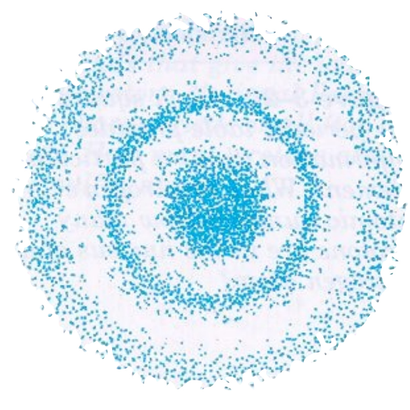
Ch07

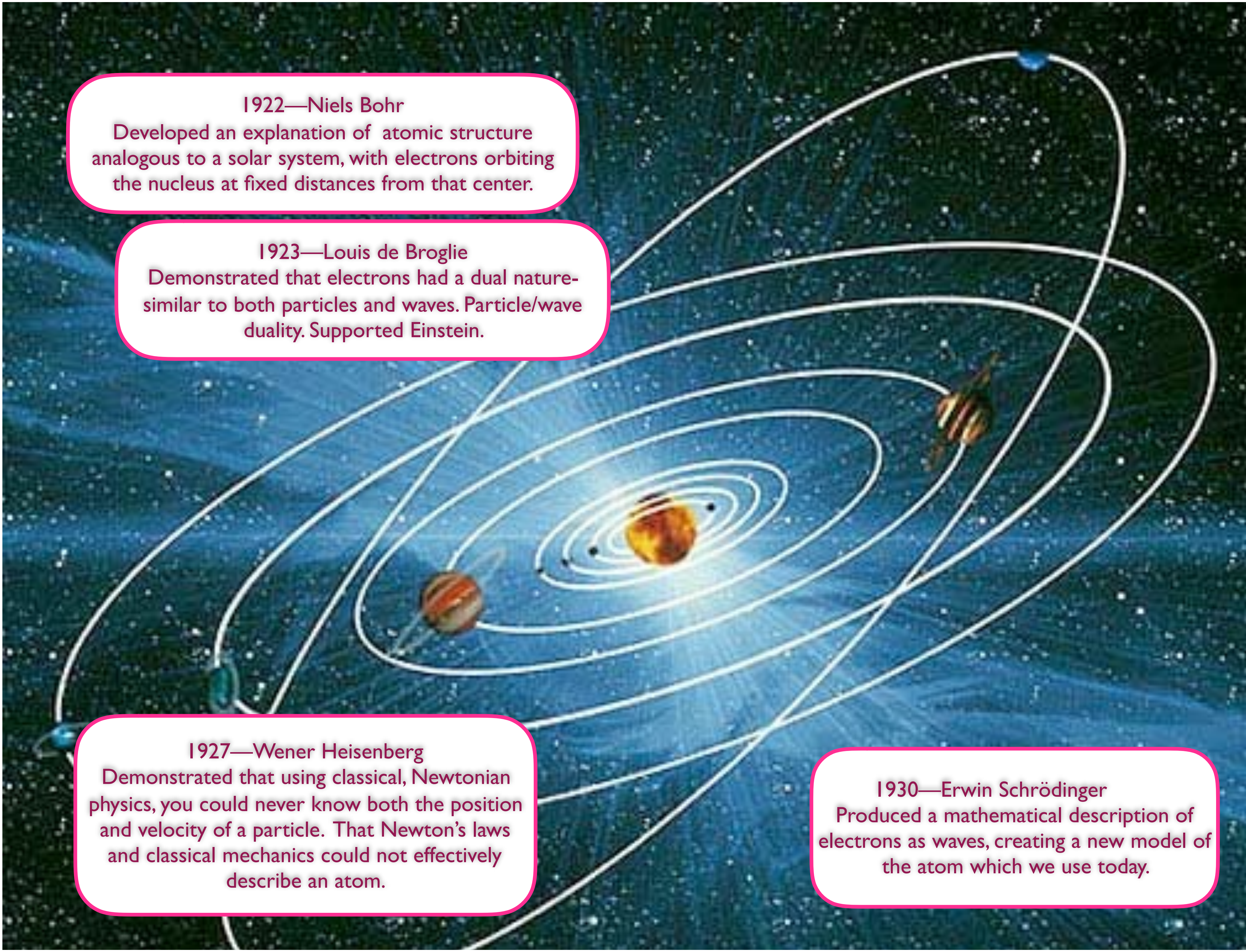
The Quantum Atom

A new kind of math

…gives us a new kind of atom.

version 1.5




1922—Niels Bohr
Developed an explanation of atomic structure analogous to a solar system, with electrons orbiting the nucleus at fixed distances from that center.
1923—Louis de Broglie
Demonstrated that electrons had a dual nature- similar to both particles and waves. Particle/wave duality. Supported Einstein.
1927—Wener Heisenberg
Demonstrated that using classical, Newtonian physics, you could never know both the position and velocity of a particle. That Newton's laws and classical mechanics could not effectively describe an atom.
1930—Erwin Schrödinger
Produced a mathematical description of electrons as waves, creating a new model of the atom which we use today.

The Wave Nature of Matter

- Problems with the Bohr Model
- New Math & the Wave nature of Matter
  - The de Broglie Hypothesis
    - Davisson-Thomson Experiment
  - Heisenberg & Uncertainty
- The Schrödinger Equation
  - Energy Levels
    - Allowed States
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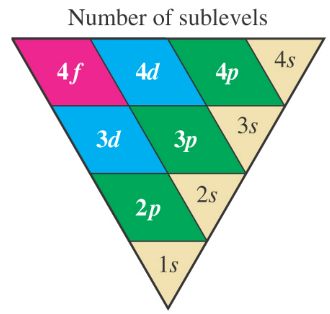
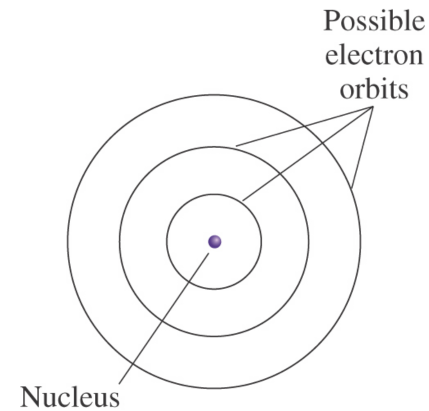
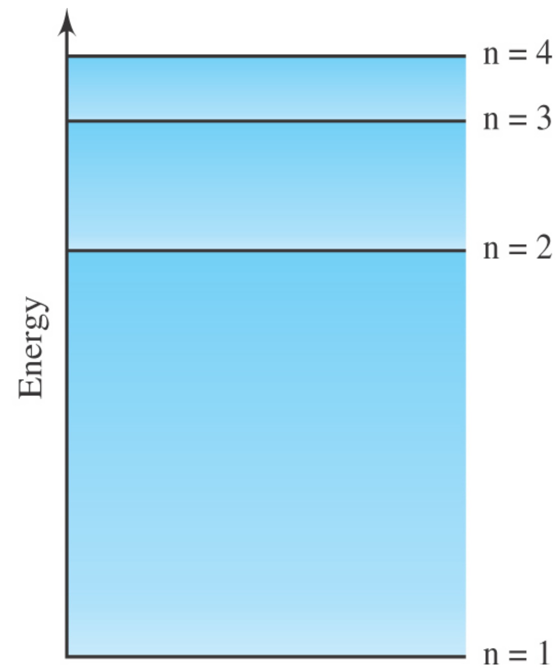
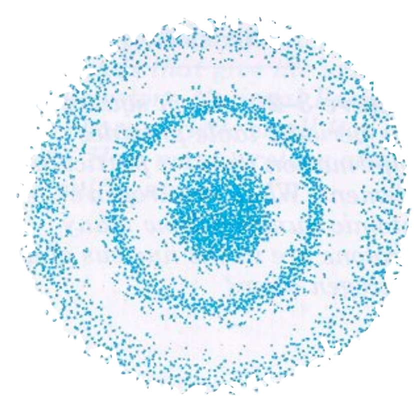
  - Orbital Phases
  - Atomic Shape & Orbital Size



