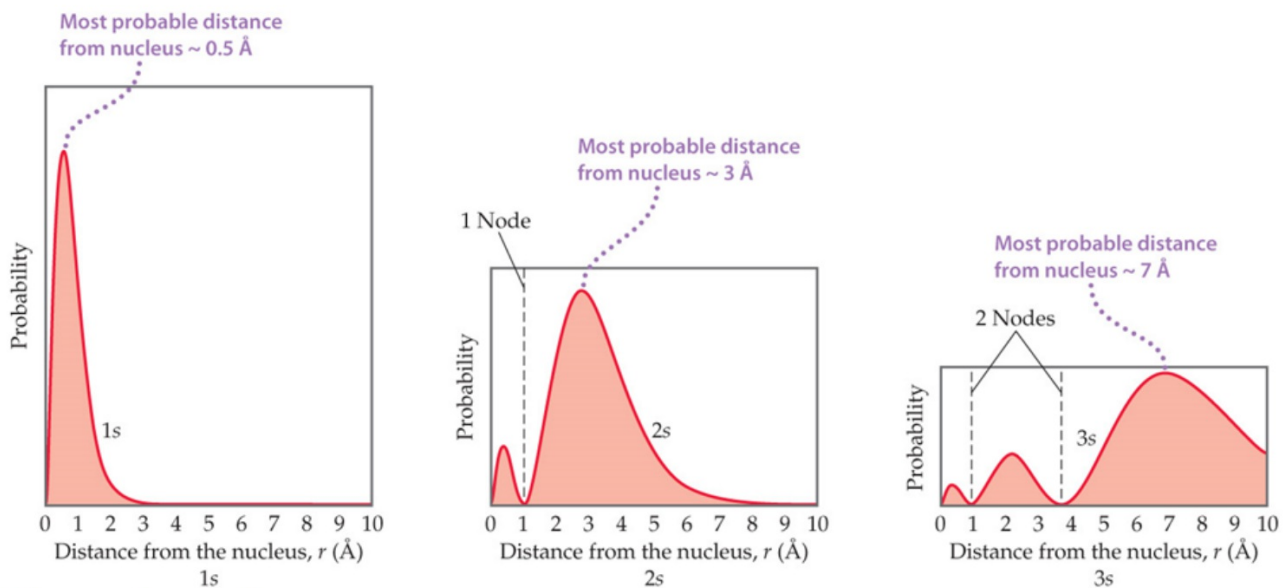
$n = 3$  shell has three subshells composed of nine orbitals

# Representations of Orbitals



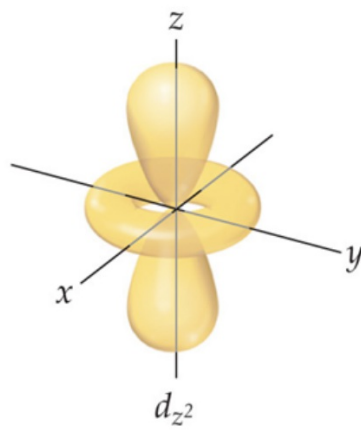
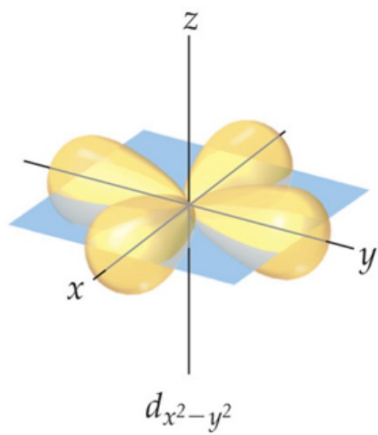
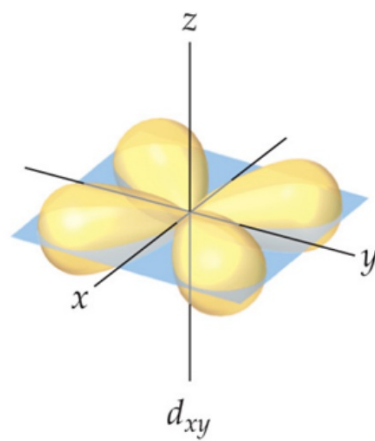
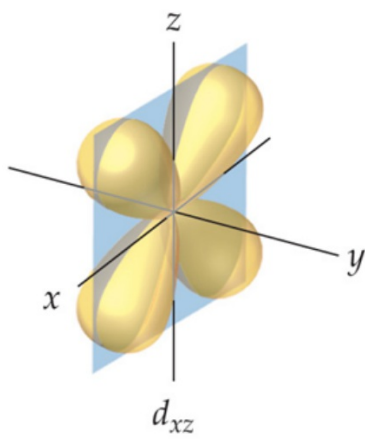
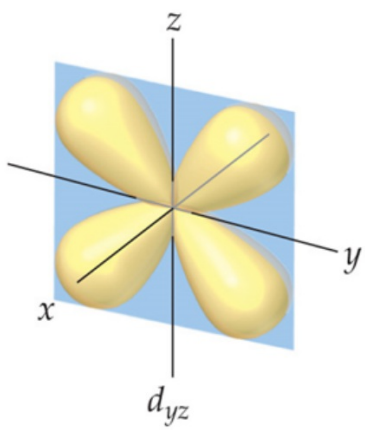
How do these orbitals change based on the energy level?

