Modern
Atomic Theory

Section 4.2 (atoms-first) and Section 11.1 (chemistry-first)

The Mysterious Electron

An Introduction to Chemistry

by Mark Bishop

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.

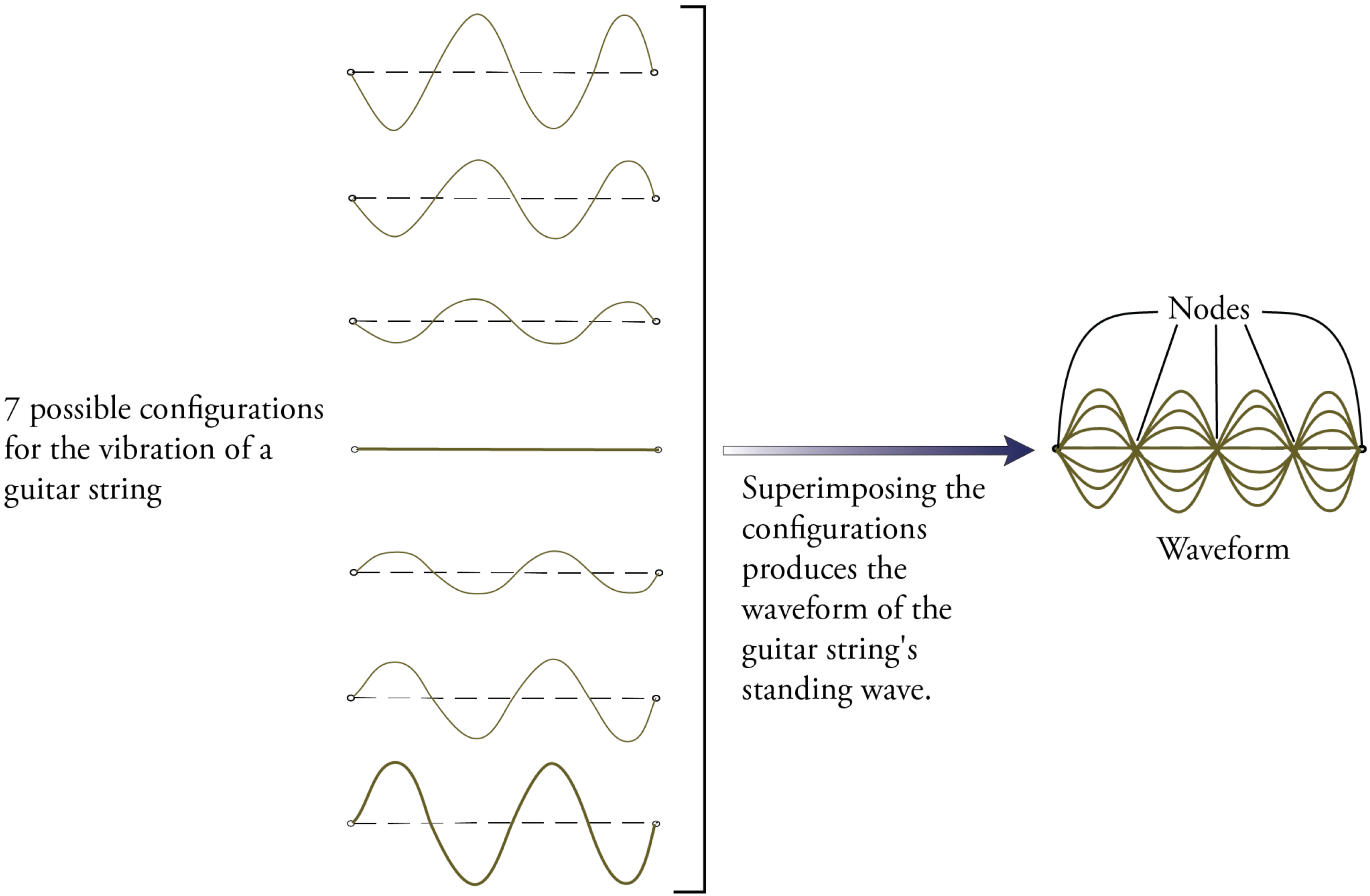
Strangeness of Tiny Particles

- 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.

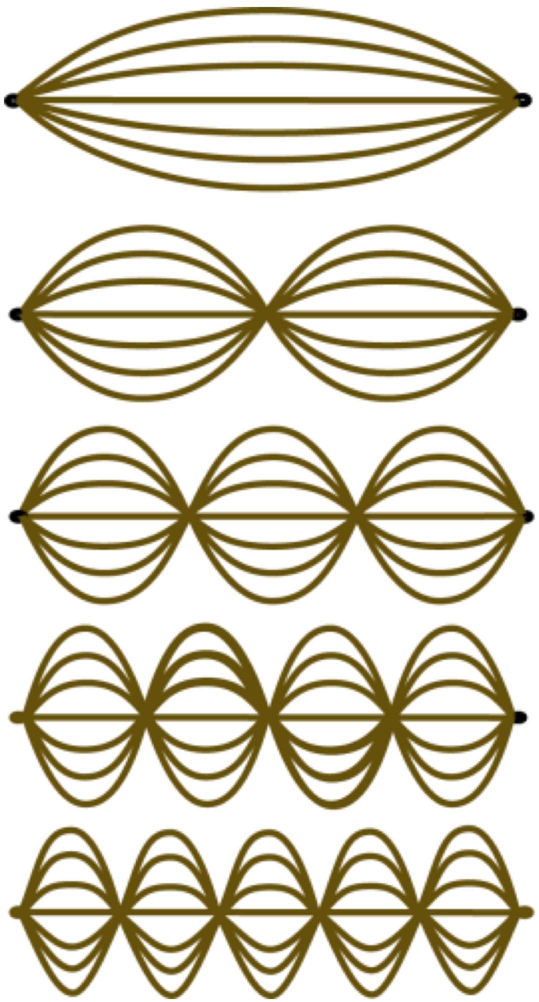
Ways to deal with Complexity and Uncertainty