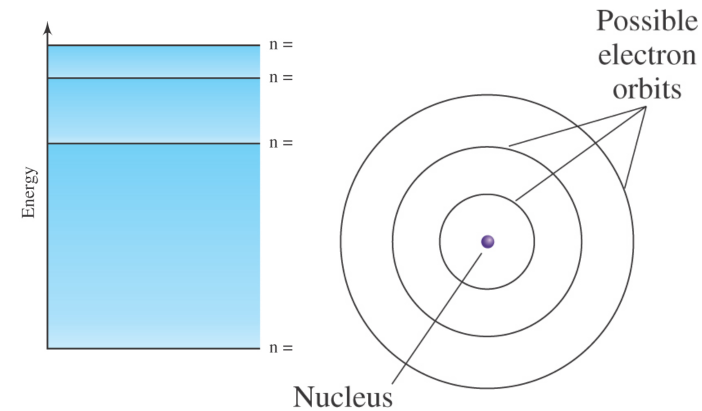


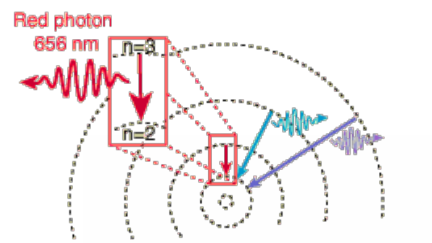




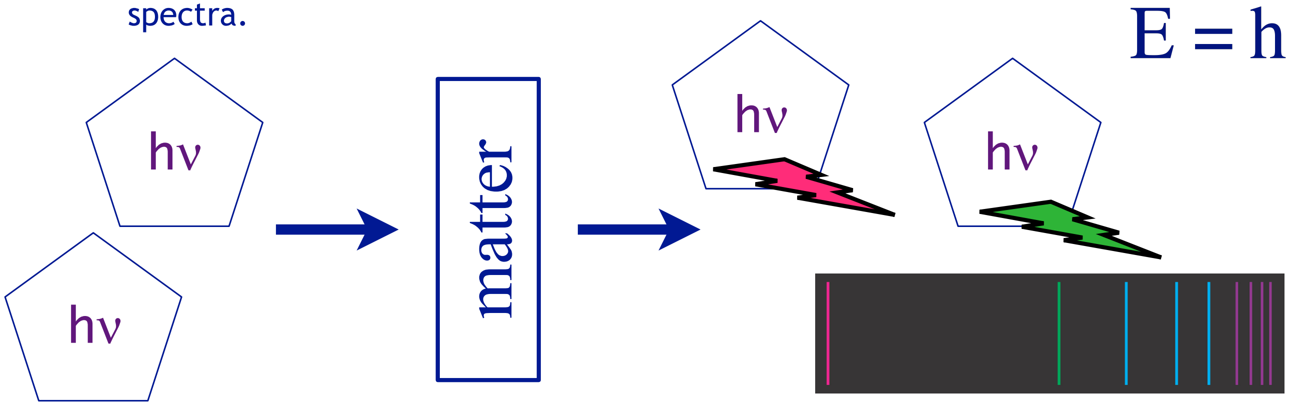
Line Spectra of the Elements

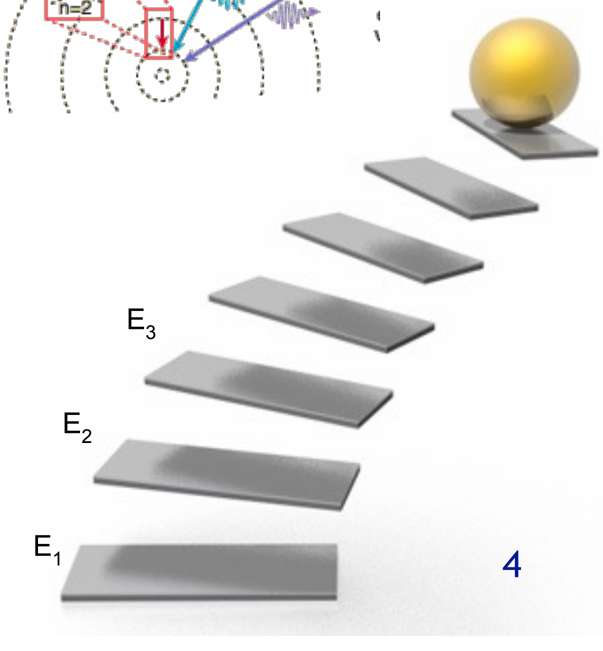
- At high temperature or voltages, elements in their pure state emit light
  - That light is special.
- Unlike most sources of light, it contains only discrete frequencies.
- Each element emits light with a unique set of frequencies.
- Niels Bohr started with Rutherford's model that electrons floated around a heavy positively charged nucleus.
- He postulated that much the same way planets orbit the sun in only orbits of a fixed distance, that electrons are also constrained to orbits of a fixed distance from the nucleus.
- He suggested that when an electron falls from a higher orbit to a lower energy orbit, it emits a photon.
- The color of that light depends on the wavelength, which depends on the energy difference between the two levels.
- With this model, only photons of with energy that equals the difference between levels can be emitted.
- This would explain why only discrete colors are seen in the line spectra.





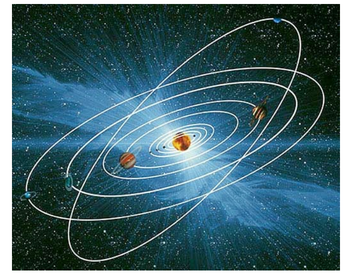
$$E = h\nu$$

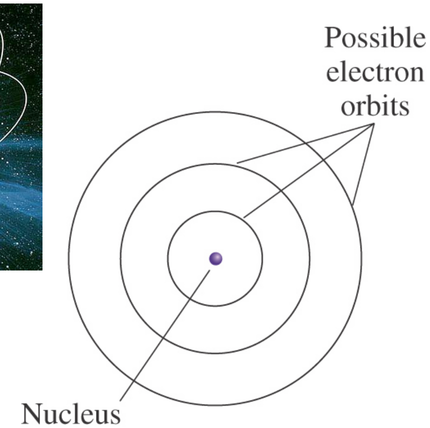


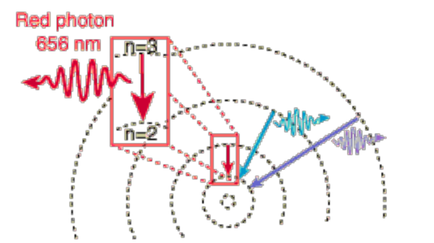


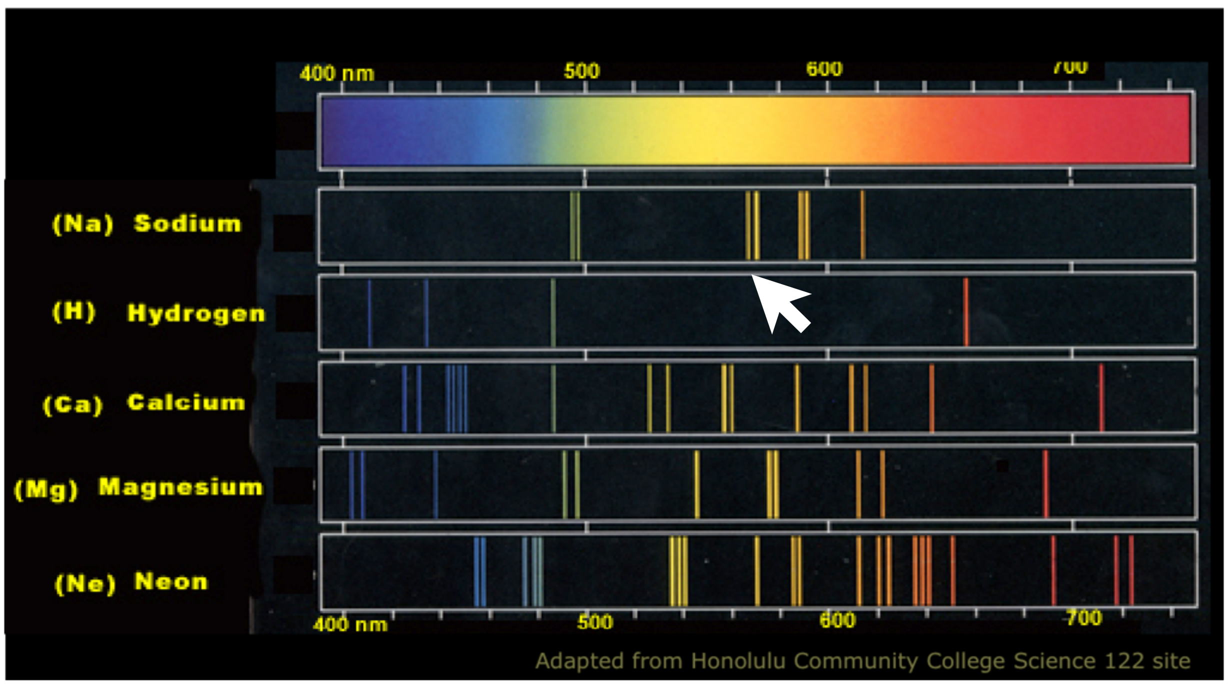
Problems with the Bohr Model

- The Bohr model was a huge step forward in atomic theory.
- It explained the line spectra and gave us insight into how electrons were arranged inside the atom.
- Bohr knew it was an incomplete model.
- His postulate that only certain orbits were allowed was unexplained.
- His model only predicted line spectra perfectly for the hydrogen atom.
- The line spectra of other elements showed splitting that wasn't explained by the Bohr model.

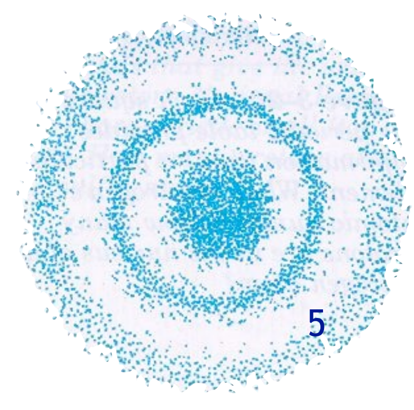




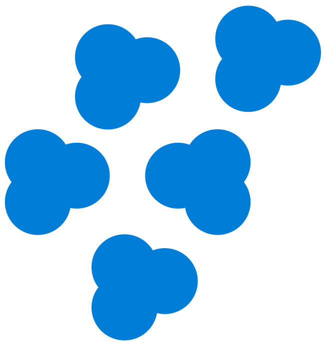




Adapted from Honolulu Community College Science 122 site

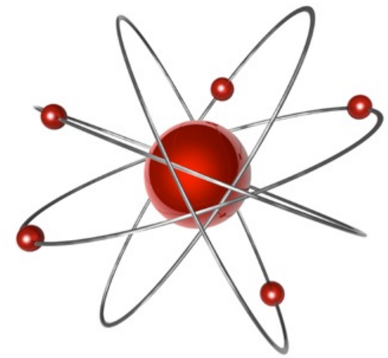


Evolution of the atom.

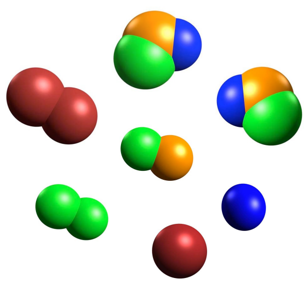


Atomos.

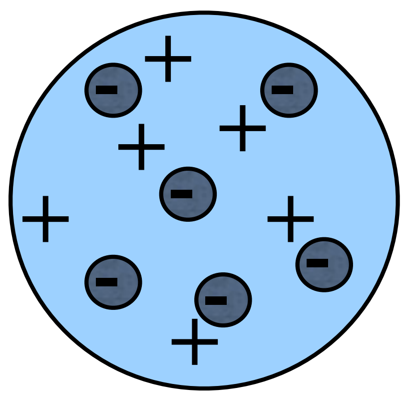
The quantum atom.



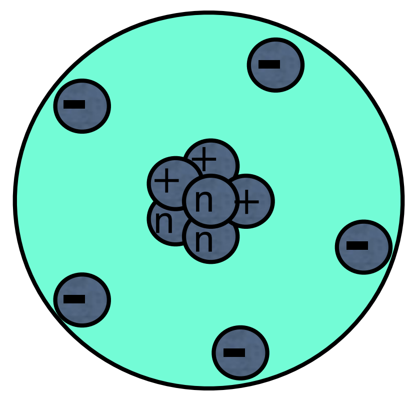
The planetary model.



Molecules & Compounds.
Elements, flavors of the atom.



The plum pudding model.



The nuclear atom.

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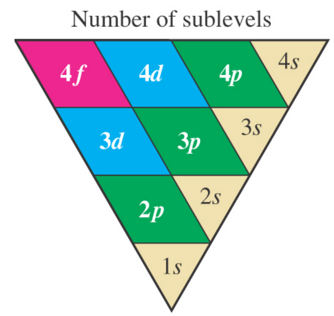
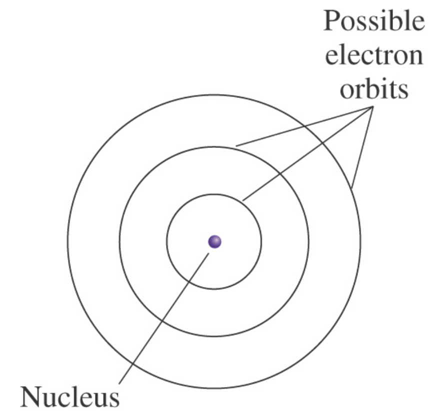
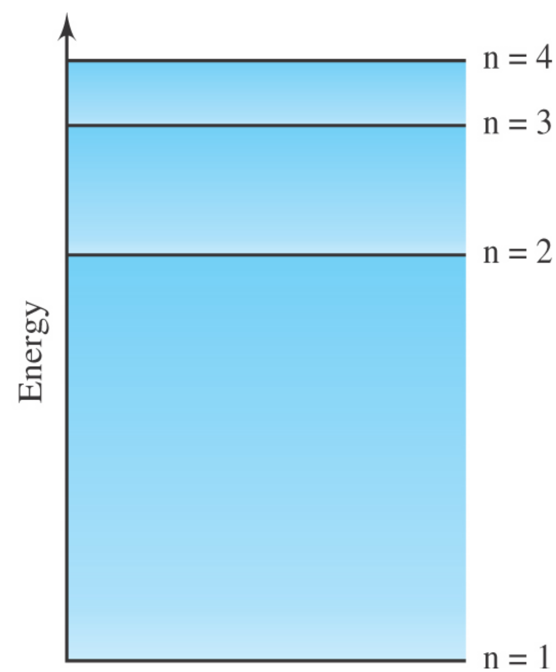
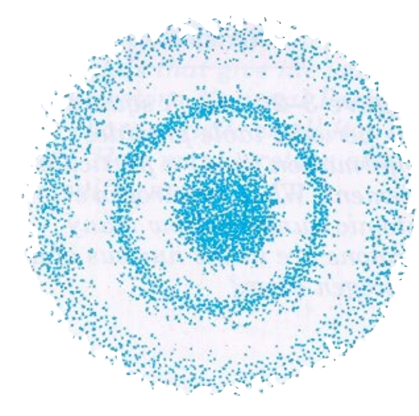