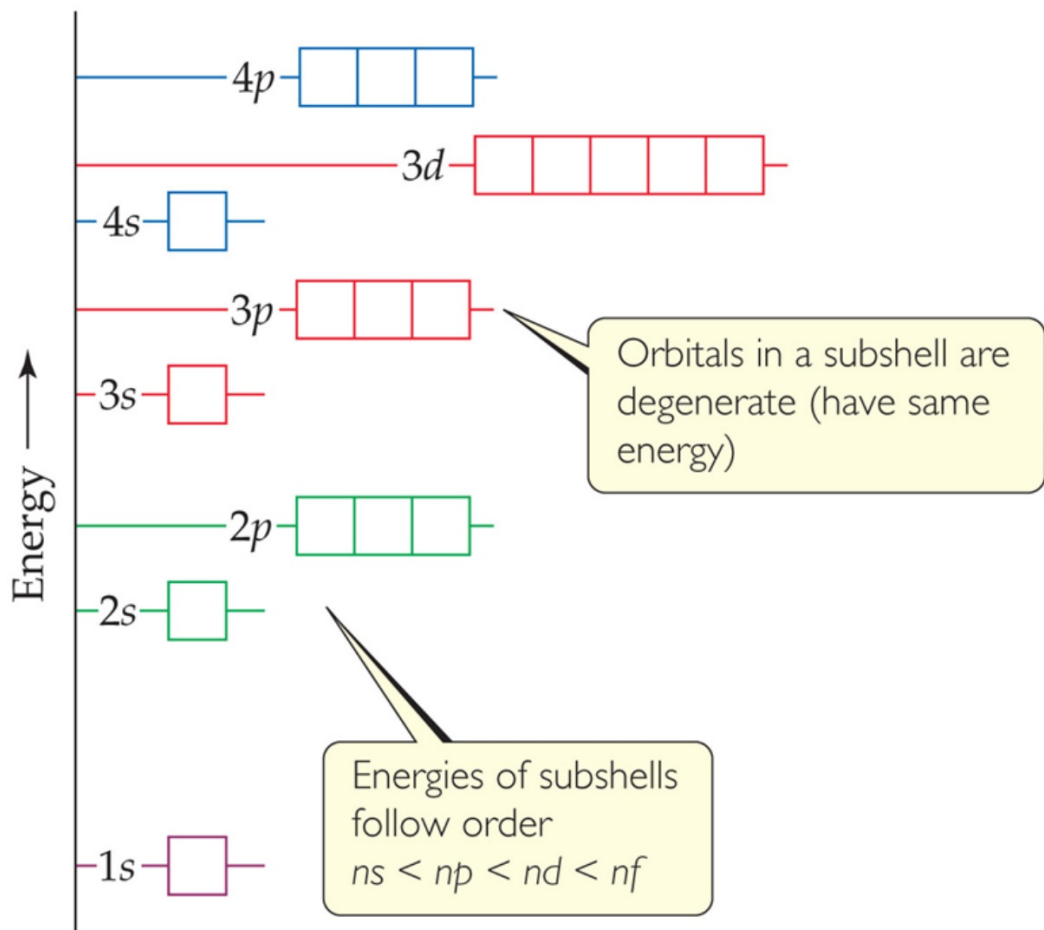
# Radial Probability (function) Density



## Three trends:

1. The # of peaks increases with increasing "n", the outermost peak being larger than the inner ones.
2. The # of nodes increases with increasing "n".
3. The electron density becomes more spread out with increasing "n".



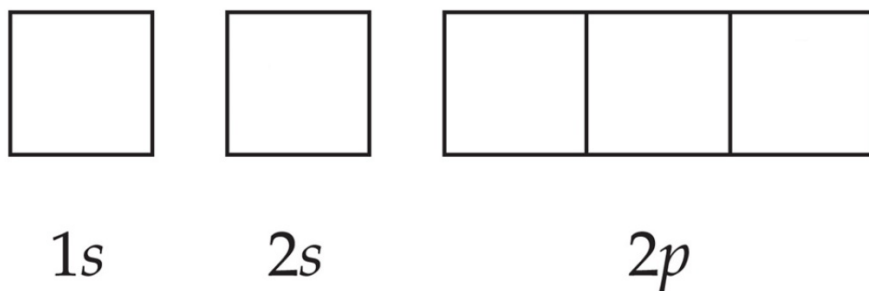


## Rules for Filling Orbital Diagrams

Aufbau Principal: Electrons occupy the **lowest energy level** possible (are as close to the nucleus as possible)

Hund's Rule: Electrons will occupy each orbital with the same spin (direction) before occupying an orbital with the opposite spin (direction)

Pauli Exclusion Principal: No two electrons can have the same quantum number. (They must be traveling in opposite directions if they are in the same orbital.)