- **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



Allowed Vibrations for a Guitar String

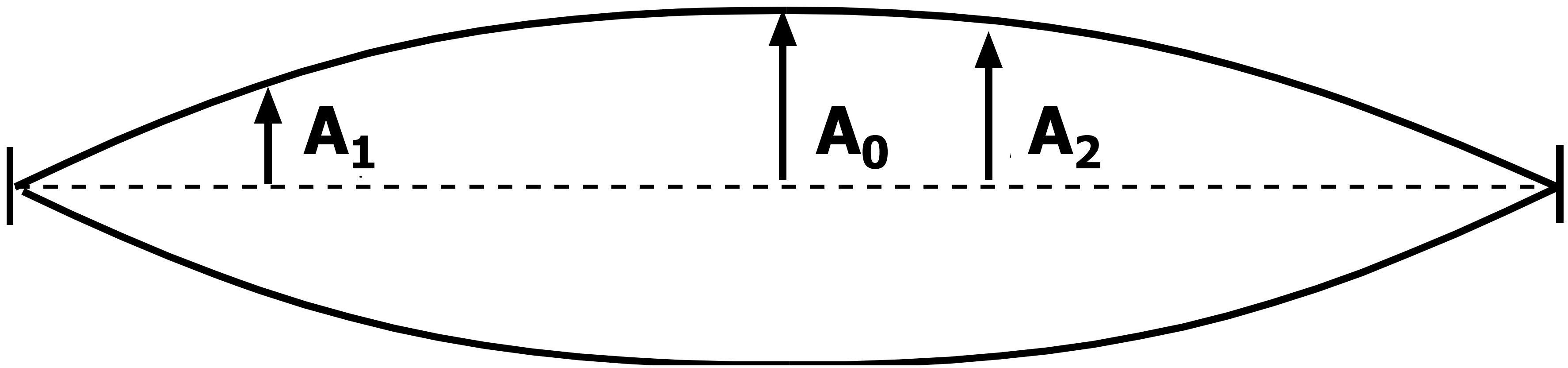


Equation for Guitar String

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

- 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

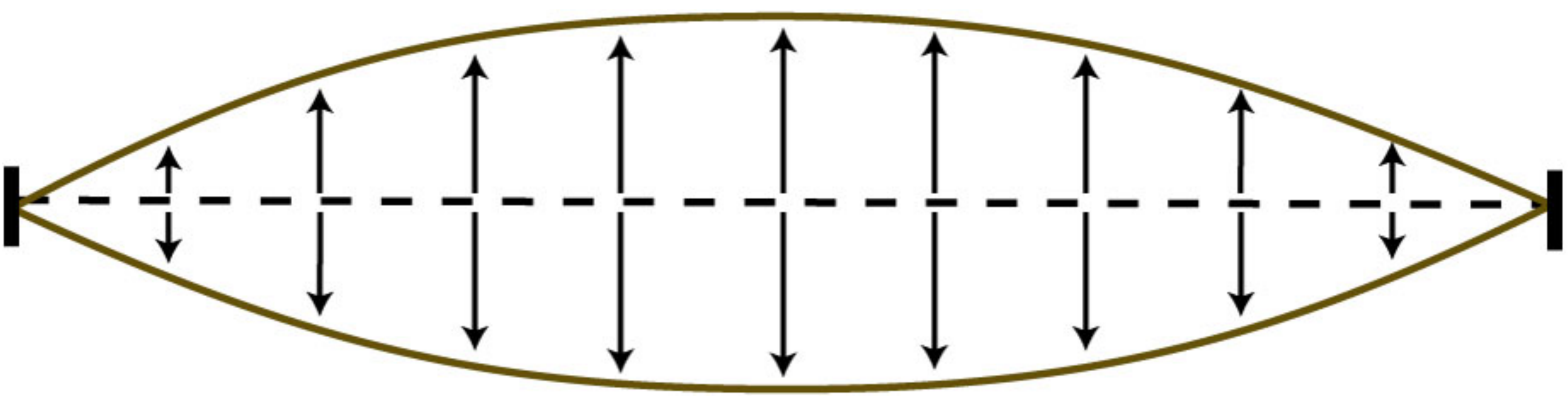
Guitar String Amplitudes



Guitar String Waveform 1

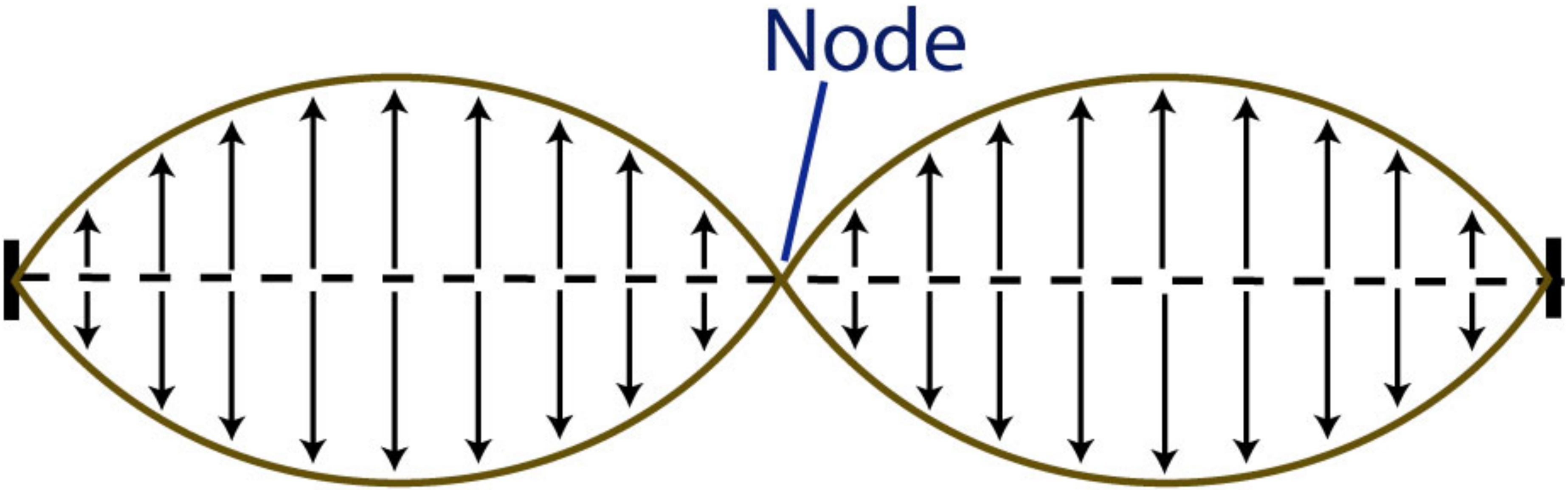
