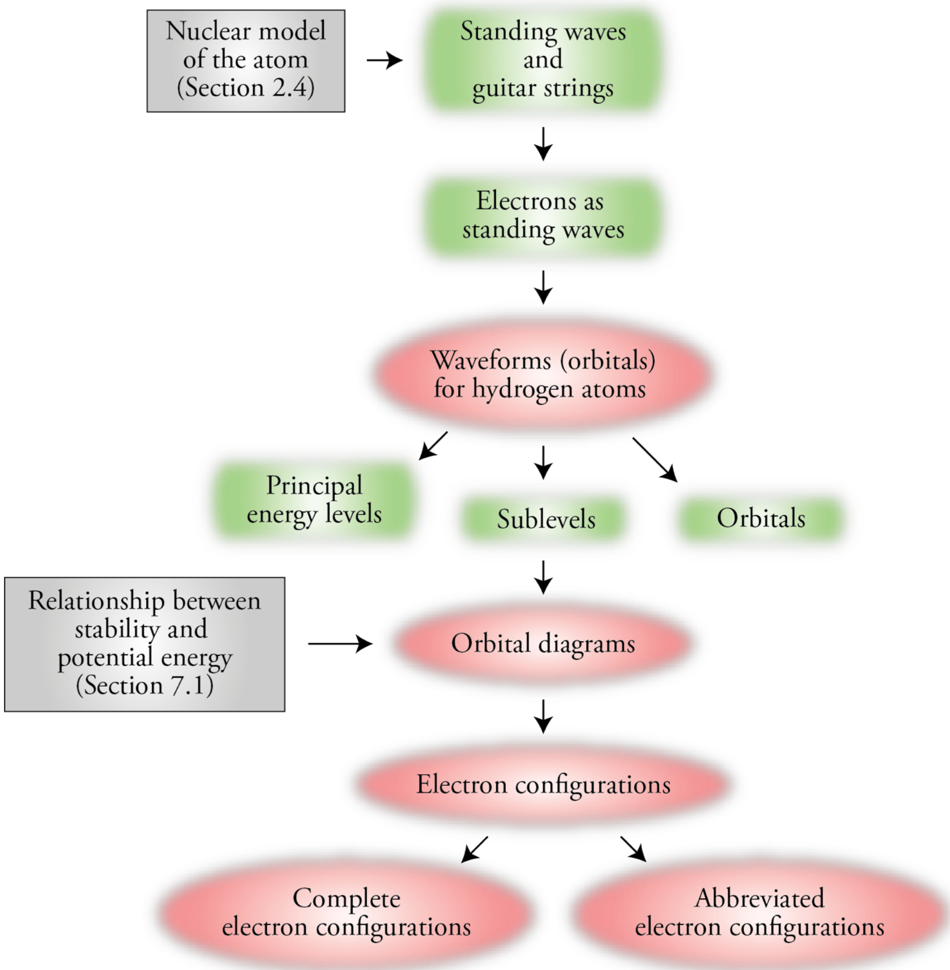
Chapter 11
Modern Atomic Theory

An Introduction to Chemistry
by Mark Bishop

Chapter Map



Nuclear model of the atom (Section 2.4)
Standing waves and guitar strings
Electrons as standing waves
Waveforms (orbitals) for hydrogen atoms
Principal energy levels
Sublevels
Orbitals
Relationship between stability and potential energy (Section 7.1)
Orbital diagrams
Electron configurations
Complete electron configurations
Abbreviated electron configurations

Atomic Theory

- *To see a World in a Grain of Sand*
  And a Heaven in a Wild Flower
  Hold Infinity in the palm of your hand
  And Eternity in an hour
  William Blake   Auguries of Innocence
- *Thus, the task is not so much to see what no one has yet seen, but to think what nobody has yet thought, about that which everybody sees.*
  Erwin Schrodinger

Particle and Wave Nature

- All matter has both particle and wave character.
- The less massive the particle, the more important its wave character.
- The electron has a very low mass, low enough to have significant wave character.

A Problem

- **Problem:** We have a barrier to our understanding, and things with significant wave character are to some degree outside that barrier. This means that the behavior of electrons is non-intuitive.

How We Solve the Problem

- One way we have been able to “describe” things outside our barrier of understanding is through mathematics.
- We describe things outside our barrier of understanding with mathematical equations, we solve the equations, we drag the results back under our barrier, and we apply them to things we do understand.
- If this helps us explain things or predict things, we assume we are on the right track.

Strangeness of Tiny Particles

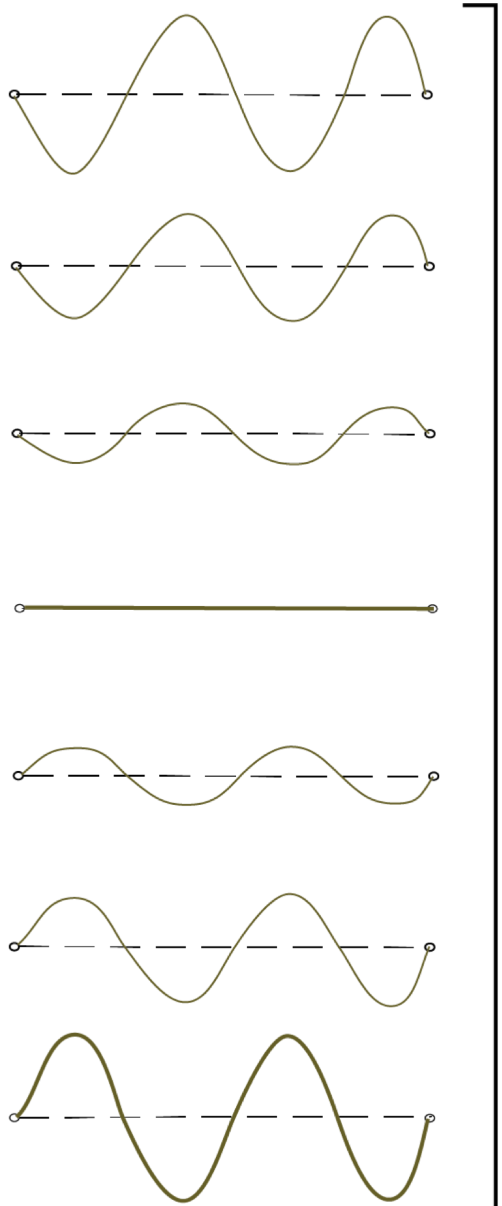
- Things become very strange in the realm of the very, very small.
- One element of this strangeness is that we lose the possibility of being able to predict with certainty where small particles are going to be and how they are moving.
- Thus we shift from talking about where tiny things will be to where they will probably be.

Ways to deal with Complexity and Uncertainty

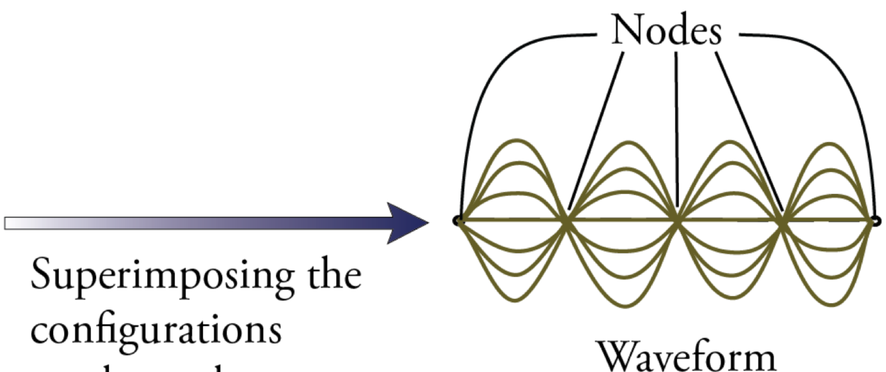
- **Analogies** In order to communicate something of the nature of the electron, scientists often use analogies. For example, in some ways, electrons are *like* vibrating guitar strings.
- **Probabilities** In order to accommodate the uncertainty of the electron's position and motion, we refer to where the electron *probably is* within the atom instead of where it definitely is.

Guitar String Waveform

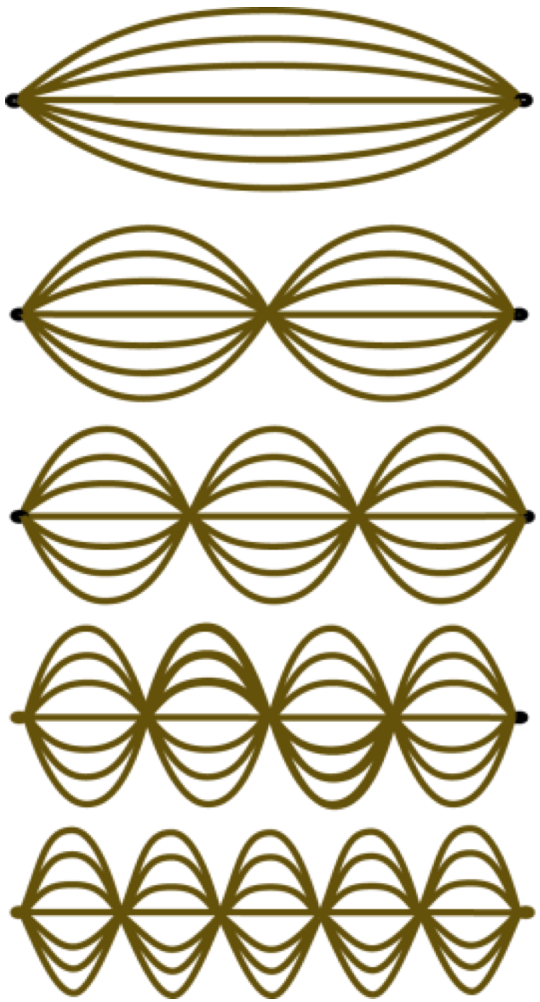
7 possible configurations for the vibration of a guitar string



Superimposing the configurations produces the waveform of the guitar string's standing wave.