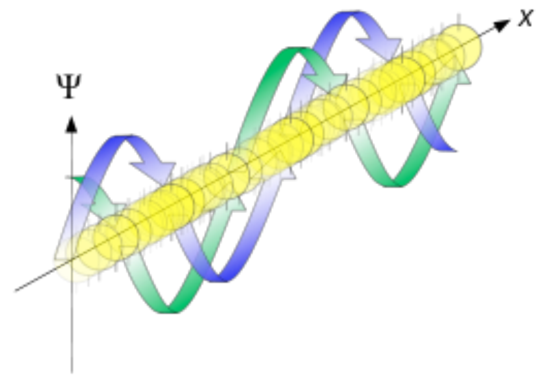




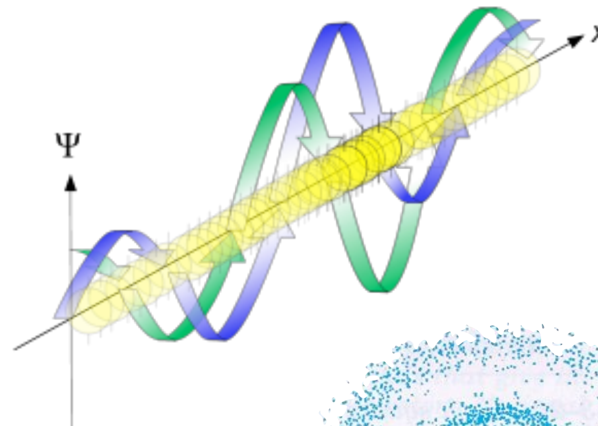
Louis de Broglie & Matter Waves

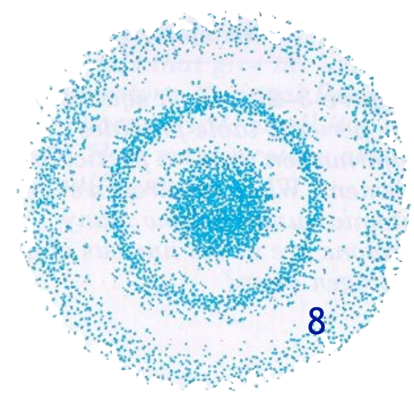
- Einstein had shown us it was sometimes useful to treat energy as if it was matter.
- He showed us that if we treated light like a particle, it could explain the photo-electric effect.
- A math student (still in graduate school) asked the question, would there be any advantages to treating matter as if it were energy?
- Louis de Broglie created a mathematical structure for coming up with the "wavelength" of physical objects and invited us to apply wave mechanics to matter.
- For most objects, this turns out to be valid but not very interesting.
- For very small objects, like electrons, it turns out to be amazing.

$$\Psi = Ae^{i(px - \omega t)}$$



$$\Psi = \sum_n A_n e^{i(p_n x - \omega_n t)}$$





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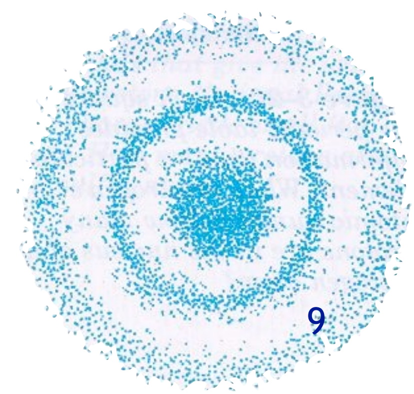
- For most objects, this turns out to be valid but not very interesting.
- For very small objects, like electrons, it turns out to be amazing.
- Louis de Broglie developed the equation for representing particles as waves:

$$\lambda = \frac{h}{p} = \frac{h}{mv}\sqrt{1 - \frac{v^2}{c^2}}$$

do not memorize this

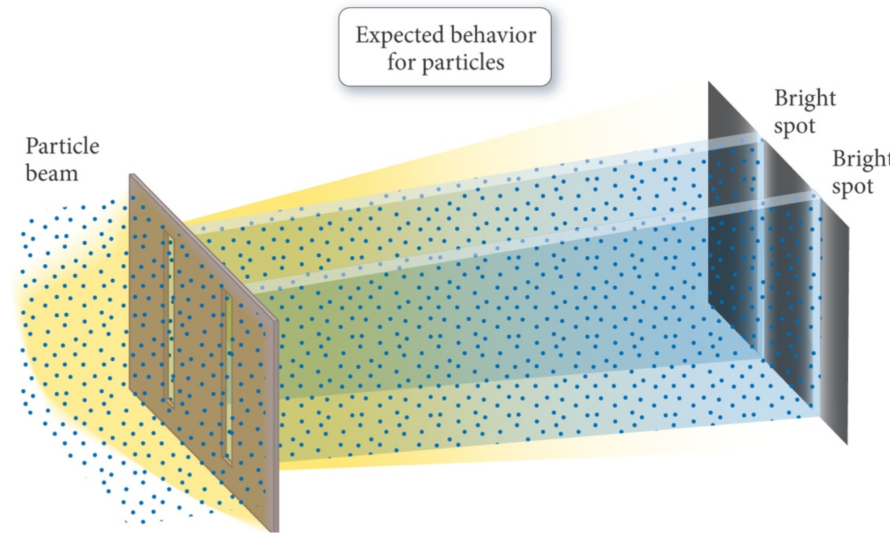
- de Broglie was a brilliant mathematician who received a nobel prize for work he did as a student. Think Google.
- When applied to electrons, matter waves unlocked a new model of atomic behavior.
- The Nobel Prize in Physics 1929 was awarded to Louis de Broglie "for his discovery of the wave nature of electrons".

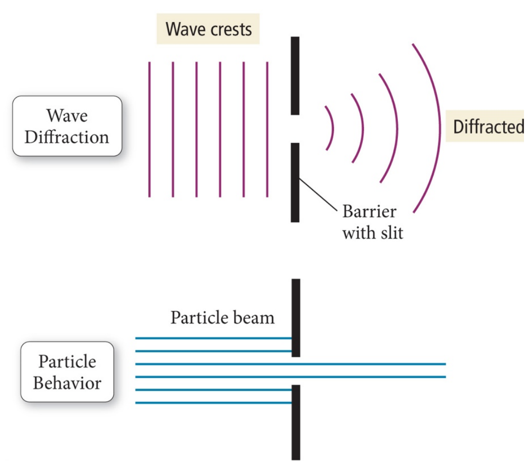
Maurice’s Little Brother

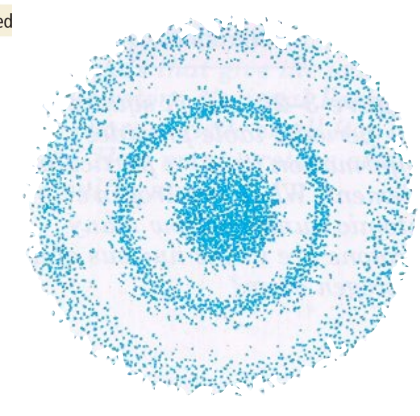


Davisson-Thomson Experiment

- Electrons are matter particles.
- They have mass and occupy space.
- An electron should pass through a diffraction grating along a predictable trajectory.
- It doesn’t.
- Very small, very fast moving particles demonstrate wave behavior.
- Electron trajectories are controlled by disturbances in the e-m field.
- Interference occurs as if a single electron was a wave.







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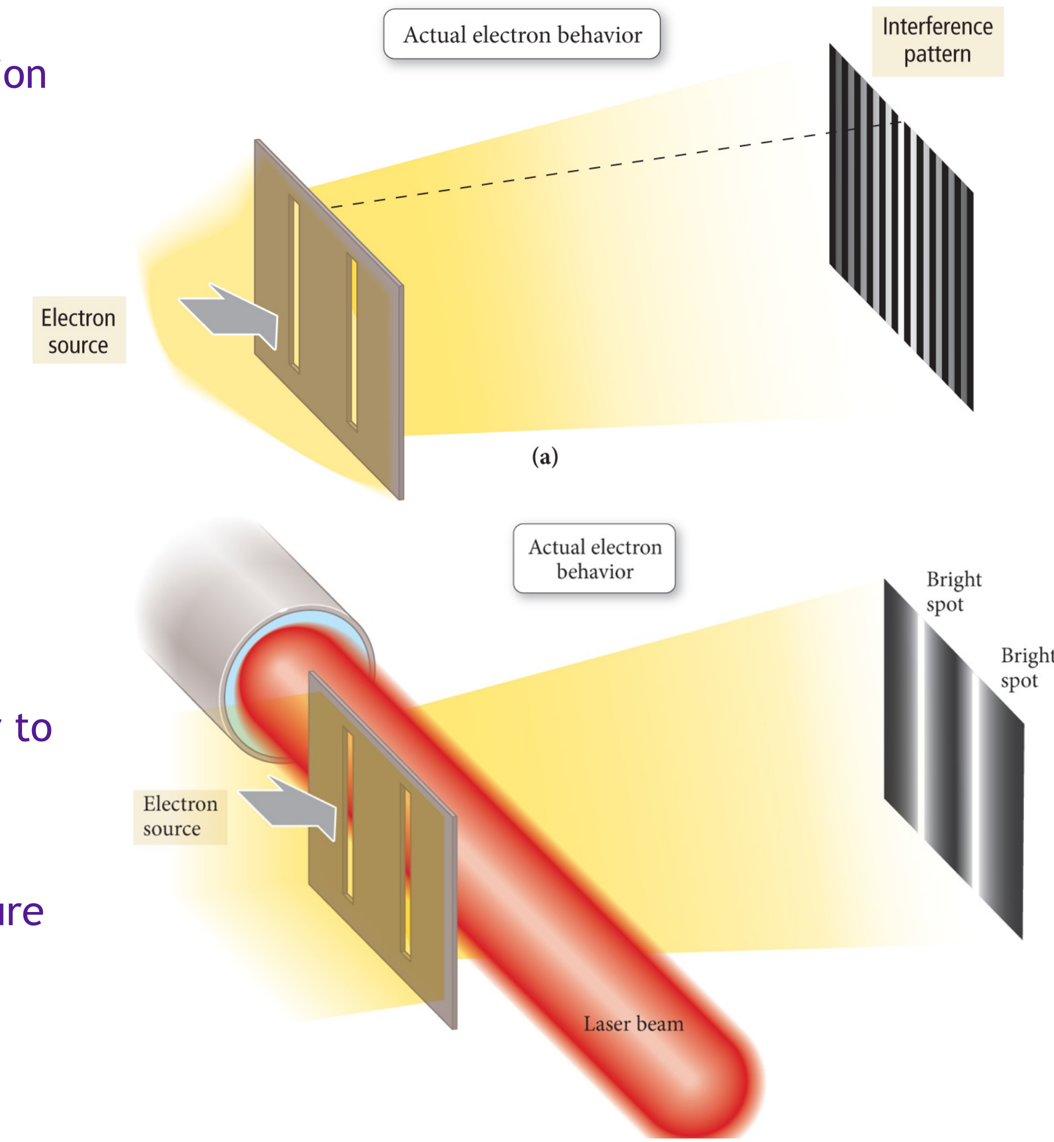
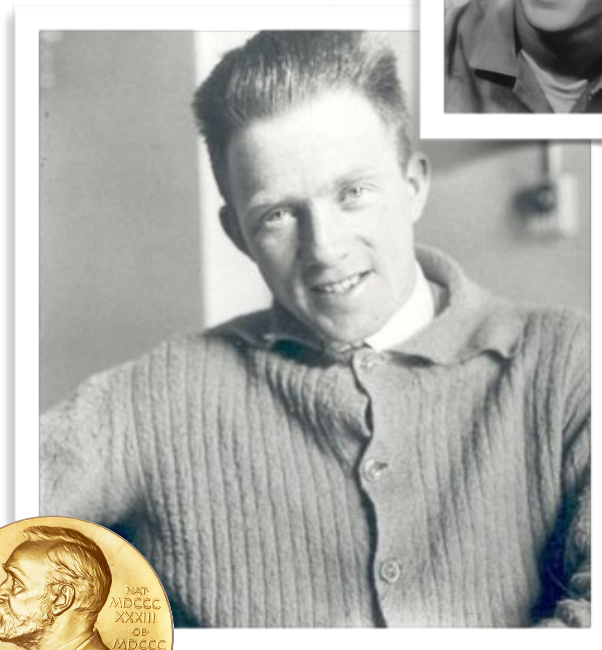
- Very small, very fast moving particles demonstrate wave behavior.
- Electron trajectories are controlled by disturbances in the e-m field.
- Interference occurs as if a single electron was a wave.
- Any attempt to observe the individual particle interacts with the e-m field.
- That interaction causes the wave behavior to collapse.
- And the electron looses it's wave nature.
- We cannot observe both the it's wave nature and particle nature at the same time.