$$A_X = A_O \sin \frac{n\pi x}{a}$$

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



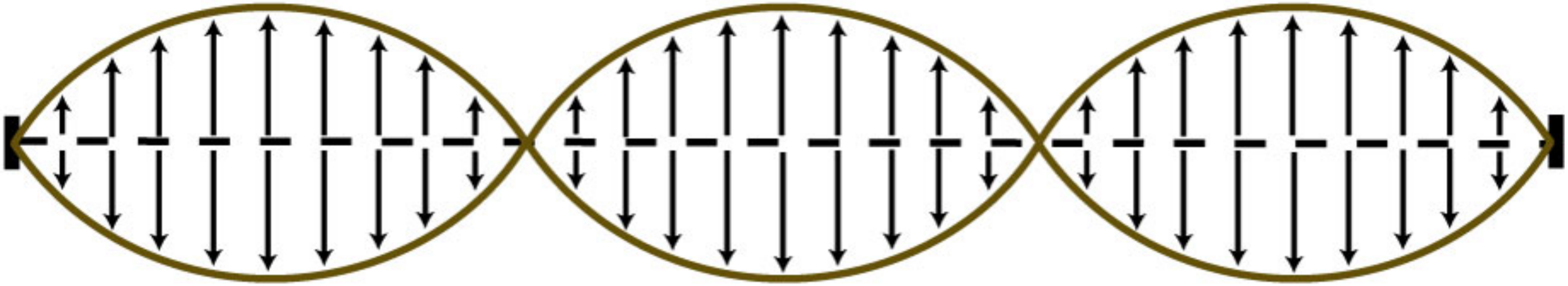
Guitar String Waveform 2

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

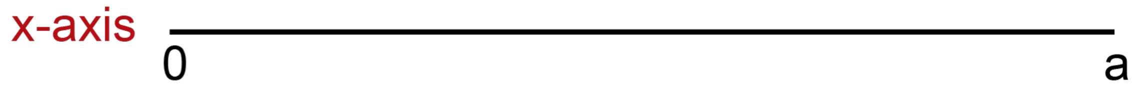


Guitar String Waveform 3

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

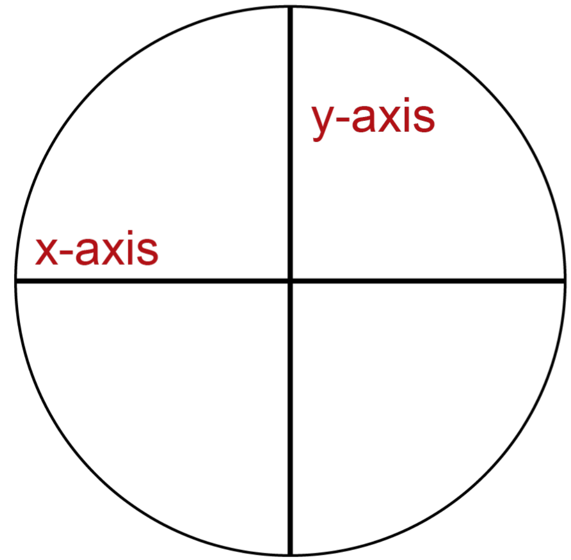


Dimensions

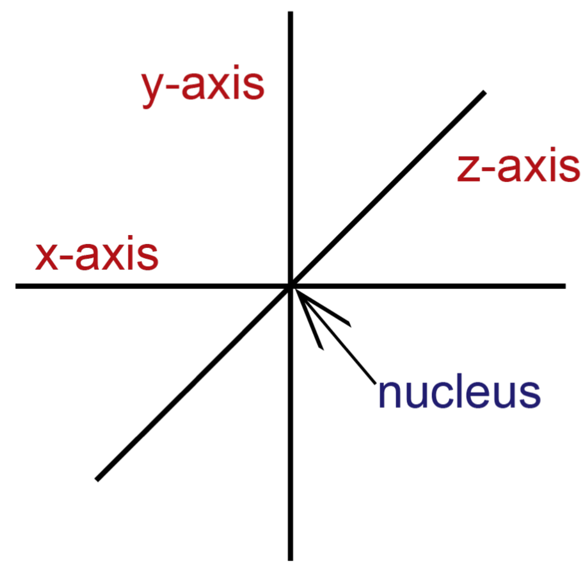