Allowed Vibrations for a Guitar String



Equation for Guitar String

$$A_x = A_o \sin \frac{n\pi x}{a}$$

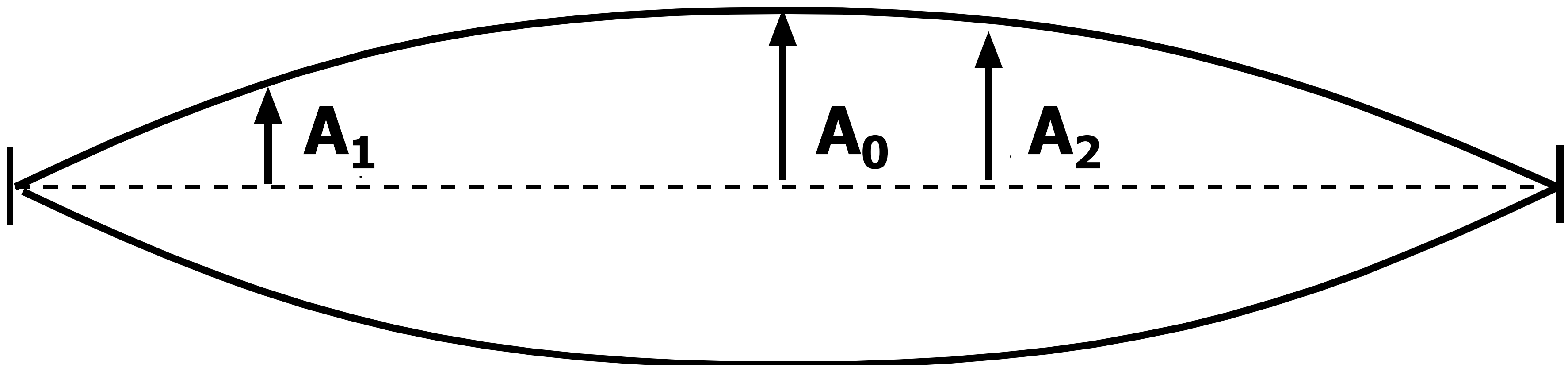
x-axis

0 a

Guitar String

- A_x = the amplitude at position x
- A_o = the maximum amplitude at any point on the string
- n = 1, 2, 3, ...
- x = the position along the string
- a = the total length of the string