Heisenberg & Uncertainty

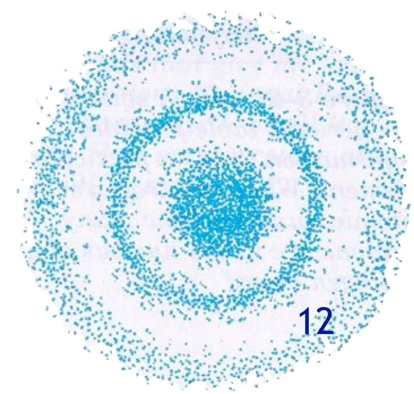


- The biggest problem with exploring the Bohr model was it was based on classical mechanics.
- It treated subatomic particles, like particles — bits of matter.
- Starting with de Broglie's matter wave equation, Werner Heisenberg showed that there was an inherent uncertainty in our knowledge of both the position and velocity of a particle.

$$\Delta x \times m\Delta v \geq \frac{h}{4\pi} \qquad \frac{h}{4\pi} = 5.27 \times 10^{-35}$$

$$\Delta x \times \Delta v \geq \frac{h}{m_e \times 4\pi} = 5.79 \times 10^{-5}$$

- Electrons move at a speed of about 5 x 10^6 m/s. If we could determine that speed to within 1% (an uncertainty of 5 x 10^4 m/s), the uncertainty in position would be a nanometer (10^{-9} m).
- The diameter of a hydrogen atom is around 10 nanometers (1.06 x 10^{-10} m).
- Heisenberg showed that classical mechanics could not even be used to demonstrate an electron remains in an atom, much less in some specific orbit within the atom.
- Werner Karl Heisenberg showed us we would have to abandon classical mechanics if we wanted to understand the atom.
- The Nobel Prize in Physics 1932 was awarded to Werner Heisenberg "for the creation of quantum mechanics, the application of which has, inter alia, led to the discovery of the allotropic forms of hydrogen".



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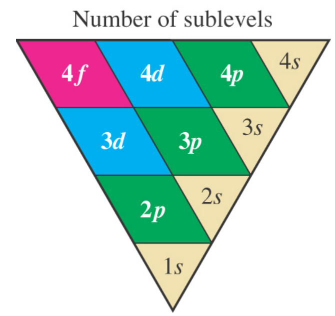
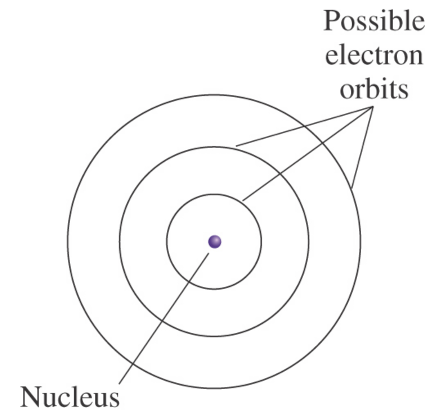
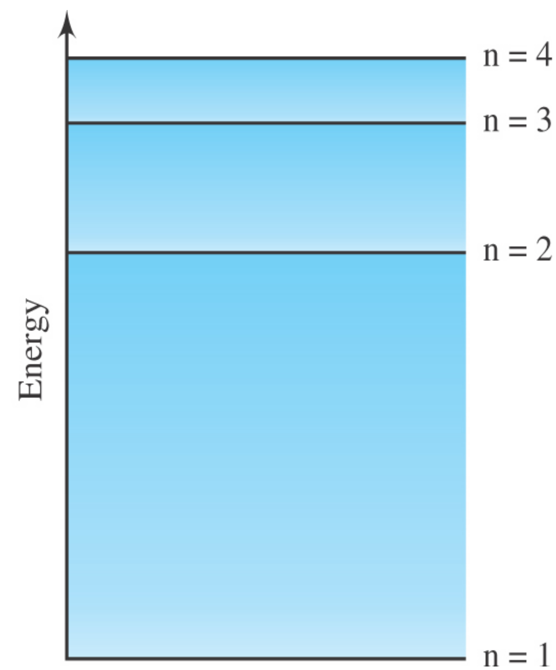
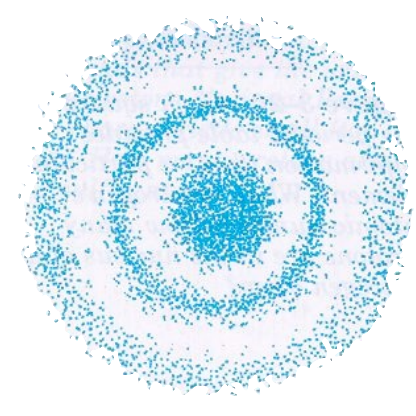


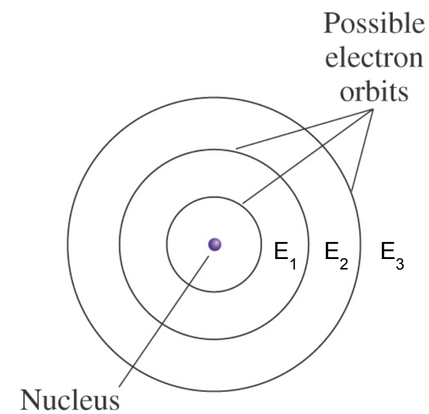


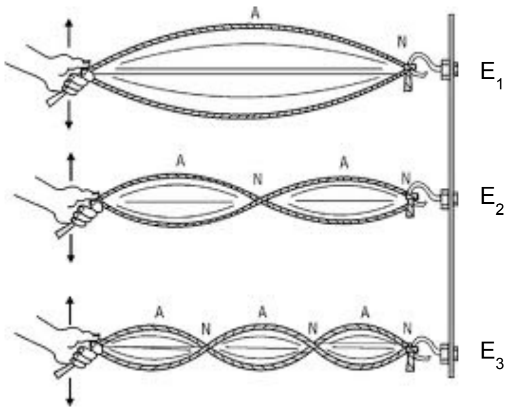


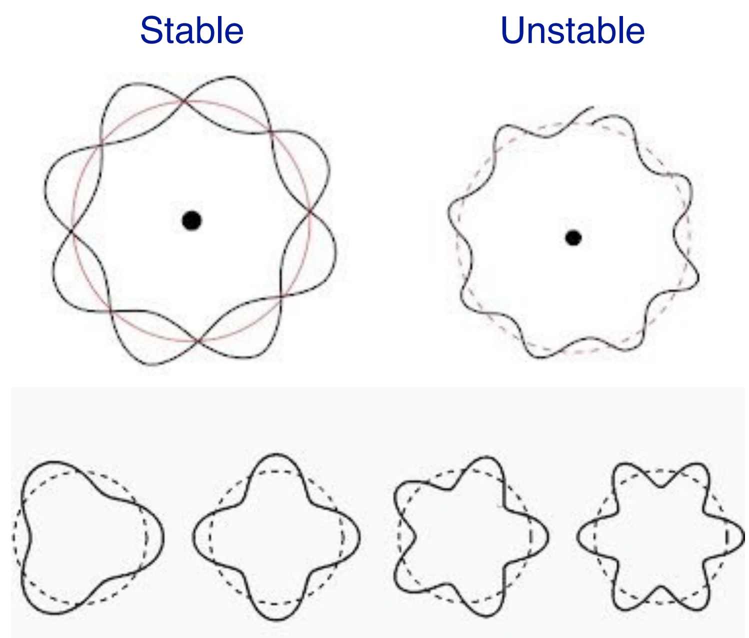


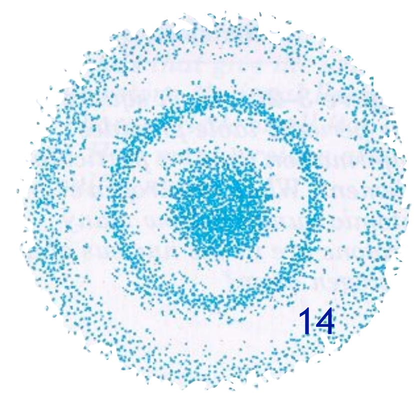
The Schrödinger Equation: Allowed Orbits

- Erwin Schrödinger produced a model of the Bohr atom that described electrons not as particles, but as waves.
- His model was based on de Broglie's mathematics.
- We won't explore the the mathematical details of that model, we'll represent it as the symbol psi (ψ).
- The first consequence of looking at electrons as waves rather than particles was to explain why only certain energy levels existed.
- Only certain energies create stable, standing waves, in a jump rope.
- Only certain energies create stable orbitals in an atom.