Guitar String

Drumhead



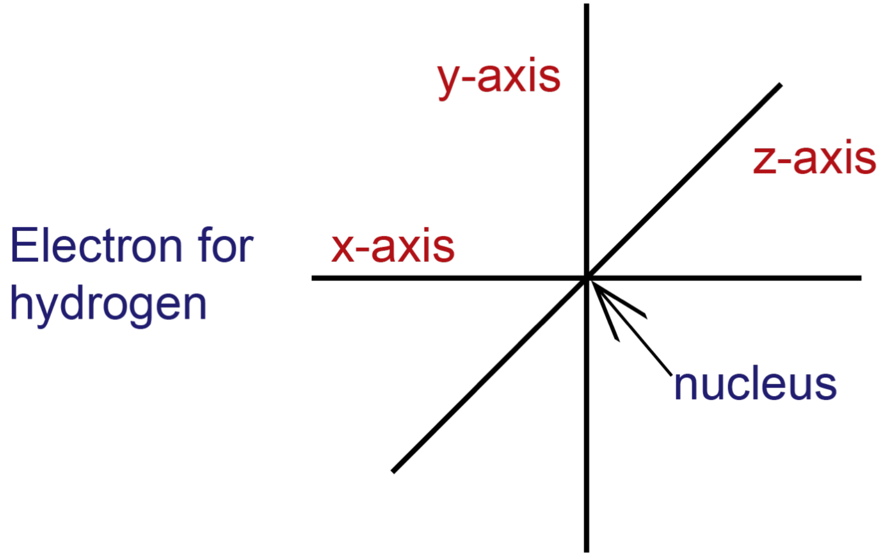
Electron for hydrogen



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

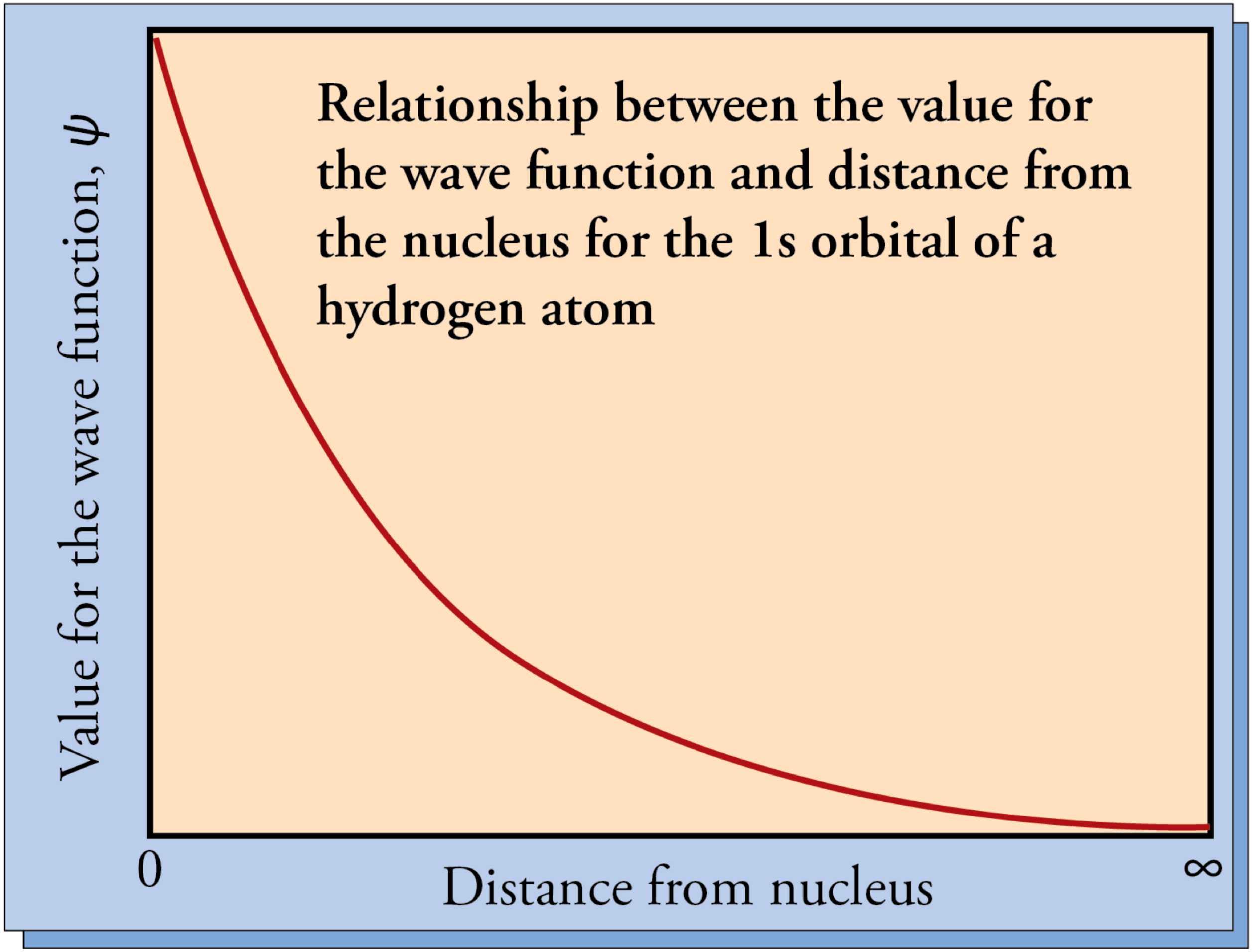
$\Psi_{2s} = f_{2s}(x,y,z)$ with 2,0,0 for quantum numbers

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

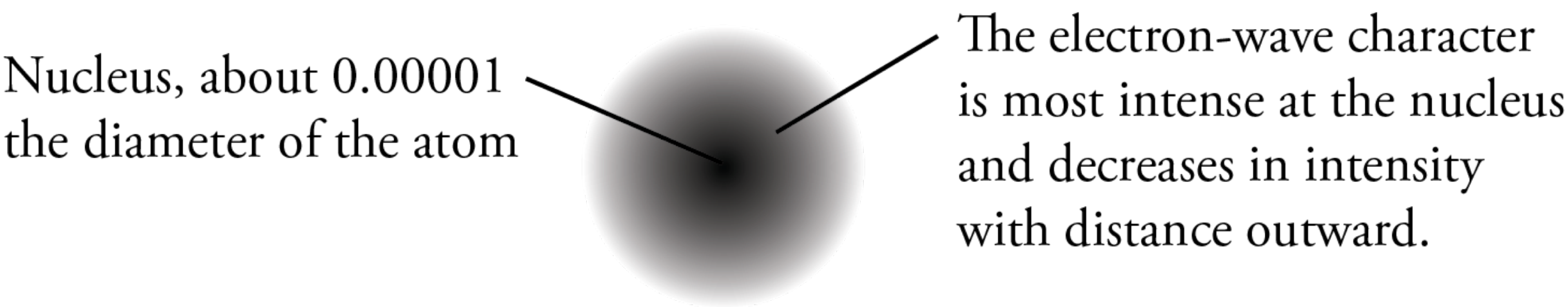
Determination of the Allowed Electron Waveforms (cont.)