# Quantum Numbers

## Summary of Quantum Numbers of Electrons in Atoms

Name	Symbol	Permitted Values	Property
principal	$n$	positive integers(1,2,3,...)	orbital energy (size)
angular momentum	$l$	integers from 0 to $n-1$	orbital shape (The $l$ values 0, 1, 2, and 3 correspond to s, p, d, and f orbitals, respectively.)
magnetic	$m_l$	integers from $-l$ to 0 to $+l$	orbital orientation
spin	$m_s$	$+1/2$ or $-1/2$	direction of $e^-$ spin

# Example 1

What is the set of quantum numbers for the last electron in a neutral carbon atom?

B = Solids    Hg = Liquids    Kr = Gases    Pm = Not found in nature

1 H 1.00794																	2 He 4.002602
3 Li 6.941	4 Be 9.012182											5 B 10.811	6 C 12.0107	7 N 14.006424	8 O 15.9994	9 F 18.9984032	10 Ne 20.1797
11 Na 22.98976928	12 Mg 24.30466											13 Al 26.9815385	14 Si 28.0855	15 P 30.973761	16 S 32.059	17 Cl 35.4527	18 Ar 39.948
19 K 39.0983	20 Ca 40.078	21 Sc 44.955912	22 Ti 47.867	23 V 50.9415	24 Cr 51.9961	25 Mn 54.938049	26 Fe 55.845	27 Co 58.933200	28 Ni 58.6934	29 Cu 63.545	30 Zn 65.39	31 Ga 69.723	32 Ge 72.61	33 As 74.92160	34 Se 78.96	35 Br 79.904	36 Kr 83.80
37 Rb 85.4678	38 Sr 87.62	39 Y 88.90585	40 Zr 91.224	41 Nb 92.90638	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 106.42	46 Pd 106.3605	47 Ag 107.8682	48 Cd 112.411	49 In 114.818	50 Sn 118.710	51 Sb 121.760	52 Te 127.60	53 I 126.90447	54 Xe 131.29
55 Cs 132.90545	56 Ba 137.327	71 Lu 174.967	72 Hf 178.49	73 Ta 180.9479	74 W 183.84	75 Re 186.207	76 Os 190.23	77 Ir 192.222	78 Pt 195.078	79 Au 196.96655	80 Hg 200.59	81 Tl 204.3833	82 Pb 207.2	83 Bi 208.98038	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226)	103 Lr (262)	104 Rf (261)	105 Db (262)	106 Sg (263)	107 Bh (262)	108 Hs (265)	109 Mt (266)	110 Ds (269)	111 Rg (272)	112 Cn (277)	113 Uut (277)	114 Uuq (277)	115 Uup (277)	116 Uuh (277)	118 Uuo (277)	
57 La 138.9055	58 Ce 140.116	59 Pr 140.90765	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.964	64 Gd 157.25	65 Tb 158.92534	66 Dy 162.50	67 Ho 164.93032	68 Er 167.26	69 Tm 168.93421	70 Yb 173.04				
89 Ac 227.0381	90 Th 232.0381	91 Pa 231.03608	92 U 238.0289	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (258)				

## Example 2

What is the set of quantum numbers for the last electron in **arsenic**?