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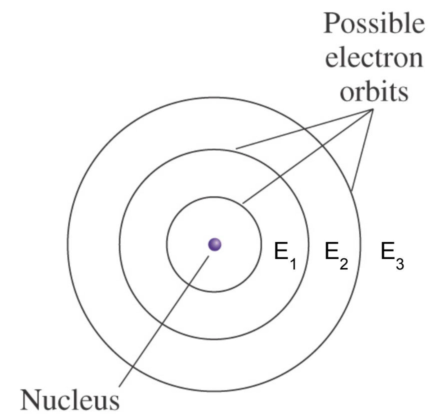
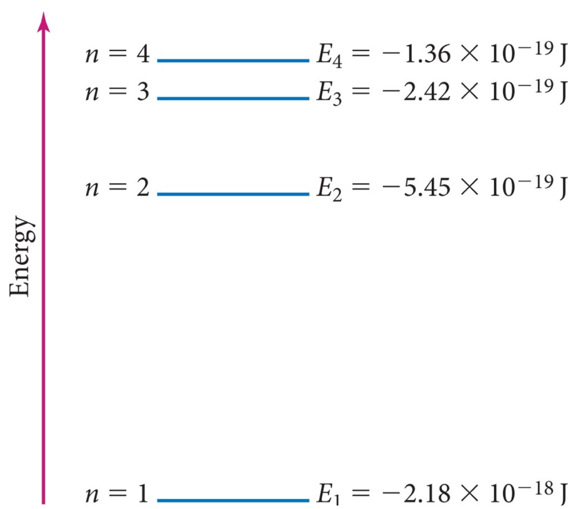
- The first consequence of looking at electrons as waves rather than particles was to explain why only certain energy levels existed.
- Only certain energies create stable, standing waves, in a jump rope.
- Only certain energies create stable orbitals in an atom.
- The allowed energy levels are defined by three numbers:
  - The Principle Quantum number (n) defines the size of the orbital.
  - The Angular Momentum Quantum number (l) defines the shape of the orbital.
  - The Magnetic Quantum number (m_l) defines the orientation of the orbital.



$$\hat{H}\psi = E\psi$$

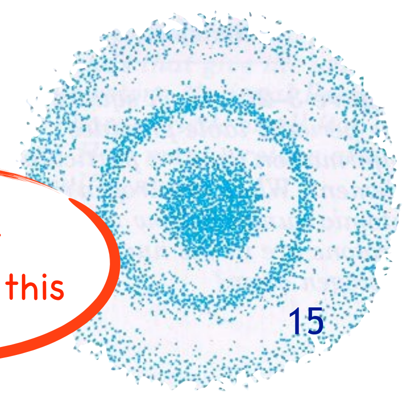


For hydrogen, the description collapses into the Rydberg Equation, which reproduces the energy levels Bohr described.

$$E_n = -2.18 \times 10^{-18} J \left(\frac{1}{n^2}\right)$$

only works for hydrogen!

do not memorize this



Calculating Energy Transitions

- How much energy is released when an electron falls from n=5 to the n=2?

$$E_5 = -2.18\times10^{-18}\,J\left(\frac{1}{5^2}\right) = -8.72\times10^{-20}\,J$$

$$E_2 = -2.18\times10^{-18}\,J\left(\frac{1}{2^2}\right) = -5.45\times10^{-19}\,J$$

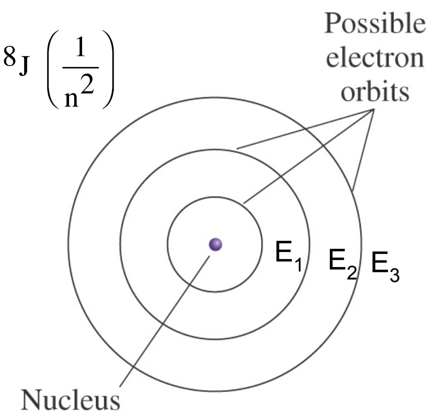
$$\Delta E = E_F - E_I = E_2 - E_5$$
$$= -5.45\times10^{-19}\,J - (-8.72\times10^{-20}\,J)$$
$$= -4.58\times10^{-19}\,J$$

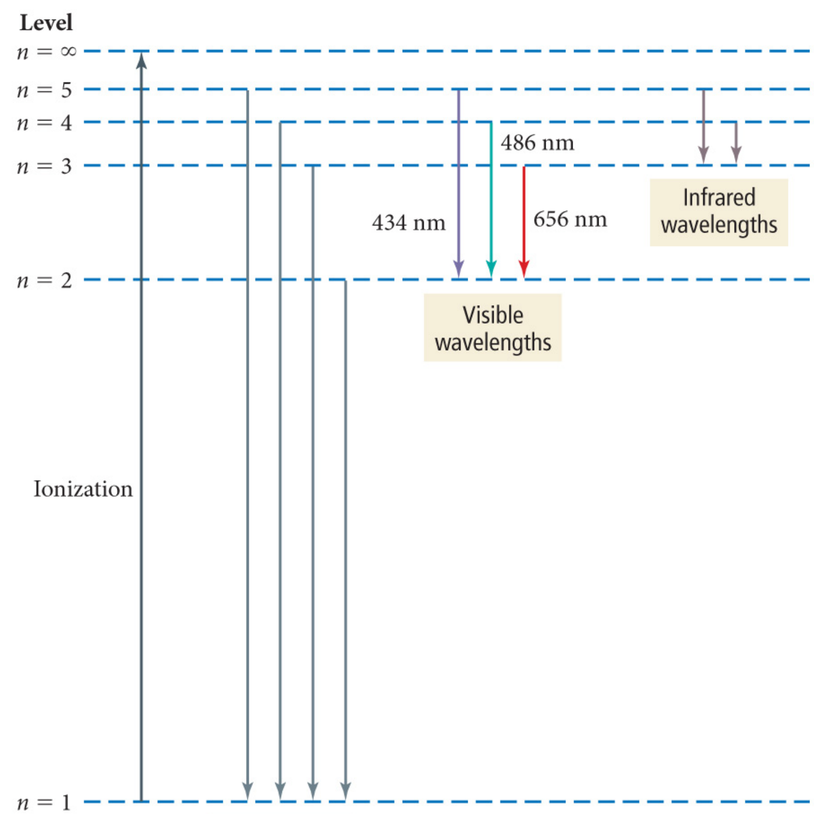
- What color light is emitted when it does?

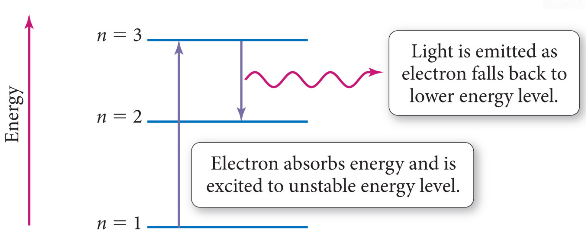
$$E = h\nu \qquad c = \lambda\nu \qquad E = \frac{hc}{\lambda}$$

$$\lambda = \frac{hc}{E} = \frac{6.626\times10^{-34}\,Js \cdot 3.00\times10^{8}\,m/s}{+4.58\times10^{-19}\,J}$$
$$= 4.34\times10^{-7}\,m \cdot \frac{n\ \ m}{10^{-9}\ m}$$
$$= 434\ nm$$

$$E_n = -2.18\times10^{-18}\,J\left(\frac{1}{n^2}\right)$$







Rydberg Equation

- The Rydberg equation predicts the energy released in an energy transition between any two states in the hydrogen atom.
- It's introduced on page 315 of the text book.
- You do not have to memorize the Rydberg equation or the Rydberg constant.
- There is one problem in the homework that requires using the Rydberg equation.

$$\Delta E = 2.178 X 10^{-18 J}\left(\frac{1}{n_{final}^2} - \frac{1}{n_{initial}^2}\right)$$

An electron in a Hydrogen atom relaxes to the n=4 level, emitting of 74 THZ. What is the value of n for the level in which the electron originated?

$$\nu = 74\ \text{THz} \cdot \frac{10^{12}\ \text{Hz}}{\text{T Hz}} = 7.4\times10^{13}\ \text{Hz}$$

$$E = h\nu = 6.626\times10^{-34}\ \text{Js} \cdot 7.4\times10^{13}\ \text{Hz}$$

$$= 4.9\times10^{-20}\ \text{J}$$

$$\Delta E = 2.178\times10^{-18}\ \text{J}\left(\frac{1}{n_F^2} - \frac{1}{n_I^2}\right)$$

$$-4.9\times10^{-20}\ \text{J} = 2.178\times10^{-18}\ \text{J}\left(\frac{1}{n^2} - \frac{1}{(4)^2}\right)$$

$$-2.3\times10^{-2}\ \frac{\text{J}}{\text{J}} = \frac{1}{n^2} - \frac{1}{16}$$

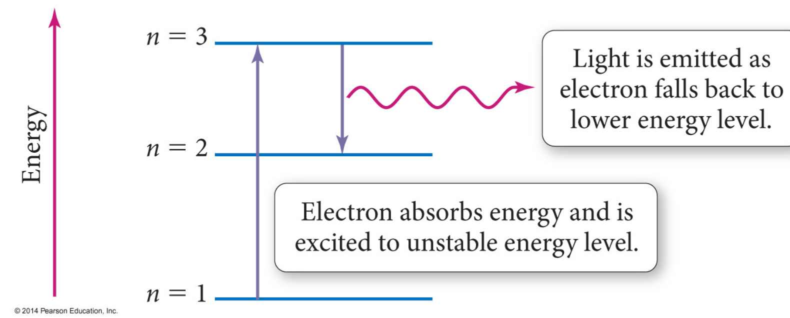
$$-2.3\times10^{-2} + 0.0625 = \frac{1}{n^2}$$

$$0.0395 = \frac{1}{n^2}$$

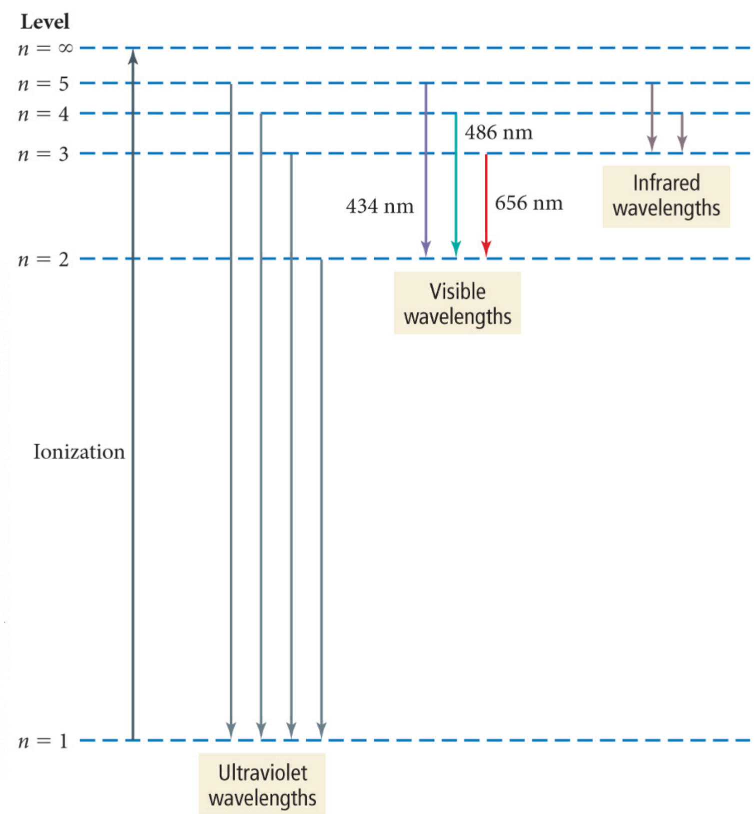
$$n^2 = \frac{1}{0.0395} = 25$$

$$n = 5$$

Excitation and Radiation



Hydrogen Energy Transitions and Radiation



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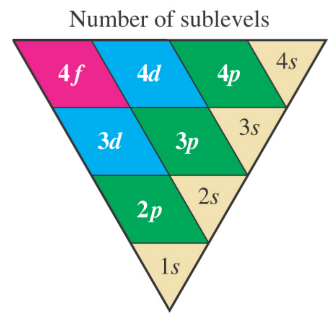