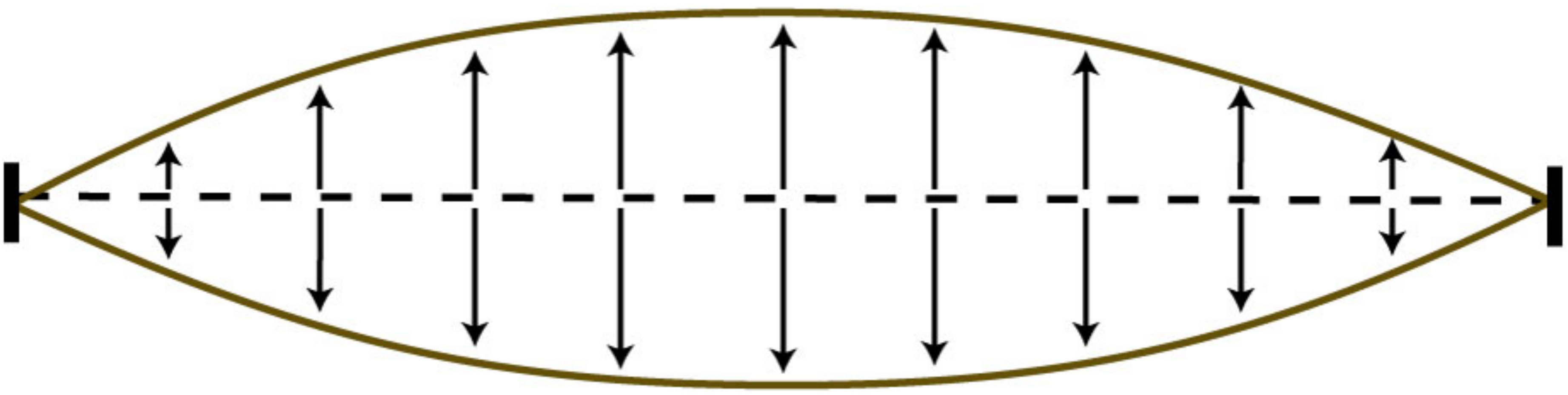
Guitar String Amplitudes



Guitar String Waveform 1

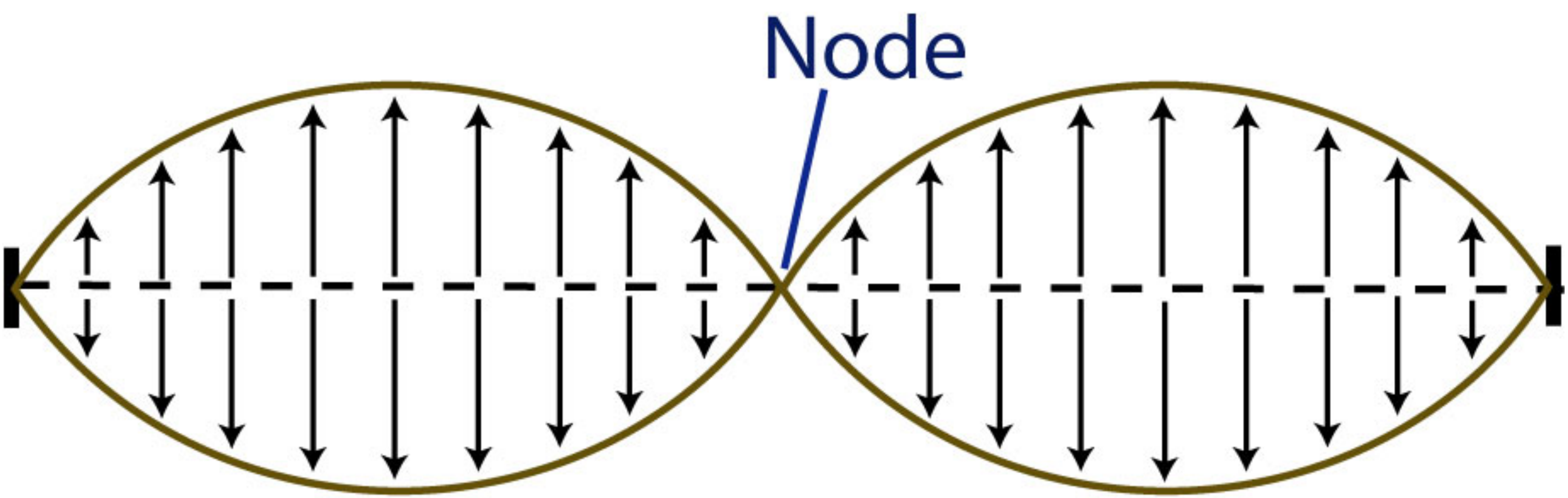
$$A_X = A_O \sin \frac{n\pi x}{a}$$

$$A_X = A_O \sin \frac{\pi x}{a}$$



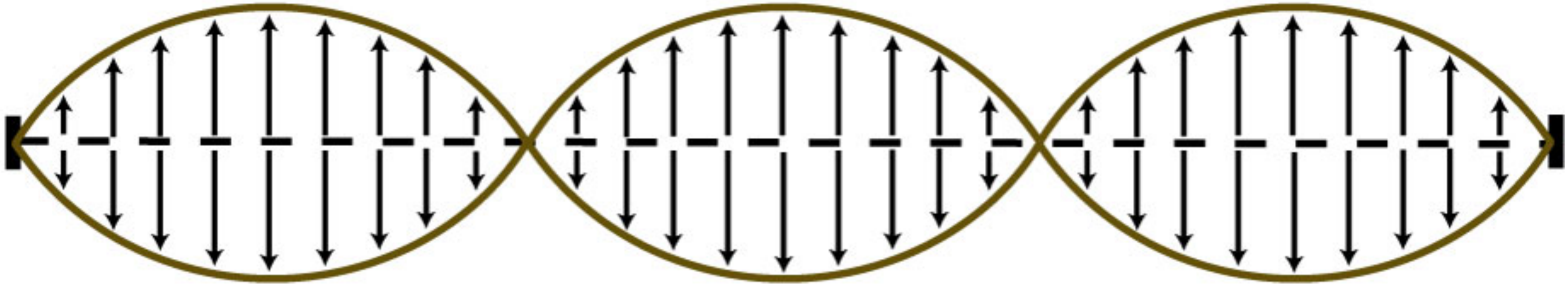
Guitar String Waveform 2

$$A_X = A_O \sin \frac{2\pi x}{a}$$

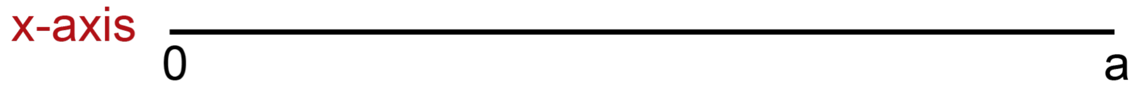


Guitar String Waveform 3

$$A_X = A_O \sin \frac{3\pi x}{a}$$

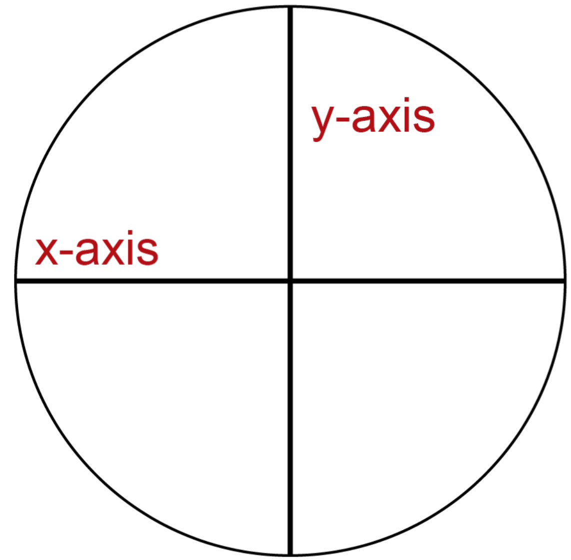


Dimensions

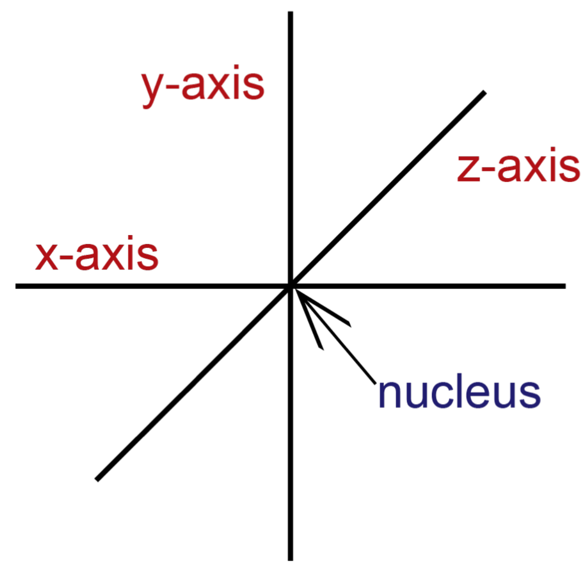


Guitar String

Drumhead



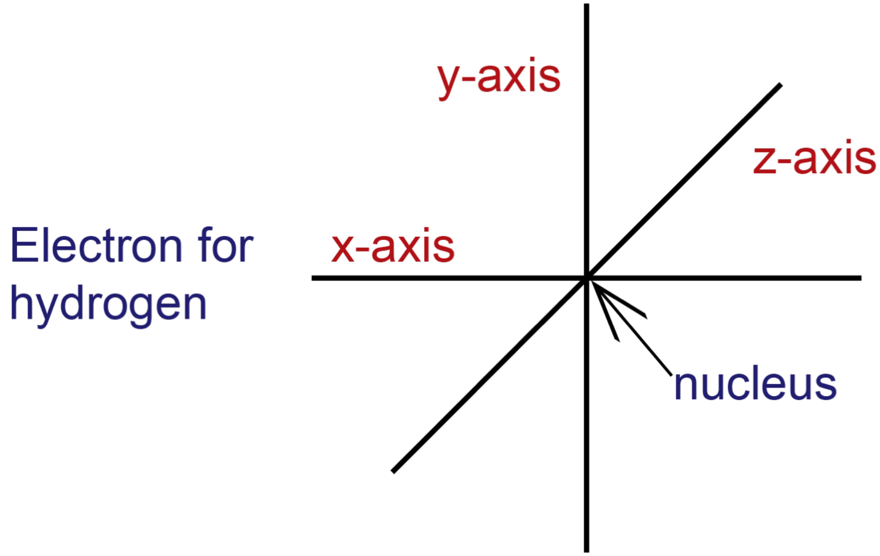
Electron for hydrogen



Determination of the Allowed Electron Waveforms

- **Step 1:** Set up the general form of the wave equation that describes the electron in a hydrogen atom. We call this equation the wave function and the values calculated from the wave equation are represented by Ψ.

$$\Psi_{x,y,z} = f(x,y,z)$$



Determination of the Allowed Electron Waveforms

- **Step 2:** Determine the forms of the general equation that fit the boundary conditions. Each equation has its own set of three quantum numbers. For example,

$\Psi_{1s} = f_{1s}(x,y,z)$ with 1,0,0 for quantum numbers

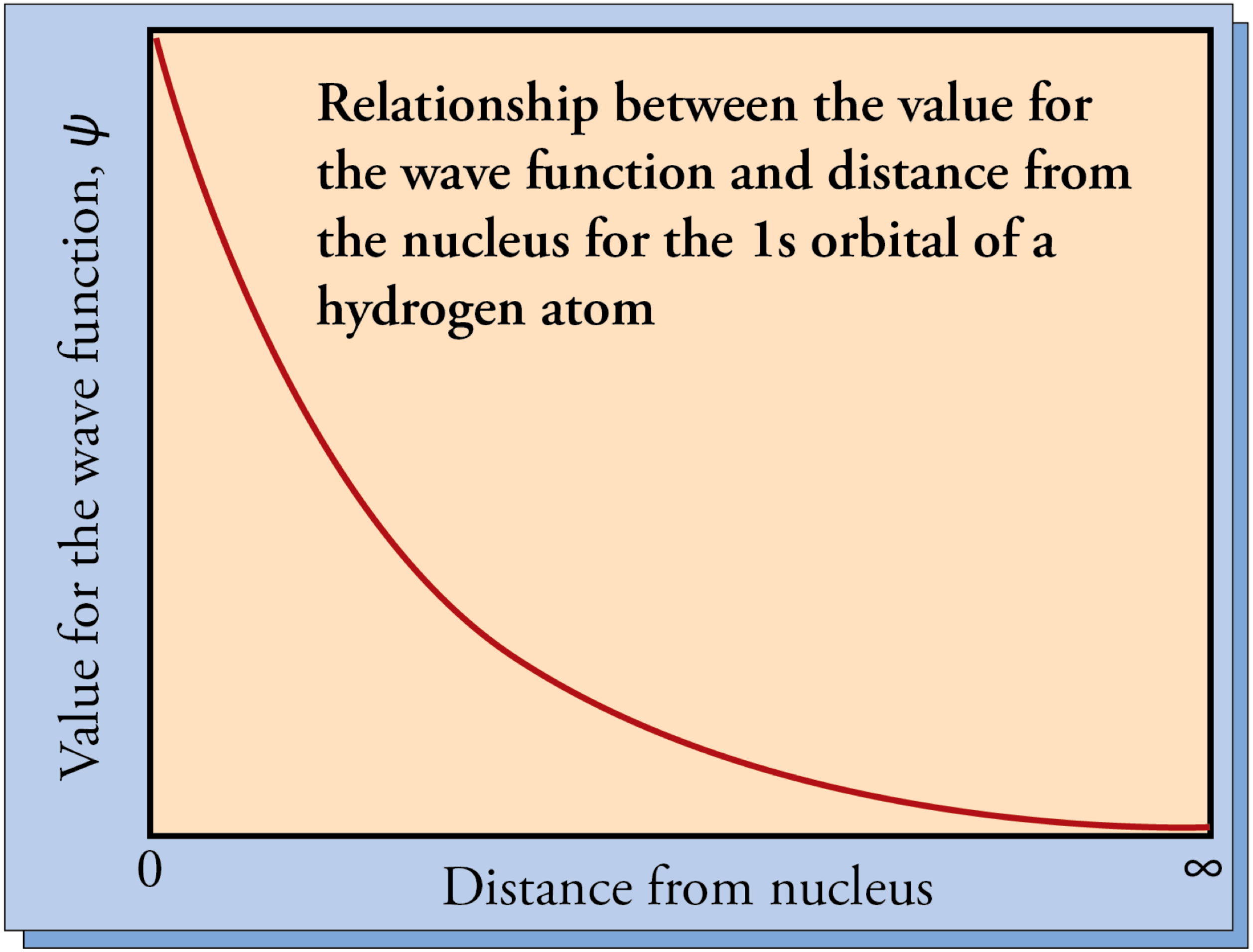
$\Psi_{2s} = f_{2s}(x,y,z)$ with 2,0,0 for quantum numbers

$\Psi_{2p} = f_{2p}(x,y,z)$ with 2,1,1 or 2,1,0 or 2,1,−1 for quantum numbers

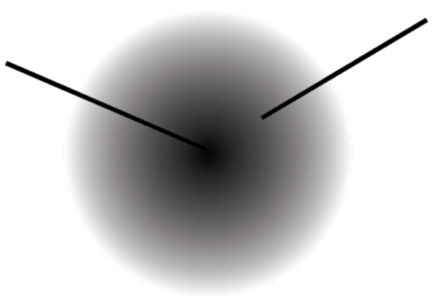
Determination of the Allowed Electron Waveforms (cont.)