*Note: save time. Only draw the sublevel where the electron exists.*

B = Solids    Hg = Liquids    Kr = Gases    Pm = Not found in nature

1 H 1.00794	2 He 4.002602											13 Al 13.00335	14 Si 12.2107	15 P 14.00642	16 S 15.9994	17 Cl 16.0045	18 Ar 19.9984																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
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Uuq 294	173 Uub 294	174 Uuh 294	175 Uuo 294	176 Uuq 294	177 Uub 294	178 Uuh 294	179 Uuo 294	180 Uuq 294	181 Uub 294	182 Uuh 294	183 Uuo 294	184 Uuq 294	185 Uub 294	186 Uuh 294	187 Uuo 294	188 Uuq 294	189 Uub 294	190 Uuh 294	191 Uuo 294	192 Uuq 294	193 Uub 294	194 Uuh 294	195 Uuo 294	196 Uuq 294	197 Uub 294	198 Uuh 294	199 Uuo 294	200 Uuq 294	201 Uub 294	202 Uuh 294	203 Uuo 294	204 Uuq 294	205 Uub 294	206 Uuh 294	207 Uuo 294	208 Uuq 294	209 Uub 294	210 Uuh 294	211 Uuo 294	212 Uuq 294	213 Uub 294	214 Uuh 294	215 Uuo 294	216 Uuq 294	217 Uub 294	218 Uuh 294	219 Uuo 294	220 Uuq 294	221 Uub 294	222 Uuh 294	223 Uuo 294	224 Uuq 294	225 Uub 294	226 Uuh 294	227 Uuo 294	228 Uuq 294	229 Uub 294	230 Uuh 294	231 Uuo 294	232 Uuq 294	233 Uub 294	234 Uuh 294	235 Uuo 294	236 Uuq 294	237 Uub 294	238 Uuh 294	239 Uuo 294	240 Uuq 294	241 Uub 294	242 Uuh 294	243 Uuo 294	244 Uuq 294	245 Uub 294	246 Uuh 294	247 Uuo 294	248 Uuq 294	249 Uub 294	250 Uuh 294	251 Uuo 294	252 Uuq 294	253 Uub 294	254 Uuh 294	255 Uuo 294	256 Uuq 294	257 Uub 294	258 Uuh 294	259 Uuo 294	260 Uuq 294	261 Uub 294	262 Uuh 294	263 Uuo 294	264 Uuq 294	265 Uub 294	266 Uuh 294	267 Uuo 294	268 Uuq 294	269 Uub 294	270 Uuh 294	271 Uuo 294	272 Uuq 294	273 Uub 294	274 Uuh 294	275 Uuo 294	276 Uuq 294	277 Uub 294	278 Uuh 294	279 Uuo 294	280 Uuq 294	281 Uub 294	282 Uuh 294	283 Uuo 294	284 Uuq 294	285 Uub 294	286 Uuh 294	287 Uuo 294	288 Uuq 294	289 Uub 294	290 Uuh 294	291 Uuo 294	292 Uuq 294	293 Uub 294	294 Uuh 294	295 Uuo 294	296 Uuq 294	297 Uub 294	298 Uuh 294	299 Uuo 294	300 Uuq 294	301 Uub 294	302 Uuh 294	303 Uuo 294	304 Uuq 294	305 Uub 294	306 Uuh 294	307 Uuo 294	308 Uuq 294	309 Uub 294	310 Uuh 294	311 Uuo 294	312 Uuq 294	313 Uub 294	314 Uuh 294	315 Uuo 294	316 Uuq 294	317 Uub 294	318 Uuh 294	319 Uuo 294	320 Uuq 294	321 Uub 294	322 Uuh 294	323 Uuo 294	324 Uuq 294	325 Uub 294	326 Uuh 294	327 Uuo 294	328 Uuq 294	329 Uub 294	330 Uuh 294	331 Uuo 294	332 Uuq 294	333 Uub 294	334 Uuh 294	335 Uuo 294	336 Uuq 294	337 Uub 294	338 Uuh 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294	422 Uuh 294	423 Uuo 294	424 Uuq 294	425 Uub 294	426 Uuh 294	427 Uuo 294	428 Uuq 294	429 Uub 294	430 Uuh 294	431 Uuo 294	432 Uuq 294	433 Uub 294	434 Uuh 294	435 Uuo 294	436 Uuq 294	437 Uub 294	438 Uuh 294	439 Uuo 294	440 Uuq 294	441 Uub 294	442 Uuh 294	443 Uuo 294	444 Uuq 294	445 Uub 294	446 Uuh 294	447 Uuo 294	448 Uuq 294	449 Uub 294	450 Uuh 294	451 Uuo 294	452 Uuq 294	453 Uub 294	454 Uuh 294	455 Uuo 294	456 Uuq 294	457 Uub 294	458 Uuh 294	459 Uuo 294	460 Uuq 294	461 Uub 294	462 Uuh 294	463 Uuo 294	464 Uuq 294	465 Uub 294	466 Uuh 294	467 Uuo 294	468 Uuq 294	469 Uub 294	470 Uuh 294	471 Uuo 294	472 Uuq 294	473 Uub 294	474 Uuh 294	475 Uuo 294	476 Uuq 294	477 Uub 294	478 Uuh 294	479 Uuo 294	480 Uuq 294	481 Uub 294	482 Uuh 294	483 Uuo 294	484 Uuq 294	485 Uub 294	486 Uuh 294	487 Uuo 294	488 Uuq 294	489 Uub 294	490 Uuh 294	491 Uuo 294	492 Uuq 294	493 Uub 294	494 Uuh 294	495 Uuo 294	496 Uuq 294	497 Uub 294	498 Uuh 294	499 Uuo 294	500 Uuq 294	501 Uub 294	502 Uuh 294	503 Uuo 294	504 Uuq 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