- **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



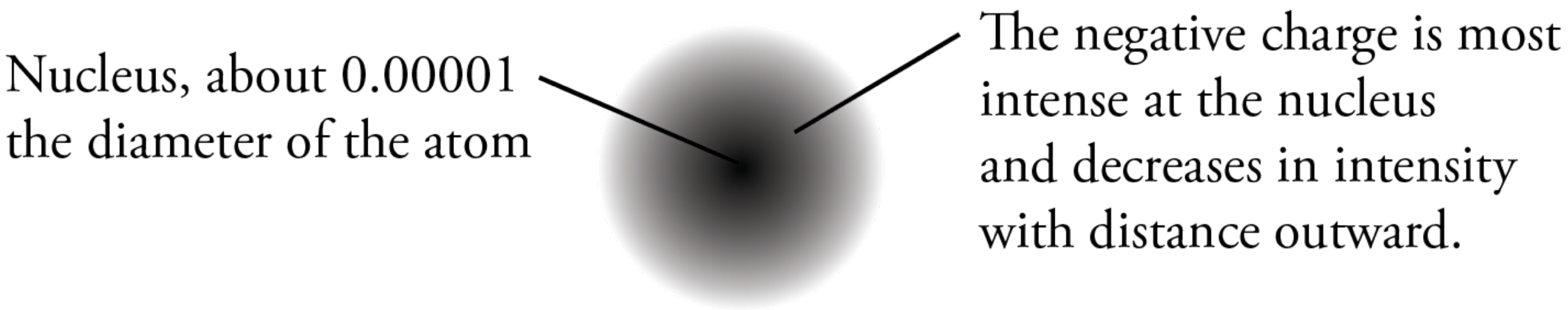
Waveform for 1*s* Electron (1,0,0)



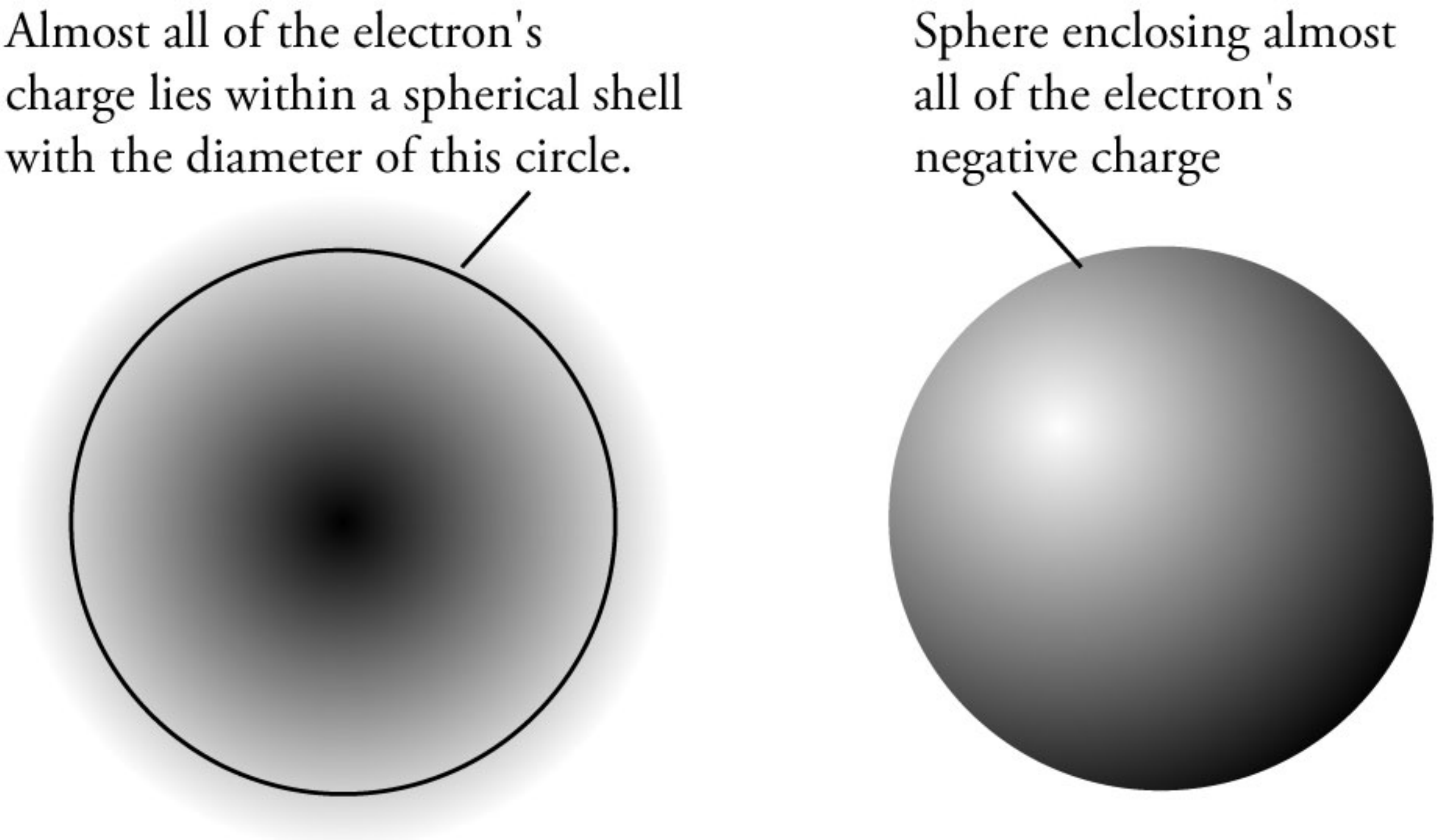
Particle Interpretation of 1*s* Orbital

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

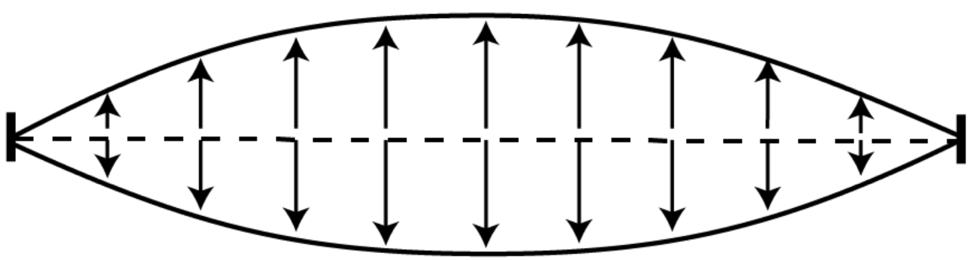

Almost all of the electron's charge lies within a spherical shell with the diameter of this circle.
Sphere enclosing almost all of the electron's negative charge

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.