- **Step 3:** Use the specific form of the wave equation to do a series of repetitive calculations to get values for many different positions outside the nucleus. Each position is represented in the equation by different x, y, and z coordinates.
- **Step 4:** We ask our computer to summarize the values calculated in two ways.

Graph for the 1,0,0 Equation



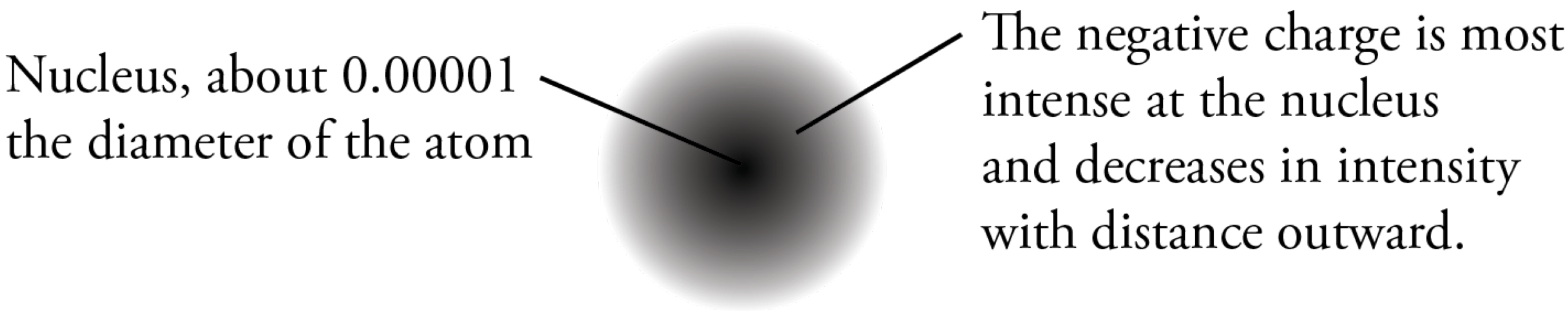
Waveform for 1*s* Electron (1,0,0)



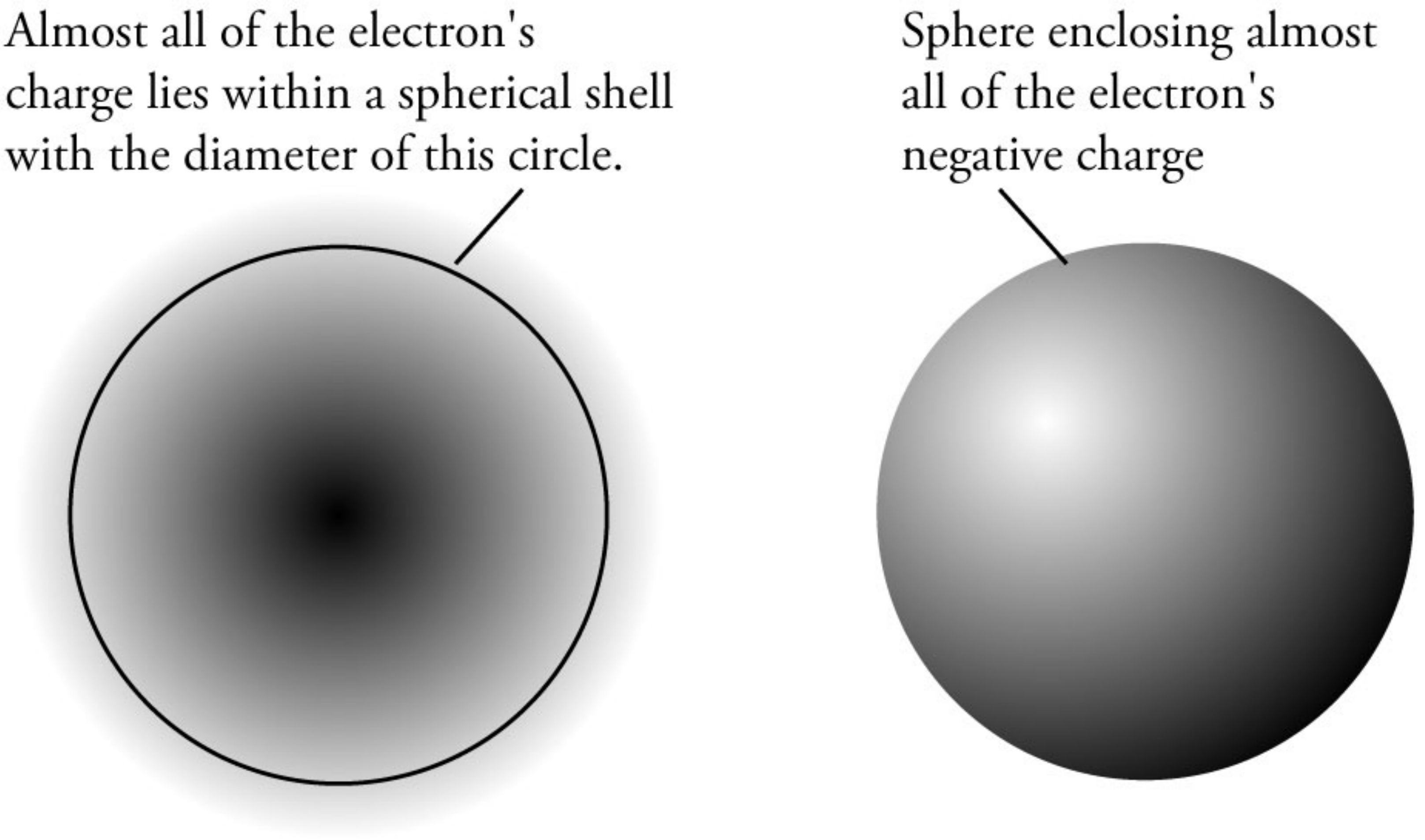
Particle Interpretation of 1*s* Orbital

A multiple exposure picture of the electron in a 1*s* orbital of a hydrogen atom might look like this.

“Just give up approach”



1*s* Orbital

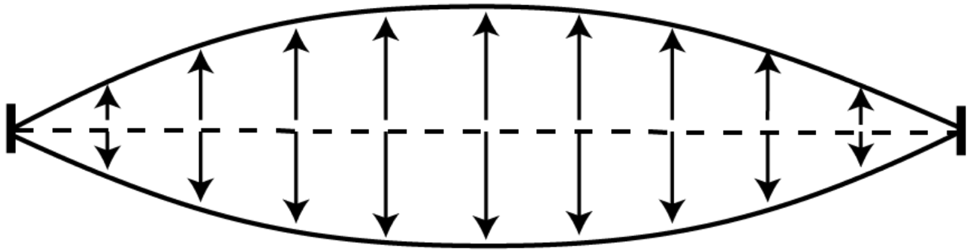

Almost all of the electron's charge lies within a spherical shell with the diameter of this circle.
Sphere enclosing almost all of the electron's negative charge

Wave Character of the Electron

- Just as the intensity of the movement of a guitar string can vary along the length of the string, so can the intensity of the negative charge of the electron vary at different positions outside the nucleus.
- We can calculate these variations by using a one-dimensional wave equation for the guitar string and a three-dimensional wave equation for the electron.

Guitar and Electron Waveforms

- The calculated variation in the intensity of the movement of the guitar string and the calculated variation in the intensity of the electron charge can be described in terms of three-dimensional standing waves.