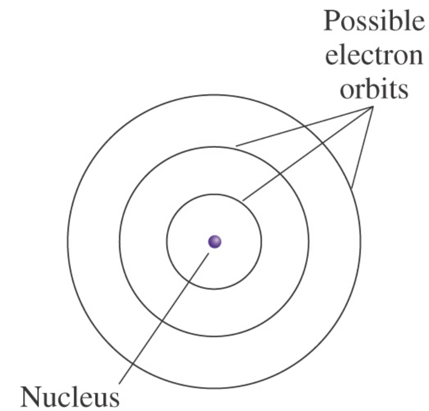

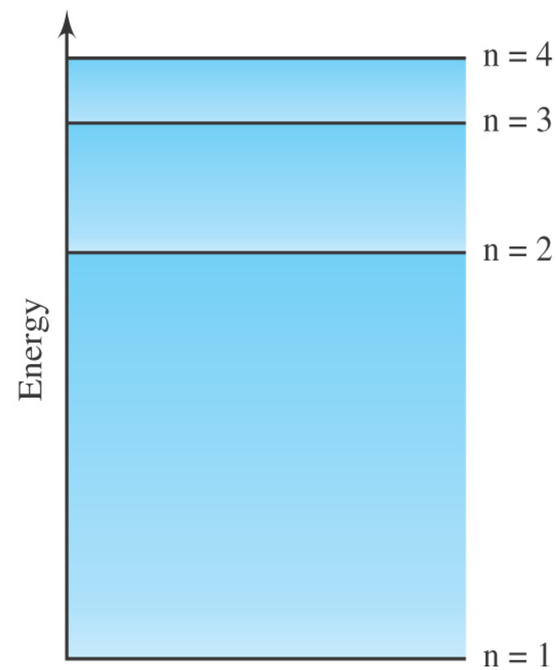

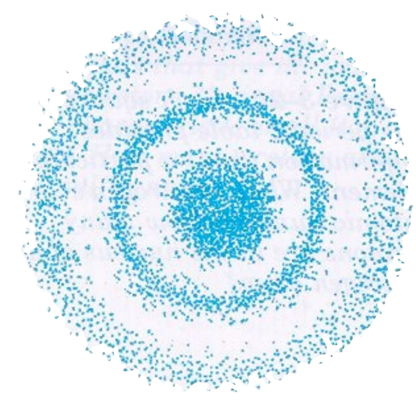

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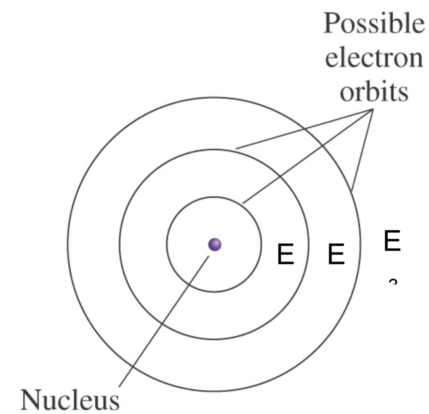

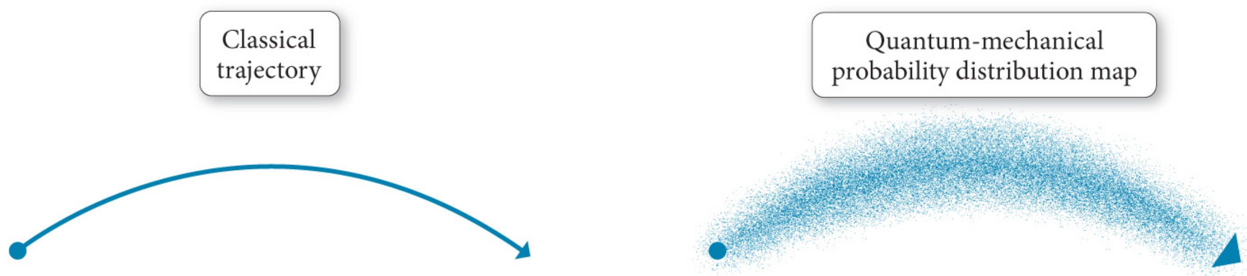

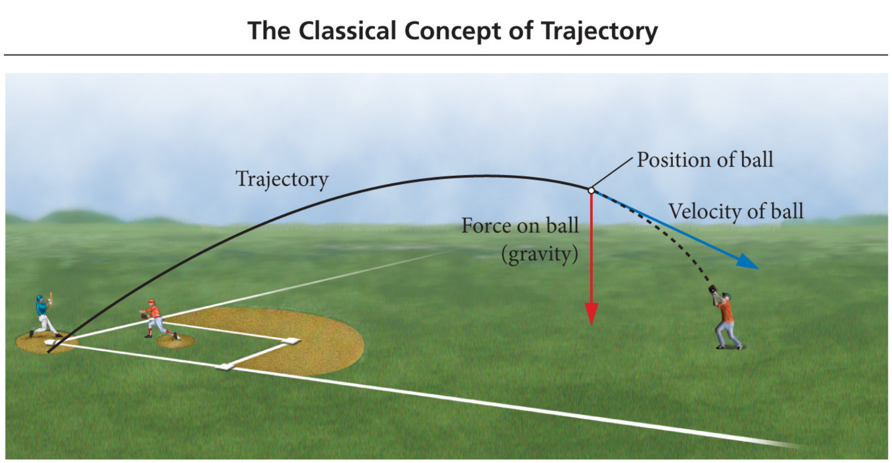

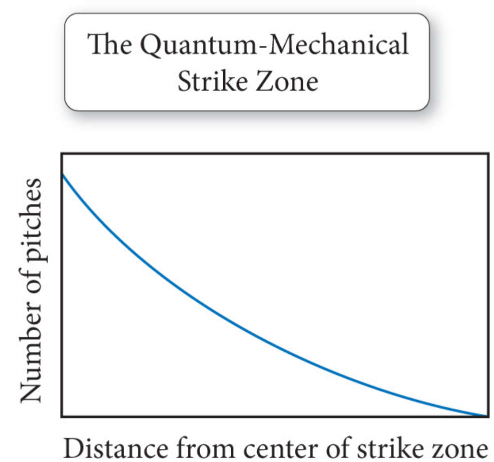

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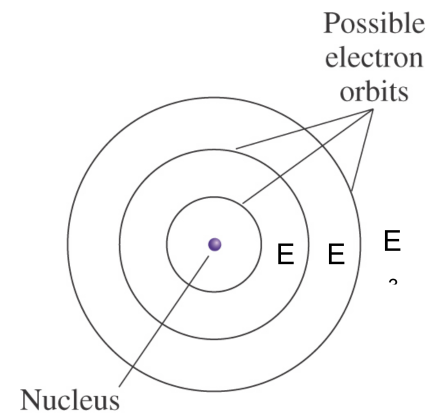