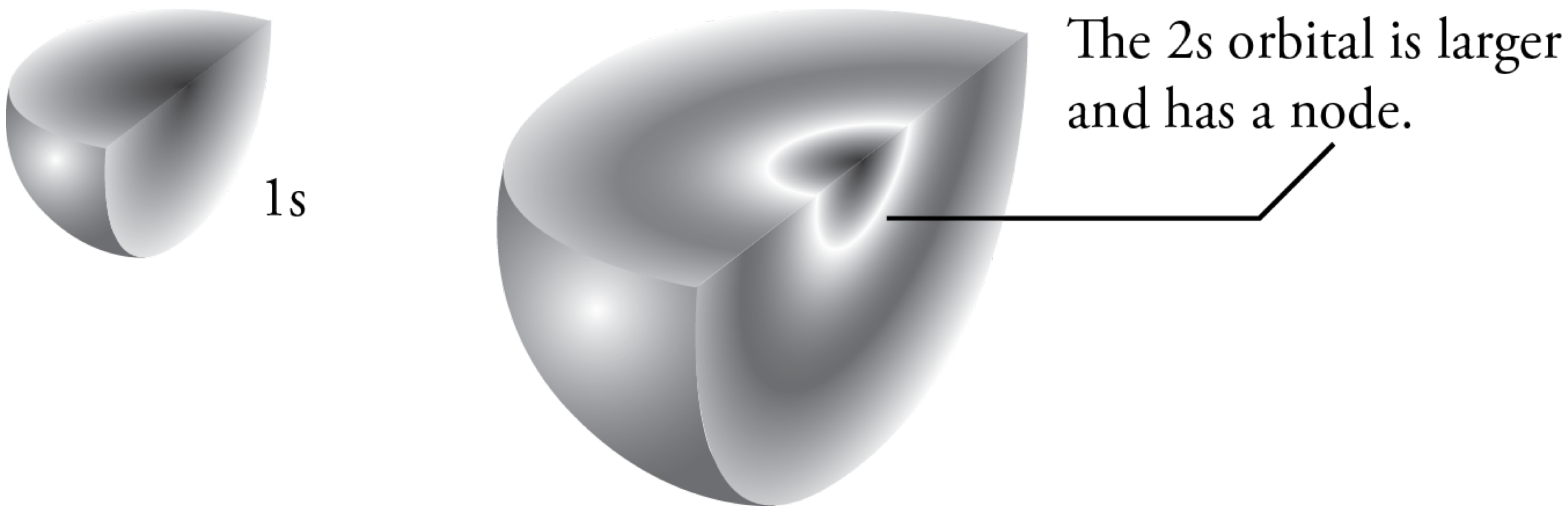
Simplest waveform for guitar string

Simplest waveform for electron 1s orbital

Wave Character of the Electron

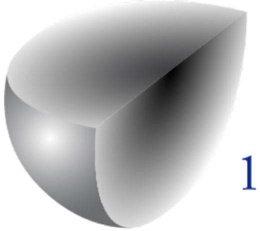
- Although both the electron and the guitar string can have an infinite number of possible waveforms, only certain waveforms are possible.
- We can focus our attention on the waveforms of varying motion of the guitar string or the varying electron charge intensity without having to think about the actual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

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

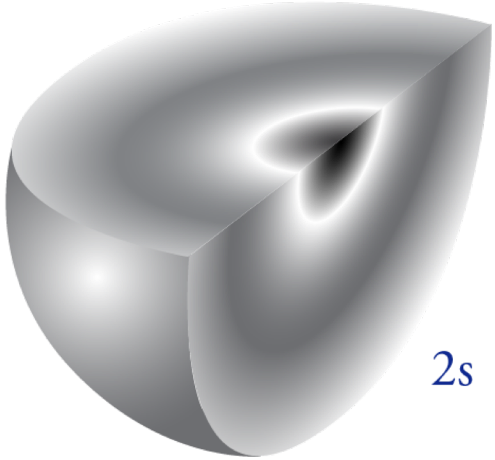


An electron in 2s is less stable and higher PE than an electron in 1s

- 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.