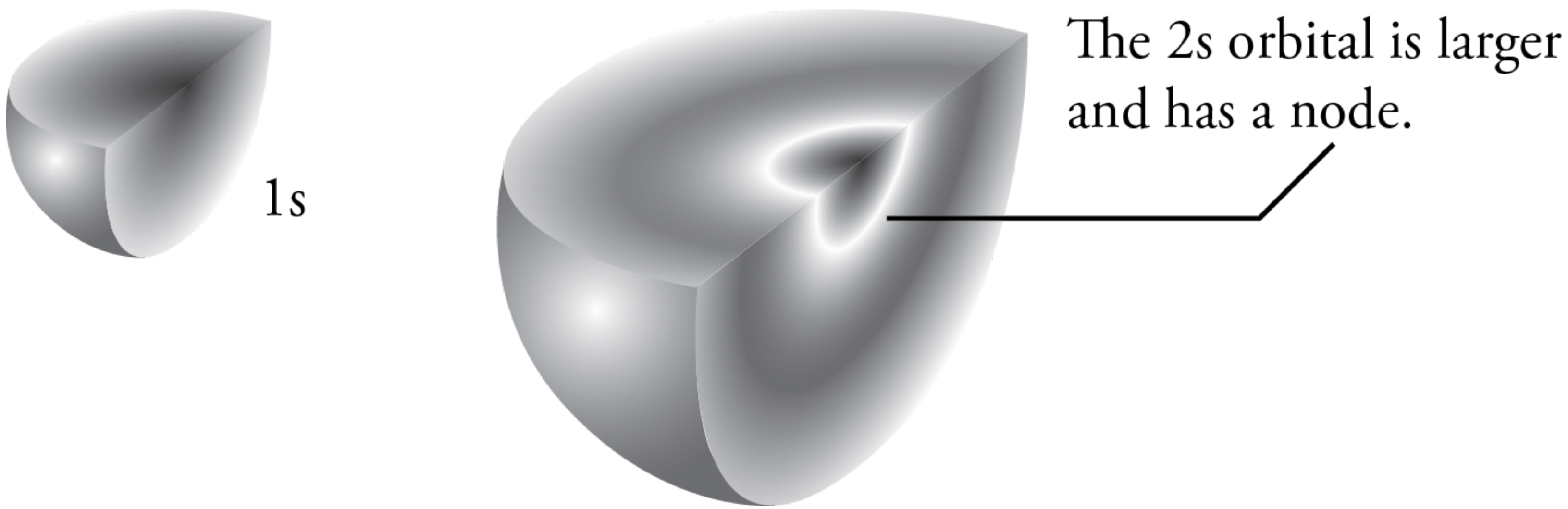
Simplest waveform for guitar string

Simplest waveform for electron 1s orbital

Wave Character of the Electron

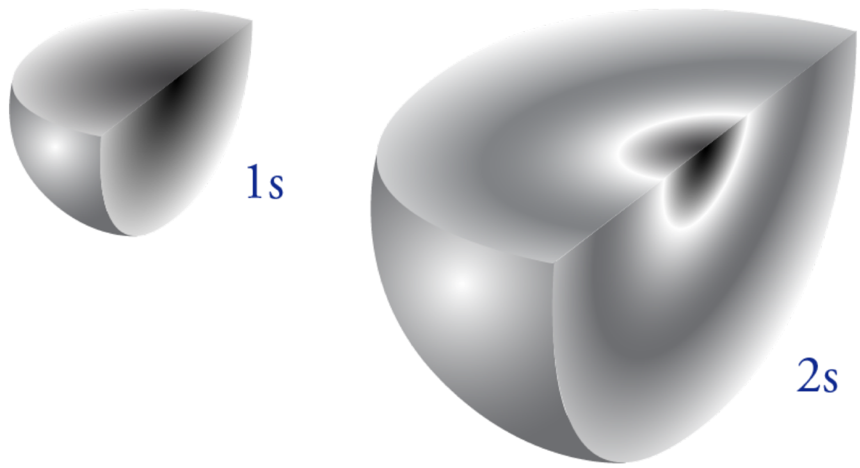
- Although both the electron and the guitar string can have an infinite number of possible waveforms, only certain waveforms are possible.
- We can focus our attention on the waveforms of varying motion of the guitar string or the varying electron charge intensity without having to think about the actual physical nature of the string or electron.

Cutaway of 1*s* and 2*s* (2,0,0) Orbitals



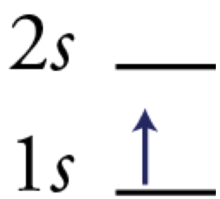
An electron in 2s is less stable and higher PE than an electron in 1s

- Electron in 2s is a greater average distance from the positive nucleus than an electron in the 1s.
- 2s electron less attracted.
- 2s electron is less stable (more likely to change).
- 2s electron is higher potential energy.
- The one electron of hydrogen is more likely to be in the smaller, more stable, and lower PE 1s orbital where it is most strongly attracted to the nucleus.

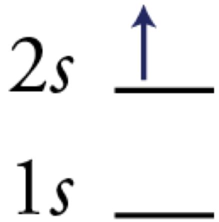


Ground State and Excited State

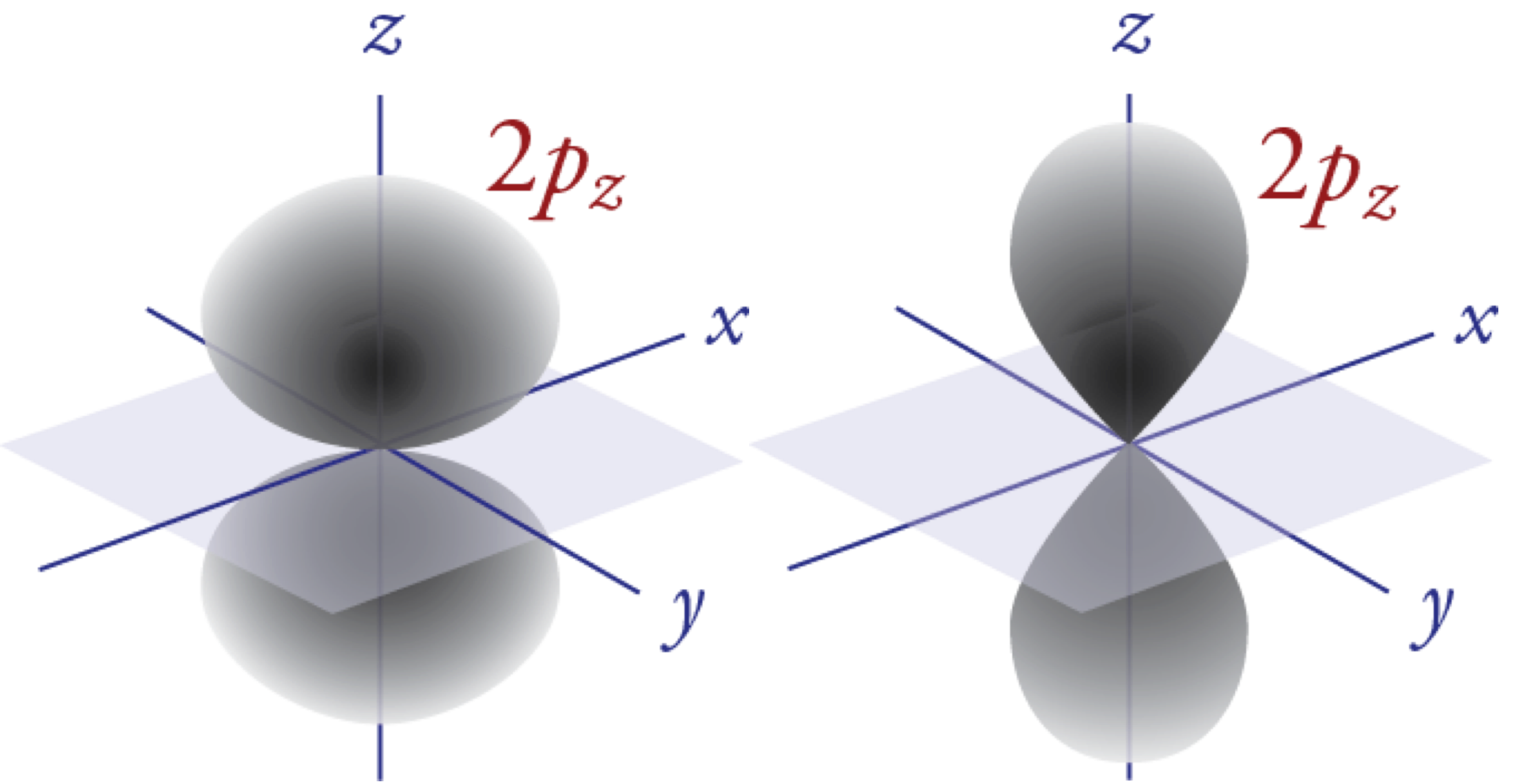
- Hydrogen atoms with their electron in the 1*s* orbital are said to be in their ***ground state***.



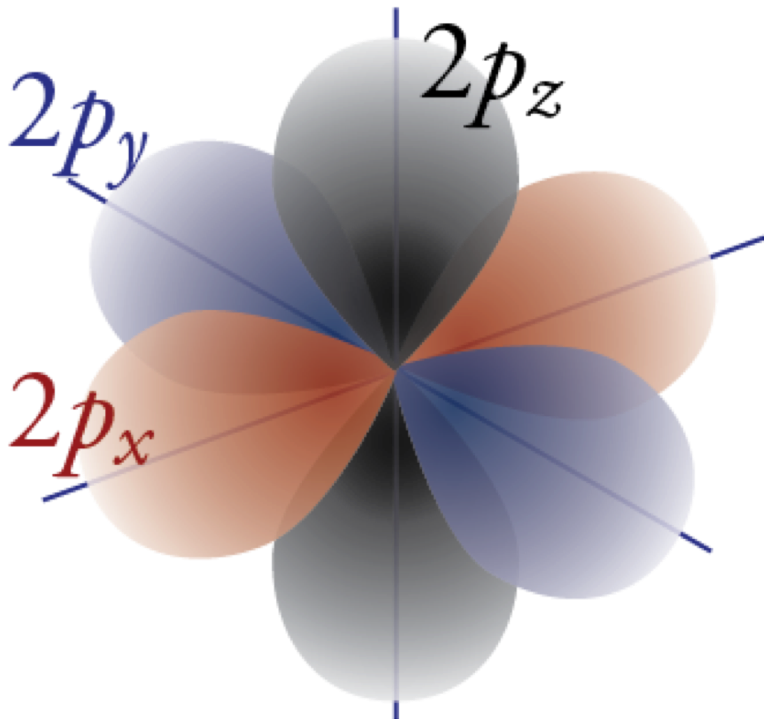
- A hydrogen atom with its electron in the 2*s* orbital is in an ***excited state***.