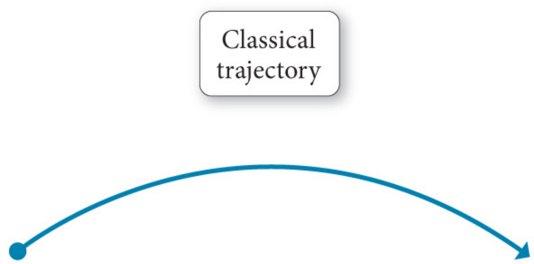

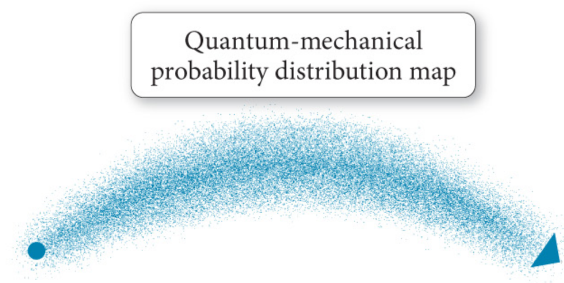

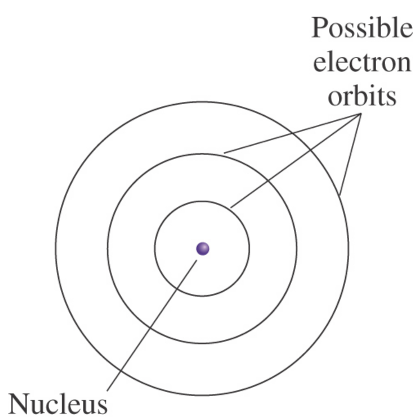

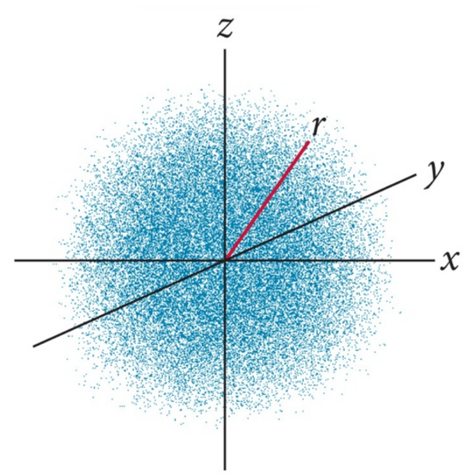

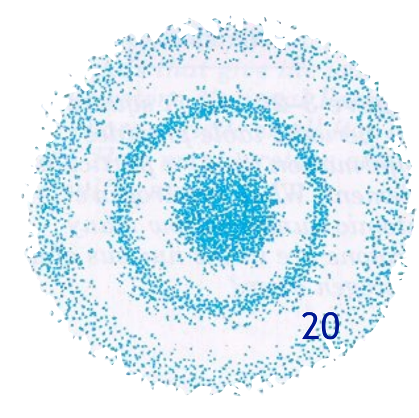

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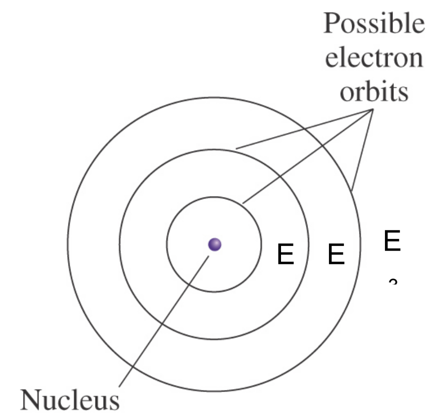
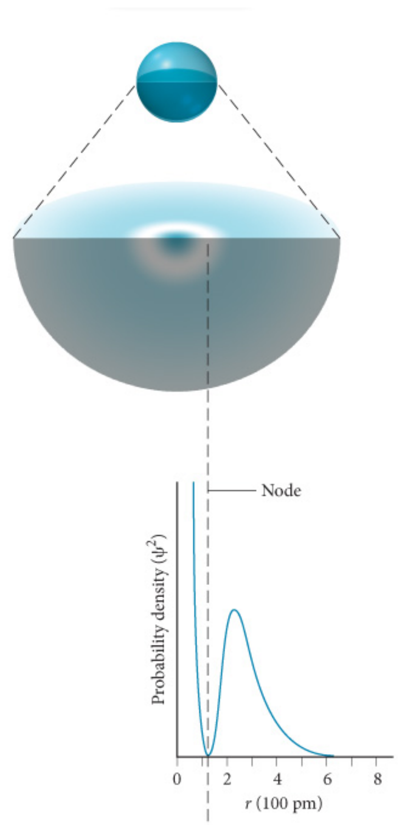
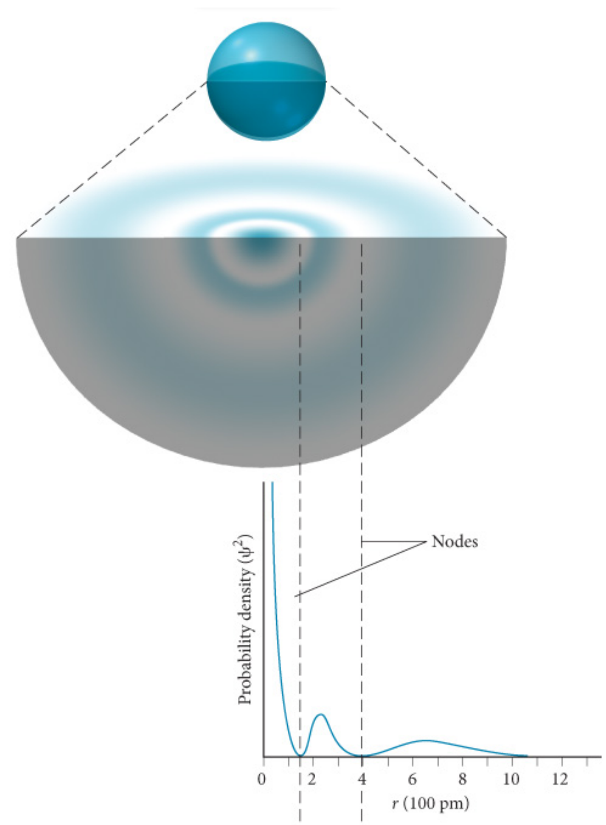
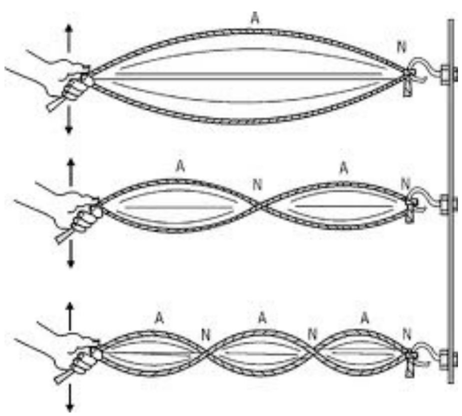
- Instead we describe electron motion as probability field, denser where the particle is more likely to be, sparse where it is less likely to be.
- As n increases, the size of the orbital increases.
- Larger orbitals encompass smaller ones.
  - n=1 orbitals are inside
  - n=2 orbitals are inside
  - n=3 orbitals etc



2s







1s

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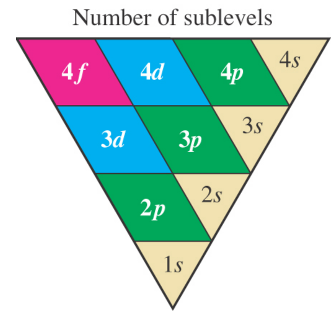
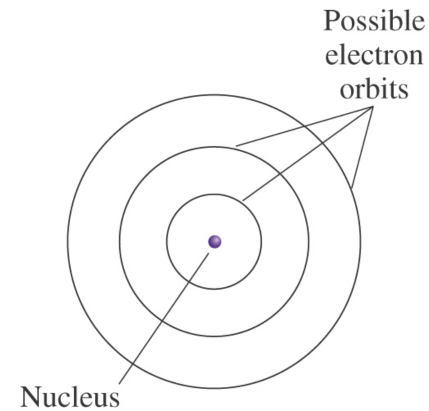
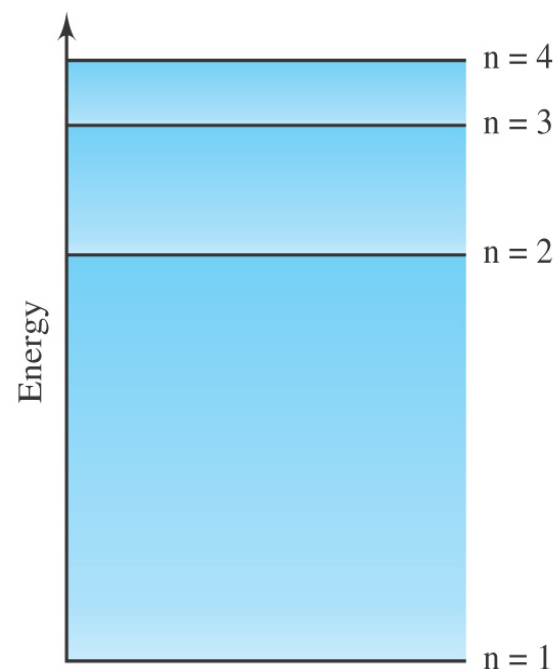
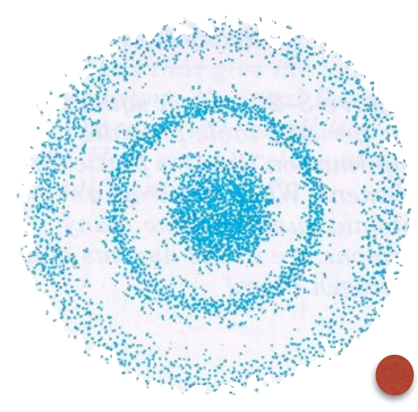
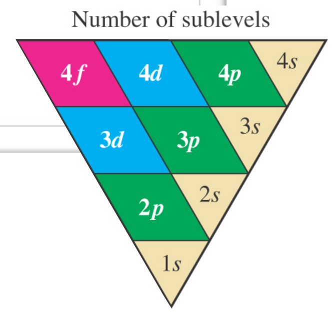




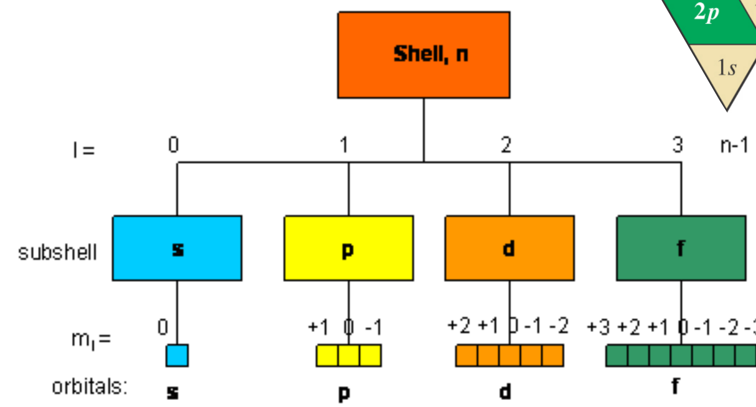




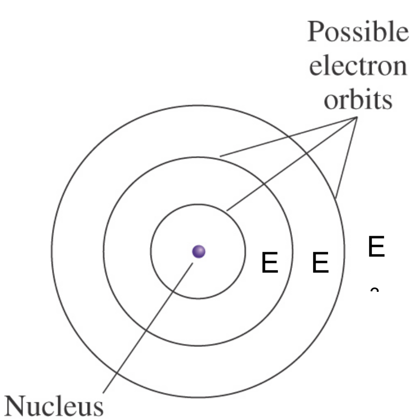
Quantum Numbers

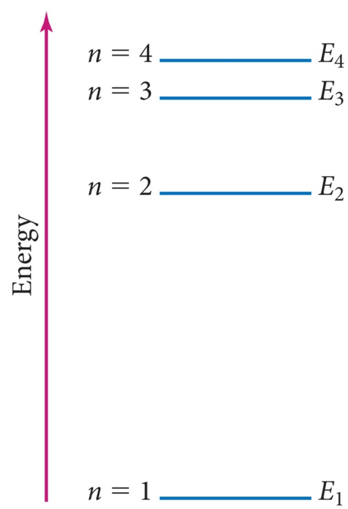


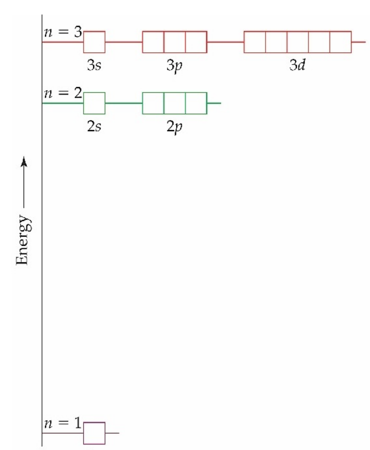
- The Principle Quantum number (n) defines the size of the orbital.
- The Angular Momentum Quantum number (l) defines the shape of the orbital.
  - l has a range of 0 to n -1
  - the shapes also have names
    - l = 0 are "s" orbitals
    - l = 1 are "p" orbitals
    - l = 2 are "d" orbitals
    - l = 3 are "f" orbitals
- The Magnetic Quantum number (m_l) defines the orientation of the orbital.
  - m_l has a range of +l to -l



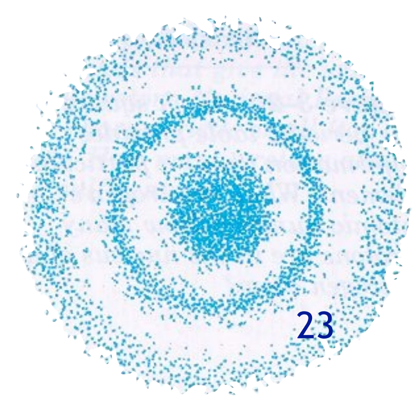
Quantum Number	Sym bol	Values	Meaning
principal	n	1,2,....	Determine size and energy level. For H, energy depend only on n. (Shell)
angular mom.	l	0,1,... ,n -1	Determine 3D shape of orbitals: 0 =s, 1=p, 2=d, 3=f (Subshell l = 0,1,2,3,.)
magnetic	m_l	-l, l-1, ... -l	Spatial orientation of orbitals.







- Their are n^2 sub-levels at each level n.
  - One at n=1
  - four at n=2
  - nine at n=3
  - sixteen at n=4, and so on.