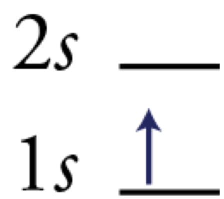
1s



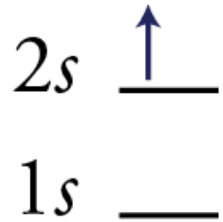
2s

Ground State and Excited State

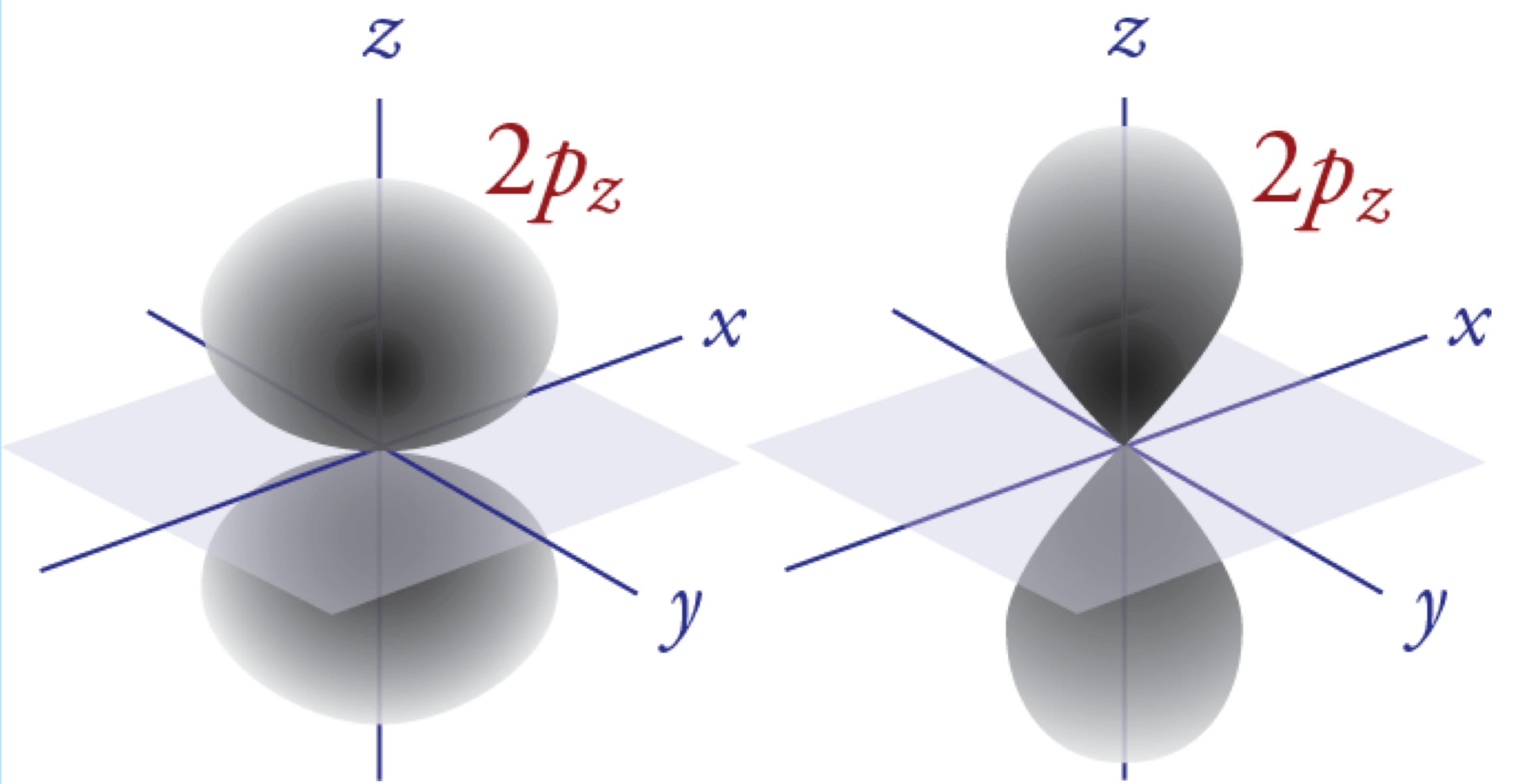
- Hydrogen atoms with their electron in the 1*s* orbital are said to be in their ***ground state***.



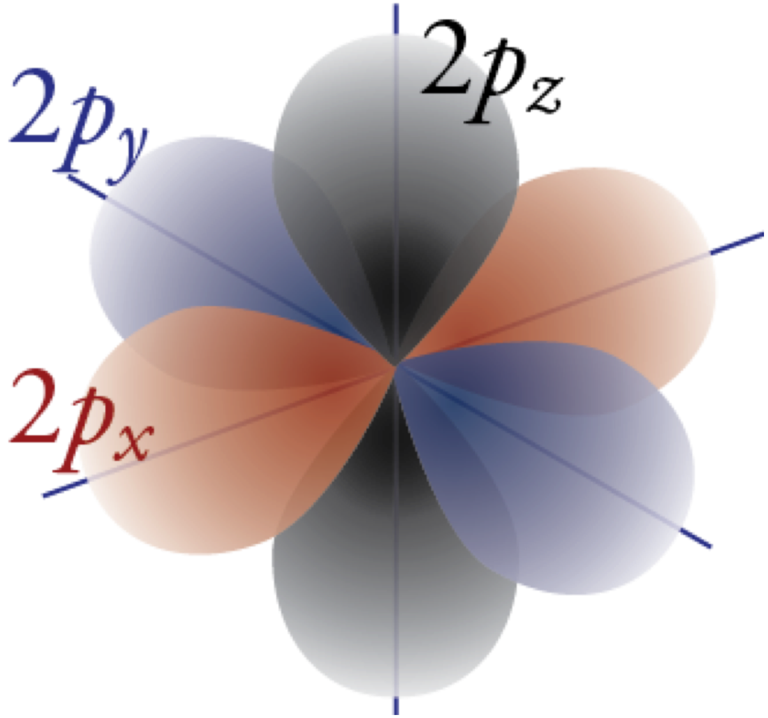
- A hydrogen atom with its electron in the 2*s* orbital is in an ***excited state***.

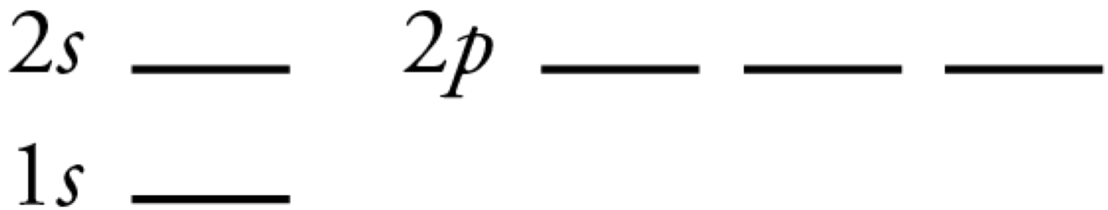


Realistic and Stylized $2p_y$ Orbital (2,1,1)