Realistic and Stylized $2p_y$ Orbital (2,1,1)



$2p_x$ (2,1,1), $2p_y$ (2,1,0), and $2p_z$ (2,1,-1) Orbitals



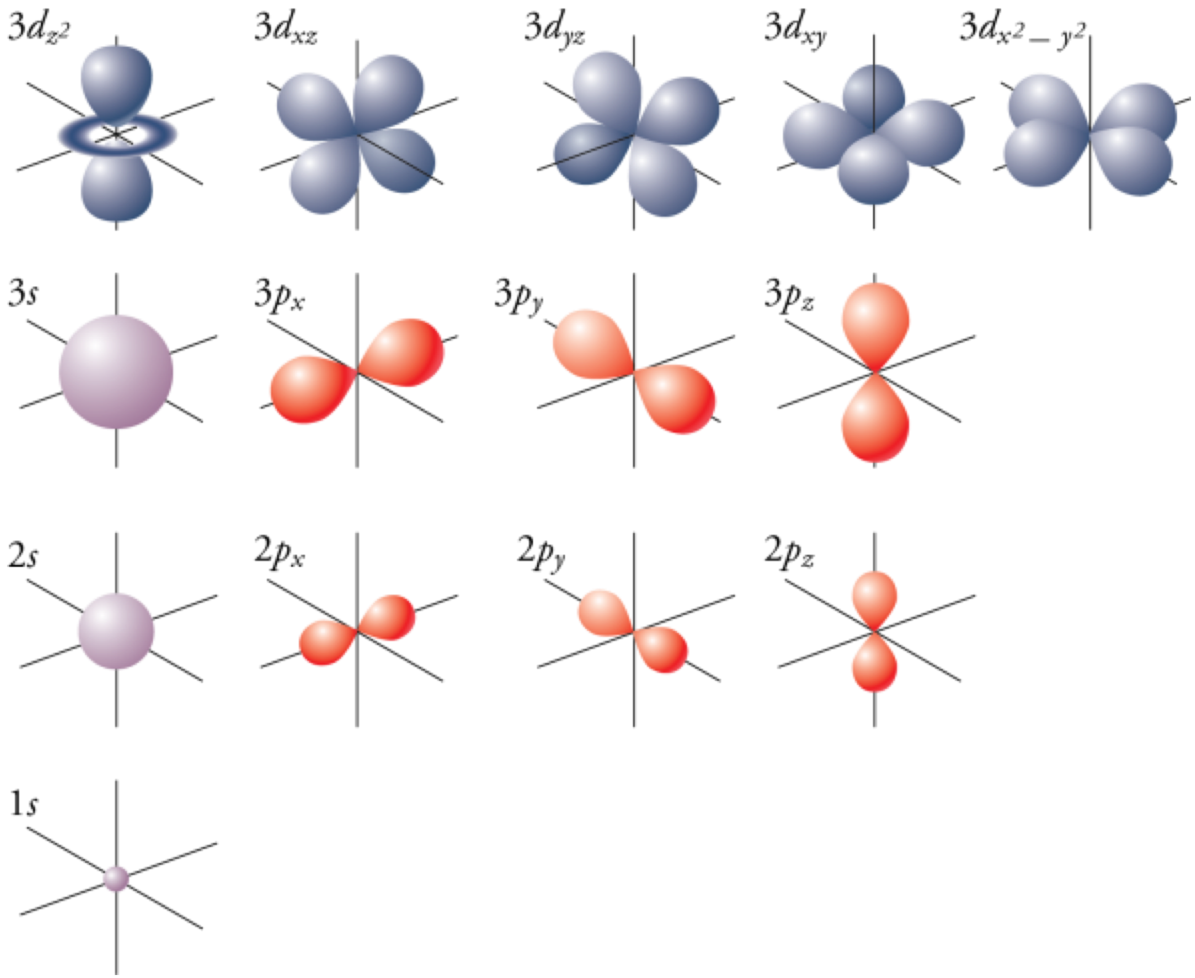
$2s$ ___ $2p$ ___ ___ ___

$1s$ ___

Sublevels

- Orbitals that have the same potential energy, the same size, and the same shape are in the same ***sublevel***.
- The sublevels are sometimes called ***subshells***.

Other Allowed Waveforms



Orbitals for Ground States of Known Elements

7*s* ___   7*p* ___ ___ ___

6*s* ___   6*p* ___ ___ ___   6*d* ___ ___ ___ ___ ___

5*s* ___   5*p* ___ ___ ___   5*d* ___ ___ ___ ___ ___   5*f* ___ ___ ___ ___ ___ ___ ___

4*s* ___   4*p* ___ ___ ___   4*d* ___ ___ ___ ___ ___   4*f* ___ ___ ___ ___ ___ ___ ___

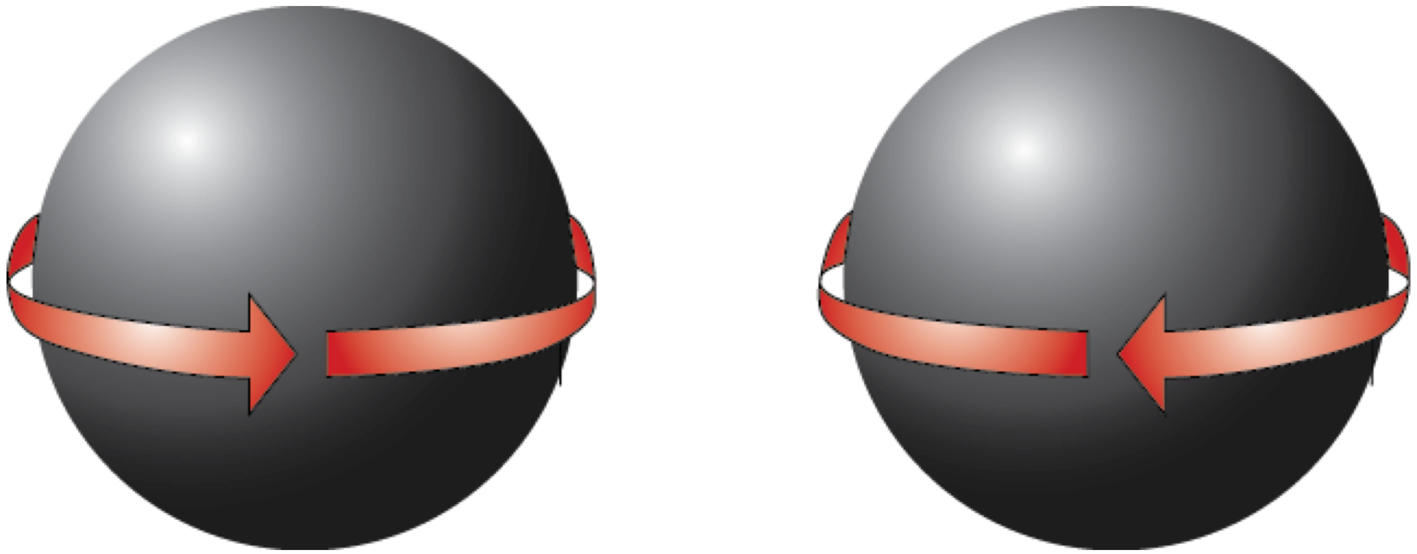
3*s* ___   3*p* ___ ___ ___   3*d* ___ ___ ___ ___ ___

2*s* ___   2*p* ___ ___ ___

1*s* ___

No other orbitals are necessary for describing the electrons of the known elements in their ground states.

Electron Spin

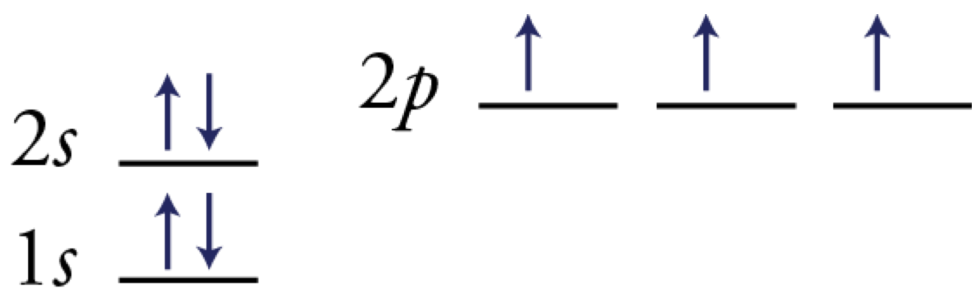


Pauli Exclusion Principle

- No two electrons in an atom can be the same in all ways.
- There are four ways that electrons can be the same:
    - Electrons can be in the same principal energy level.
    - They can be in the same sublevel.
    - They can be in the same orbital.
    - They can have the same spin.

Ways to Describe Electrons in Atoms

- Arrows are added to an ***orbital diagram*** to show the distribution of electrons in the possible orbitals and the relative spin of each electron. The following is an orbital diagram for a nitrogen atom.



- The information in orbital diagrams is often described in a shorthand notation called an ***electron configuration***.

$1s^2\ 2s^2\ 2p^3$

Electron Configurations

- The sublevels are filled in such a way as to yield the lowest overall potential energy for the atom.
- No two electrons in an atom can be the same in all ways. This is one statement of the ***Pauli Exclusion Principle***.
- When electrons are filling orbitals of the same energy, they prefer to enter empty orbitals first, and all electrons in half-filled orbitals have the same spin. This is called ***Hund's Rule***.

Electron Configurations (cont.)

