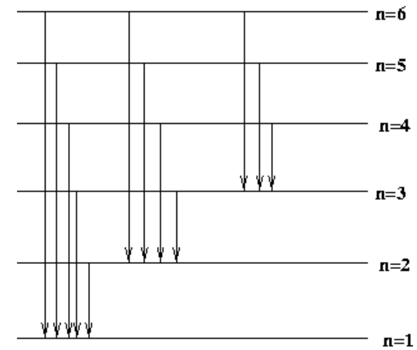
Quantum Theory

- Electrons occupy energy levels within an atom (1913 - Niels Bohr of Denmark)
- Distance between energy levels is called a quantum (so a quantum leap really isn't that far…)
  - Electrons can only occupy these levels!!!
- When the electrons of an atom are in their lowest energy state, it's called the ground state
- If the atom takes in energy, the electrons may get bumped up to higher levels, or what is called an excited state.

Spectral Emission and Energy Levels in the Atom

•Spectral emissions from gas tubes (or just a neon sign) are examples of an atom being excited and then returning to ground state. Each time the atom returns to ground state, it emits light of a specific wavelength.

•Every element emits different wavelengths because each element has a different electron configuration



n represents the energy level of the electron

Image from http://theory.uwinnipeg.ca/mod_tech/node151.html

Quantum Cont.

The electromagnetic spectrum

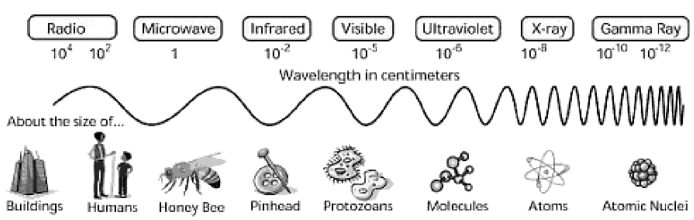
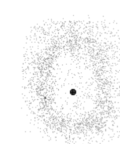


Image from: http://imagers.gsfc.nasa.gov/ems/waves3.html

- Visible light is one form of energy that our eyes have been designed to "see". There are many other similar forms of energy we cannot see.

Quantum Cont.

- Modern quantum theory is mathematical -- it doesn't tell us exactly where an electron will be -- rather it tells us the likelihood of finding an electron in a certain place
- When you plot the probable locations, you define what are called "orbitals" (or the "electron cloud") image: http://regentsprep.org/Regents/physics/phys05/catomodel/cloud.htm

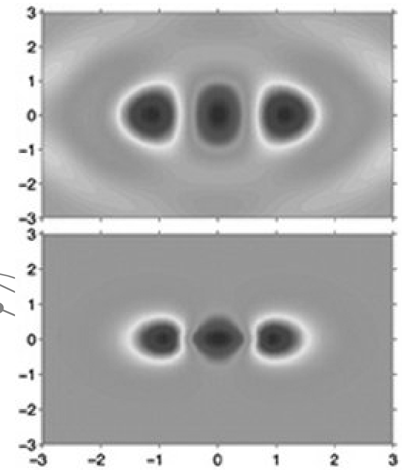


- The diagrams you will see in books and elsewhere are typically drawn to represent where you will find the electron 90% of the time.

Quantum Cont.

- How would we see an electron?
  - Photons of light bouncing off of the electron
  - Although photons have no mass, they do have energy and momentum – which would in turn affect the electron. This leads to…
- The Heisenberg Uncertainty Principle: You can't simultaneously measure the velocity and location of an electron.
  - Basically, there is a fundamental limitation to what we can measure.
- Can we see electrons, protons, and neutrons? No. We know they are there from models and experimental data.

Evidence for our quantum equations being correct? See below!



"NITRO TOPO. Outermost electron orbital of a nitrogen molecule reconstructed from molecular scans (top) closely matches the independently calculated orbital (bottom). Colors indicate peaks (toward red) and valleys (toward blue) of the orbital. Distances are in angstroms (tenths of nanometers)."

J. Itatani *et al.*/*Nature*

Image and text from http://www.phschool.com

Electron Configurations

- Electrons are described by their quantum numbers
- The principal quantum #, "n", can be 1-7. In general, the higher #, the farther away from the nucleus
  - Quantum # n is the energy level (related to row on periodic table)
  - Higher # = higher energy level
- The shapes of the orbitals are represented by the second quantum # (angular momentum quantum number), "l".

Possible values and letters for the second quantum number				
Value of "l"	0	1	2	3
Letter used	s	p	d	f

Electron Configs. Cont.

- The s orbital can have 1 pair of electrons (each with opposite spin)
- The p orbitals can have 3 pairs of electrons (px, py, pz)
- The d orbitals can have 5 pairs of electrons (dxz, dyz, dxy, dx^2-y^2, dz^2)
- The f orbitals can have 7 pairs of electrons

Electron Configs. Cont.

- The third quantum number is m_l – the magnetic quantum number. This tells us which orbital (orientation) that the electron is in.
  - Can have integer values -l to l
  - s subshell (l=0) has one orbital: $m_l = 0$
  - p subshell (l=1) has three orbitals: $m_l = -1, 0, 1$
  - d subshell (l=2) has five orbitals: $m_l = -2, -1, 0, 1, 2$
  - f subshell (l=3) has seven orbitals: $m_l = -3, -2, -1, 0, 1, 2, 3$
- The final quantum number is m_s – the spin quantum number (positive or negative spin)
  - Can have values of -1/2 and +1/2

Electron Configurations

- We can view some images of orbitals at the following website:

http://winter.group.shef.ac.uk/orbitron/index.html

Electron Configs. Cont.

- Pauli Exclusion Principle: Only two electrons can occupy the same orbital, and these two electrons must have opposite spin
- Hund's Rule: When filling the pairs for each orbital, the electrons will fill all orbitals unpaired (with the same spin direction) before pairing begins. (by convention write as spin up)
  - This is due to the fact that the most stable arrangement of electrons is that with the most parallel spins

Electron Configs.

- Example configurations:

		1s	2s	2p		
H	$1s^1$	↑				
He	$1s^2$	↑↓				
Li	$1s^2 2s^1$	↑↓	↑			

Electron Configs. Cont.

		1s	2s	2p
Be	$1s^2 2s^2$	↑↓	↑↓	[ ] [ ] [ ]
B	$1s^2 2s^2 2p^1$	↑↓	↑↓	[↑] [ ] [ ]
N	$1s^2 2s^2 2p^3$	↑↓	↑↓	[↑] [↑] [↑]
O	$1s^2 2s^2 2p^4$	↑↓	↑↓	[↑↓] [↑] [↑]