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

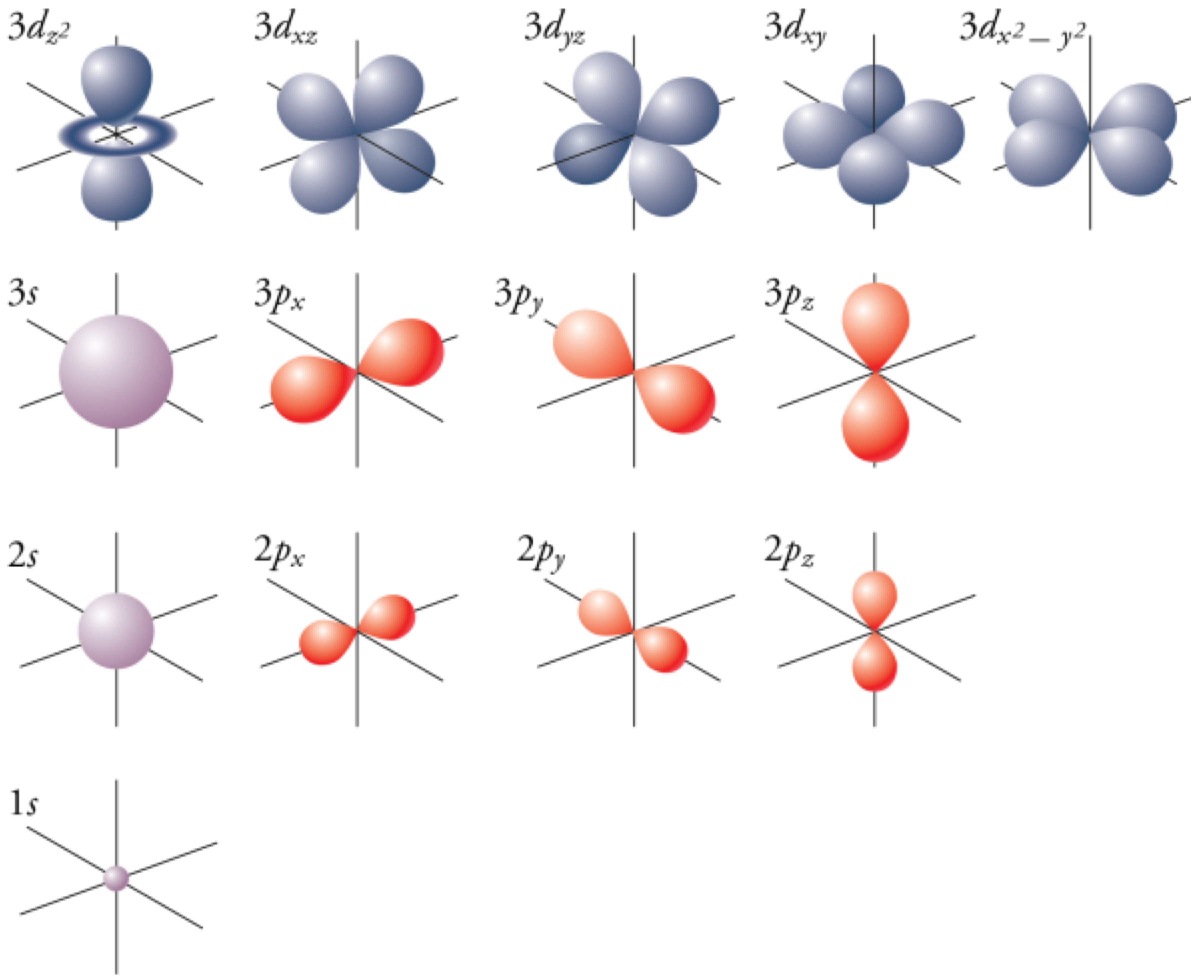




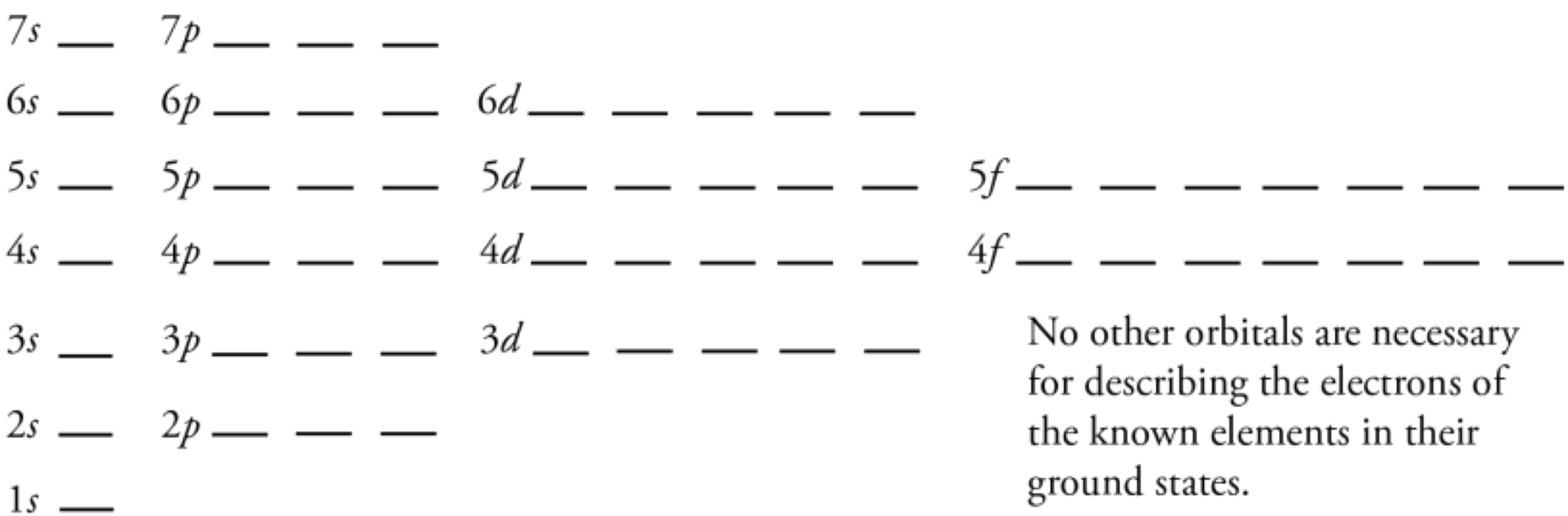
Sublevels

- 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



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