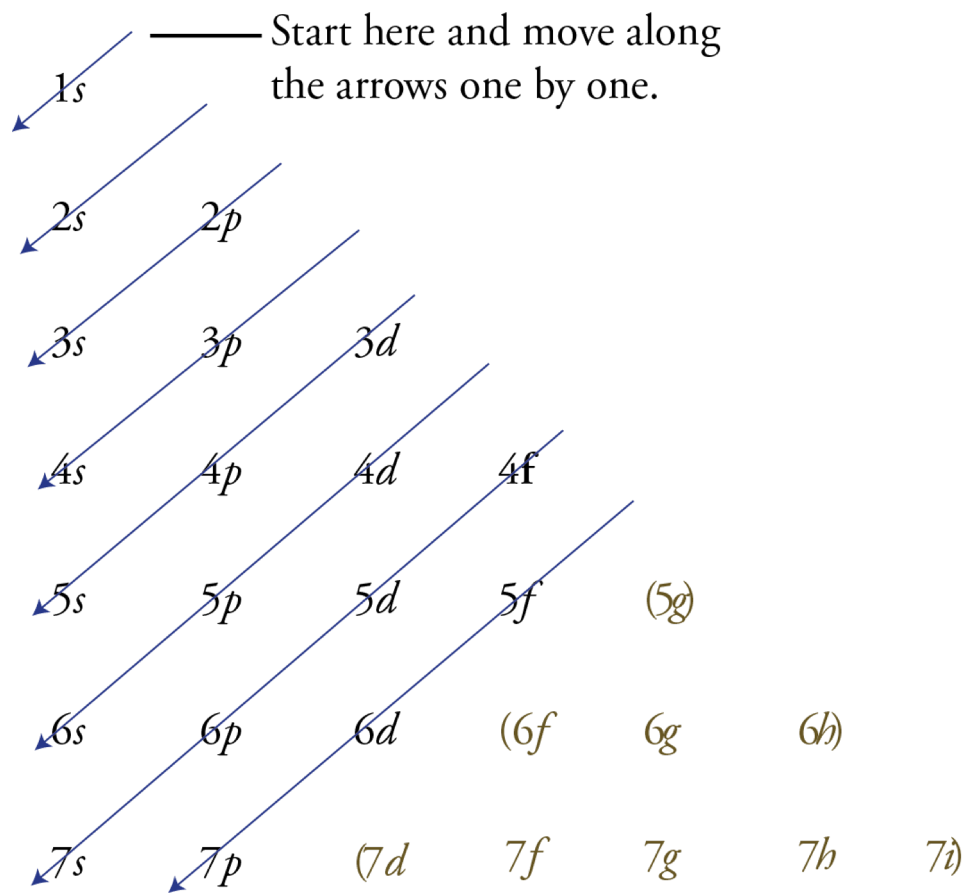
Represents the principal energy level

$1s^2$

Shows the number of electrons in the orbital

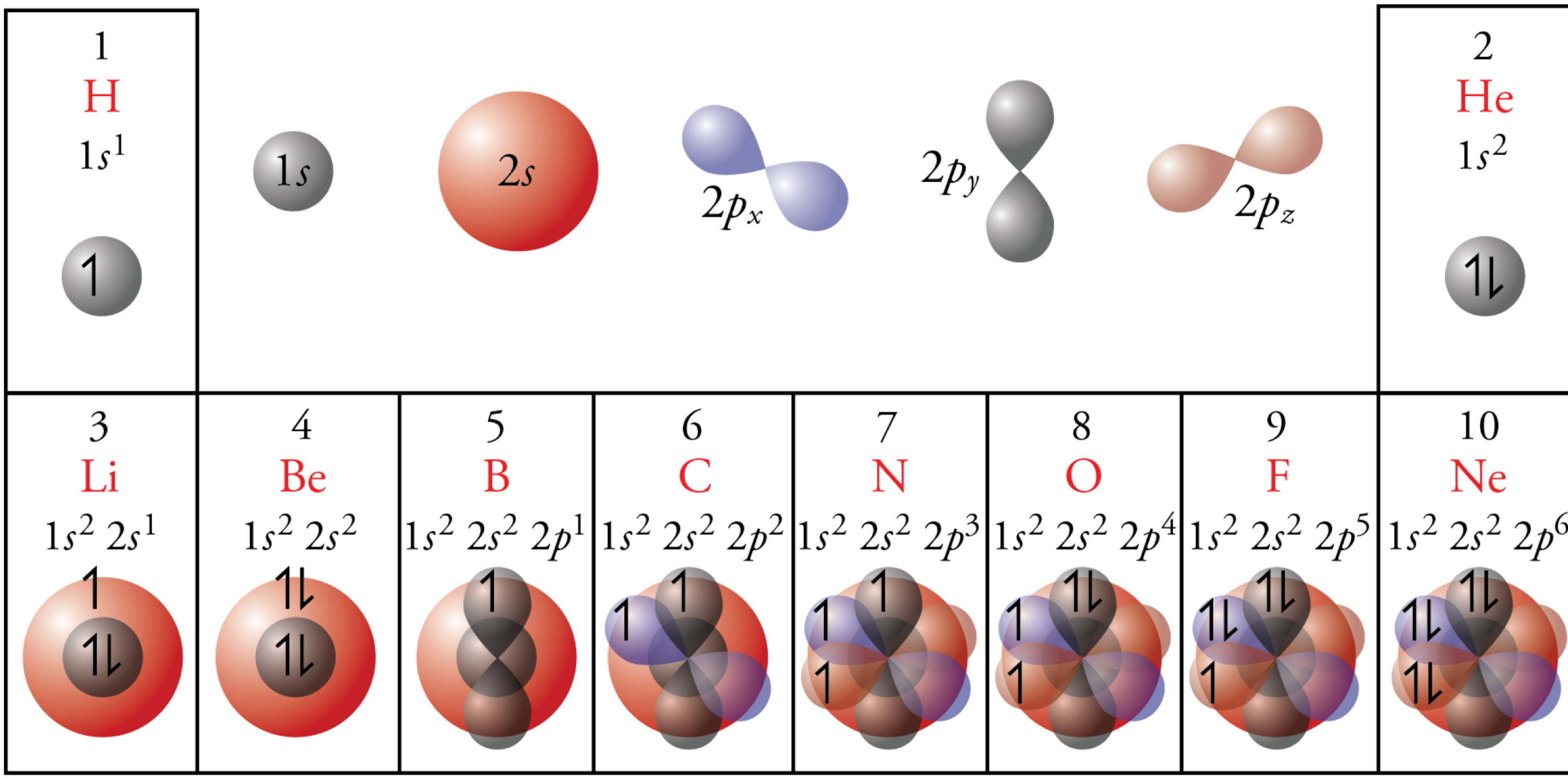
Indicates the shape of the orbital

Order of Orbital Filling



1*s* 2*s* 2*p* 3*s* 3*p* 4*s* 3*d* 4*p* 5*s* 4*d* 5*p* 6*s* 4*f* 5*d* 6*p* 7*s* 5*f* 6*d* 7*p*

Second Period Electron Configurations



Writing Electron Configurations

- Determine the number of electrons in the atom from its atomic number.
- Add electrons to the sublevels in the correct order of filling.
- Add two electrons to each *s* sublevel, 6 to each *p* sublevel, 10 to each *d* sublevel, and 14 to each *f* sublevel.
- To check your complete electron configuration, look to see whether the location of the last electron added corresponds to the element's position on the periodic table.

Order of Filling from the Periodic Table

s block | d block | p block

	1	2		3	4	5	6	7	8	9	10	11	12		13	14	15	16	17	18
	1A	2A		3B	4B	5B	6B	7B	8B	8B	8B	1B	2B		3A	4A	5A	6A	7A	8A
											1s	1								2
2s	3	4												2p	5	6	7	8	9	10
3s	11	12												3p	13	14	15	16	17	18
4s	19	20	3d	21	22	23	24	25	26	27	28	29	30	4p	31	32	33	34	35	36
5s	37	38	4d	39	40	41	42	43	44	45	46	47	48	5p	49	50	51	52	53	54
6s	55	56	5d	71	72	73	74	75	76	77	78	79	80	6p	81	82	83	84	85	86
7s	87	88	6d	103	104	105	106	107	108	109	110	111	112	7p	113	114	115	116	117	118

f block

4f	57	58	59	60	61	62	63	64	65	66	67	68	69	70
5f	89	90	91	92	93	94	95	96	97	98	99	100	101	102

Long Periodic Table

s block | *f* block | *d* block | *p* block

1 1A	2 2A															3 3B	4 4B	5 5B	6 6B	7 7B	8 8B	9 8B	10 8B	11 1B	12 2B	13 3A	14 4A	15 5A	16 6A	17 7A	18 8A
																								1 1s							2
3 2s	4																									5 2p	6	7	8	9	10
11 3s	12																									13 3p	14	15	16	17	18
19 4s	20															21 3d	22	23	24	25	26	27	28	29	30	31 4p	32	33	34	35	36
37 5s	38															39 4d	40	41	42	43	44	45	46	47	48	49 5p	50	51	52	53	54
55 6s	56	57 4f	58	59	60	61	62	63	64	65	66	67	68	69	70	71 5d	72	73	74	75	76	77	78	79	80	81 6p	82	83	84	85	86
87 7s	88	89 5f	90	91	92	93	94	95	96	97	98	99	100	101	102	103 6d	104	105	106	107	108	109	110	111	112	113 7p	114	115	116	117	118

Drawing Orbital Diagrams

- Draw a line for each orbital of each sublevel mentioned in the complete electron configuration. Draw one line for each *s* sublevel, three lines for each *p* sublevel, five lines for each *d* sublevel, and seven lines for each *f* sublevel.
- Label each sublevel.
- For orbitals containing two electrons, draw one arrow up and one arrow down to indicate the electrons' opposite spin.
- For unfilled sublevels, follow Hund's Rule.

Abbreviated Electron Configurations

- The highest energy electron are most important for chemical bonding.
- The noble gas configurations of electrons are especially stable and, therefore, not important for chemical bonding.
- We often describe electron configurations to reflect this representing the noble gas electrons with a noble gas symbol in brackets.
- For example, for sodium

$1s^2\, 2s^2\, 2p^6\, 3s^1$ goes to [Ne] $3s^1$

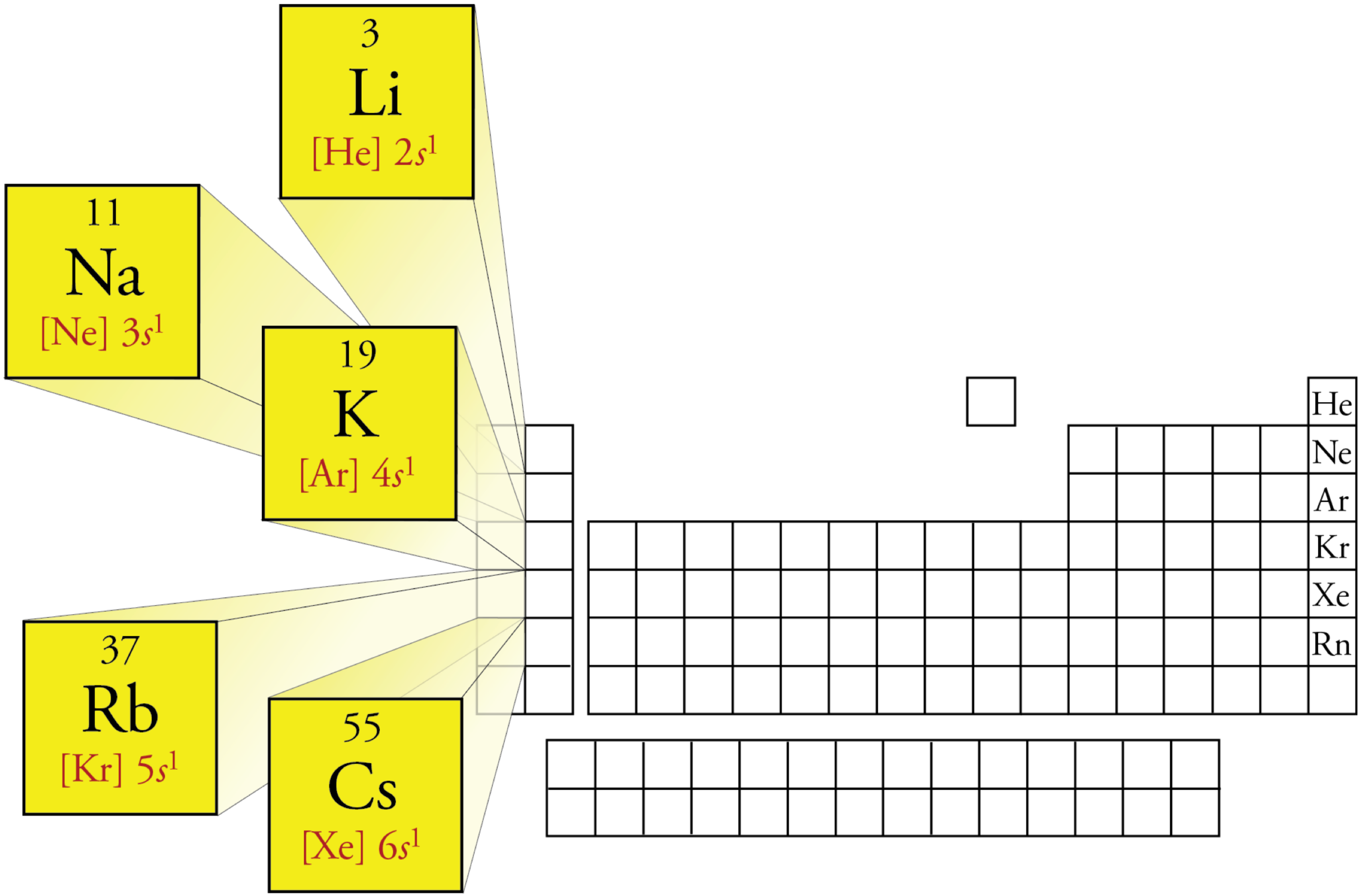
Writing Abbreviated Electron Configurations

- Find the symbol for the element on a periodic table.
- Write the symbol in brackets for the noble gas located at the far right of the preceding horizontal row on the table.
- Move back down a row (to the row containing the element you wish to describe) and to the far left. Following the elements in the row from left to right, write the outer-electron configuration associated with each column until you reach the element you are describing.

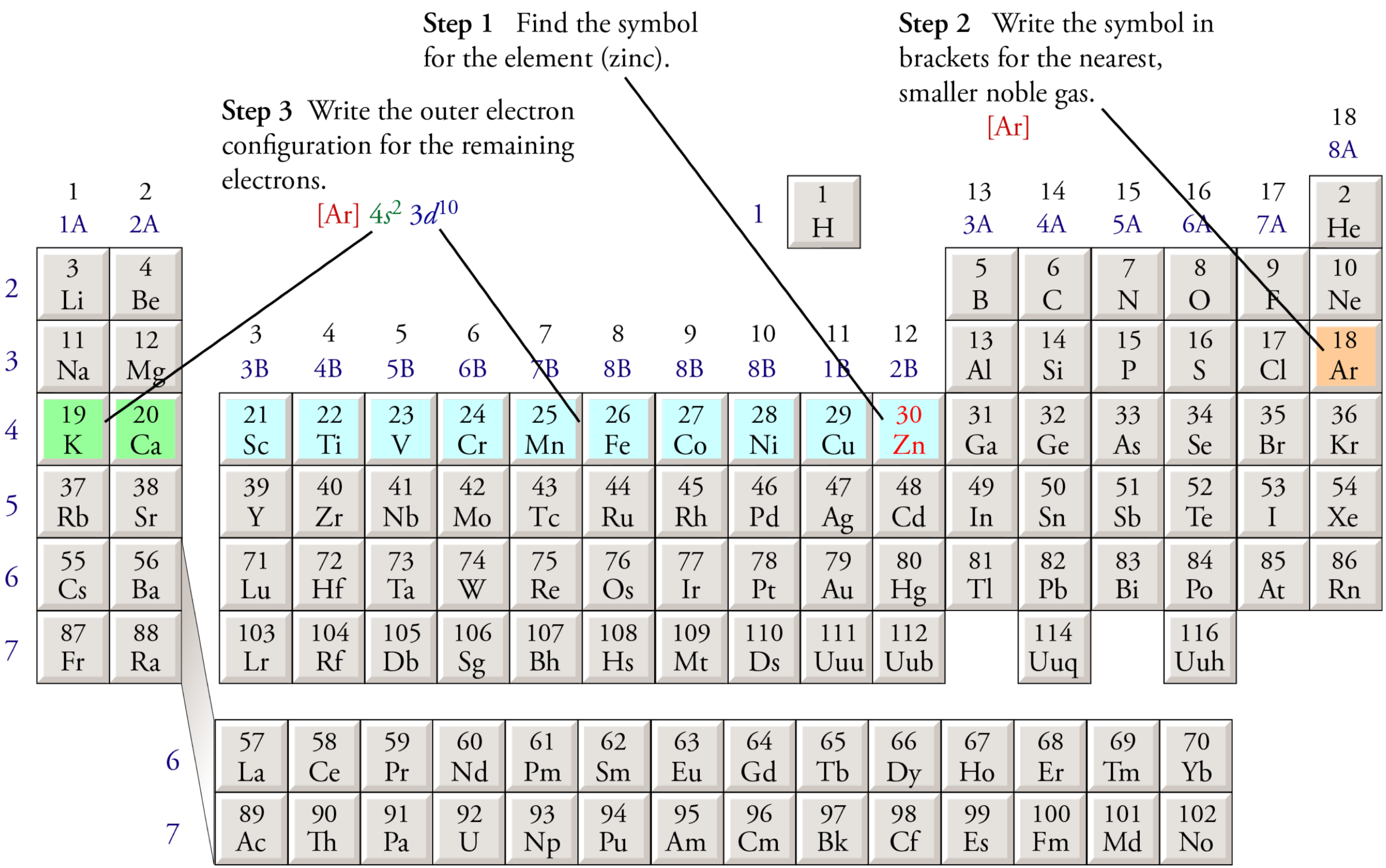
Abbreviated Electron Configurations – Optional Step

- Rewrite the abbreviated electron configuration, listing the sublevels in the order of increasing principal energy level (all of the 3's before the 4's, all of the 4's before the 5's, etc.)

Group 1 Abbreviated Electron Configurations



Abbreviated Electron Configuration Steps for Zinc



Common Mistakes

- Complete electron configurations – miscounting electrons (Use the periodic table to determine order of filling.)
- Orbital diagrams – forgetting to leave electrons unpaired with the same spin when adding electrons to the *p*, *d*, or *f* sublevels (Hund's Rule)
- Abbreviated electron configurations
  - Forgetting to put $4f^{14}$ after [Xe]
  - Forgetting to list sublevels in the order of increasing principal energy level