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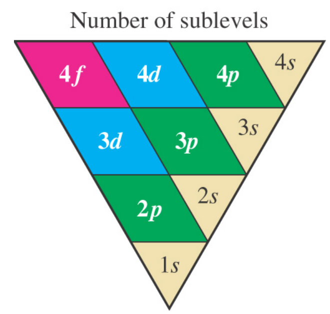
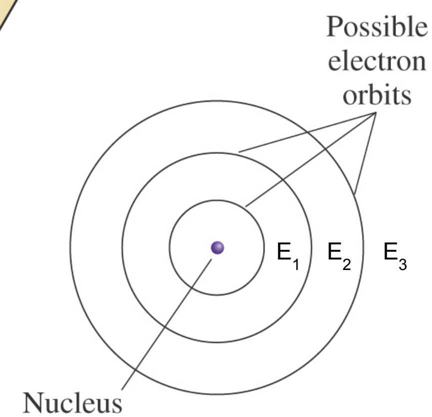
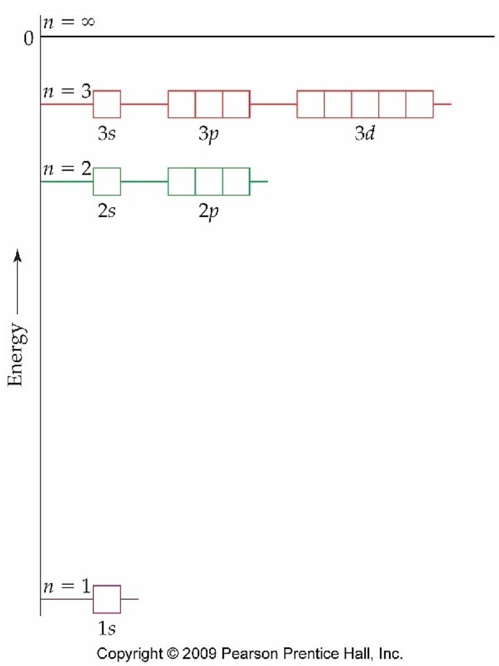
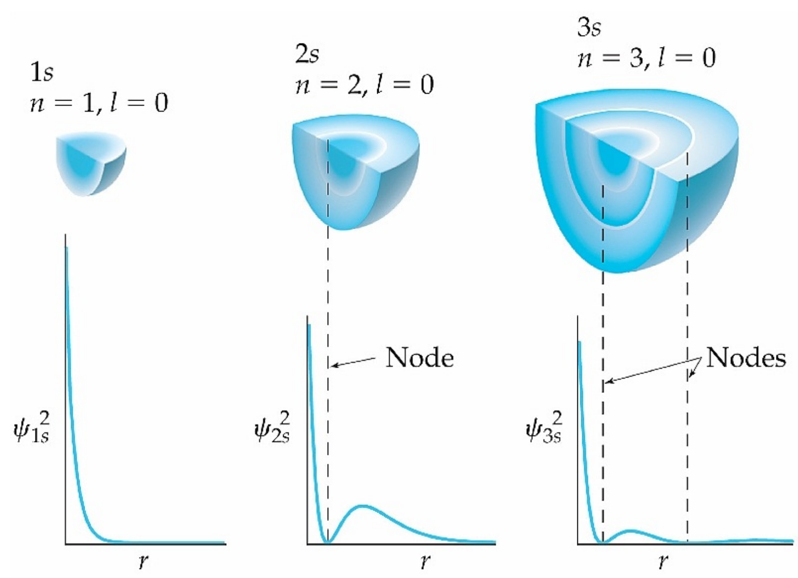
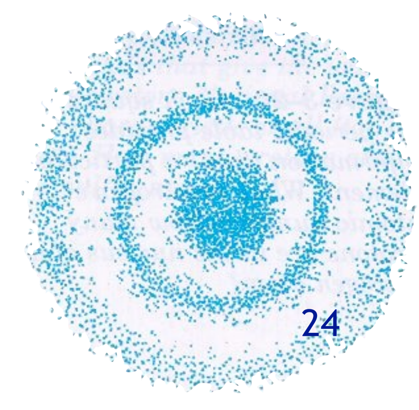






S orbitals are Spherical





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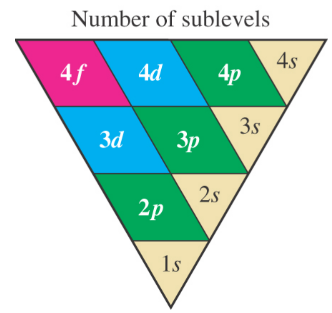
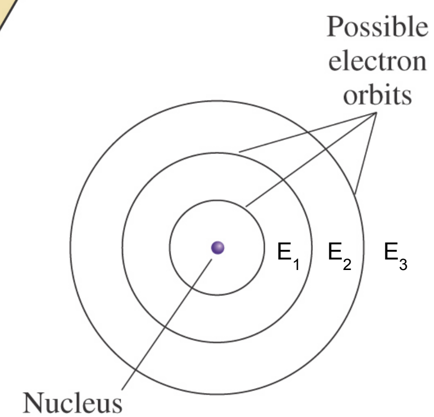
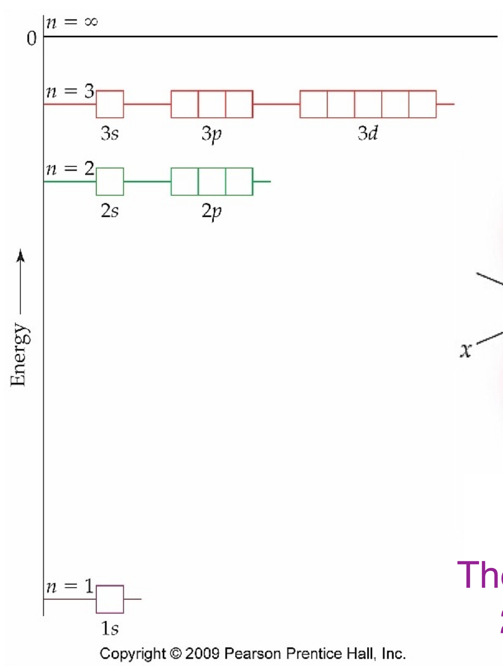
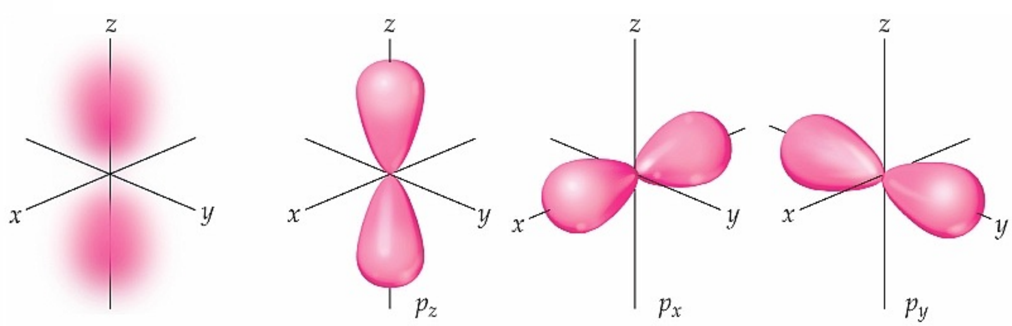




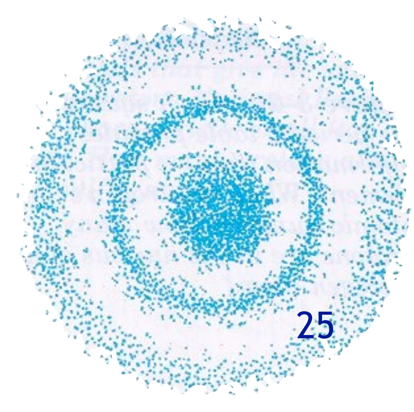


P orbitals are Pear shaped



(note each P orbital has one nodal plane)

The three sub-levels are named with x, y, and z subscripts.
$2p_z$ looks just like $3p_z$, except the n=3 orbital is larger.



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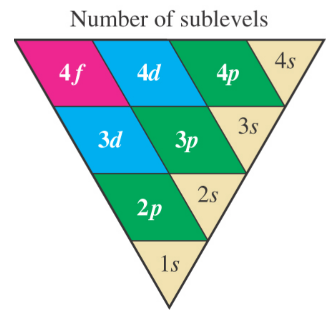

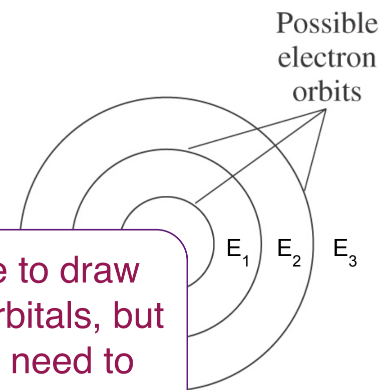

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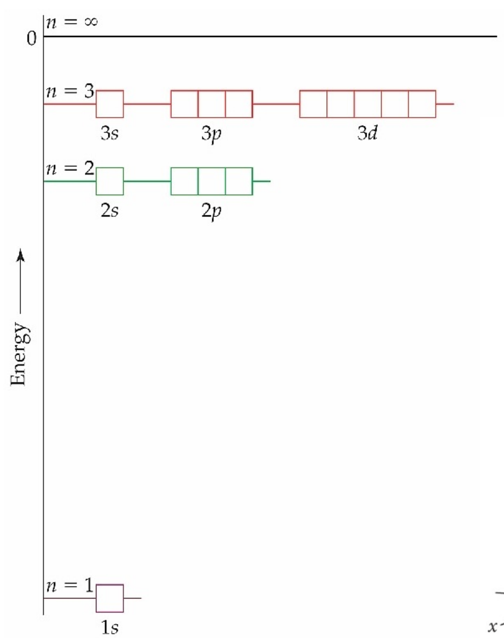
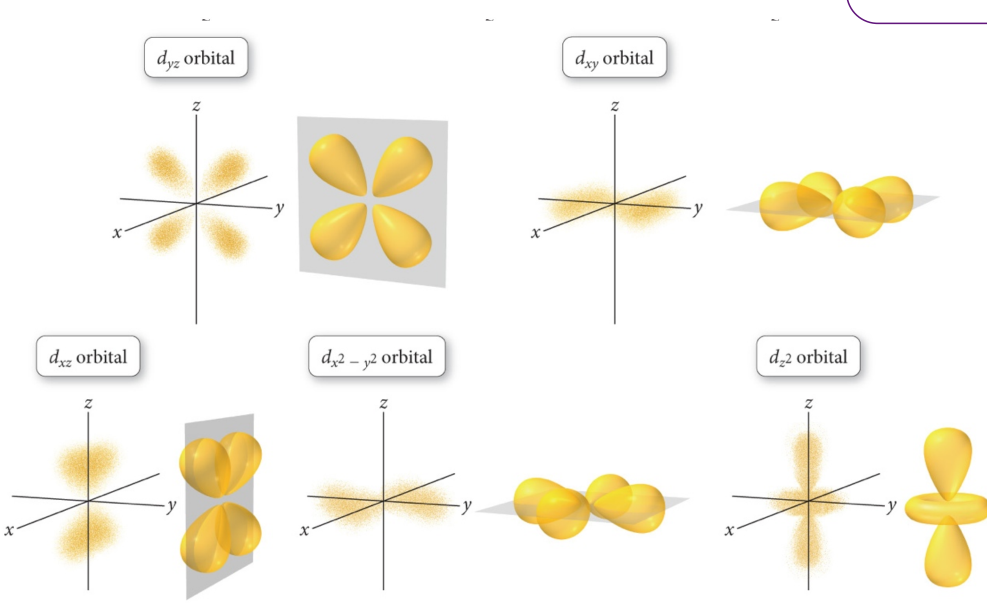
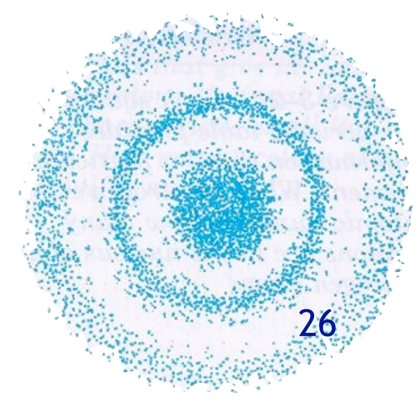
d: five orbitals
f: seven orbitals



D orbitals have Double nodal planes





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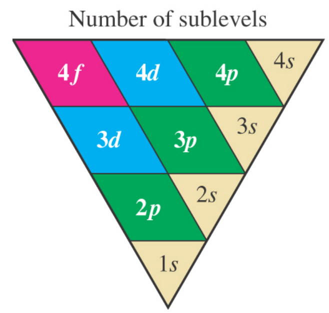

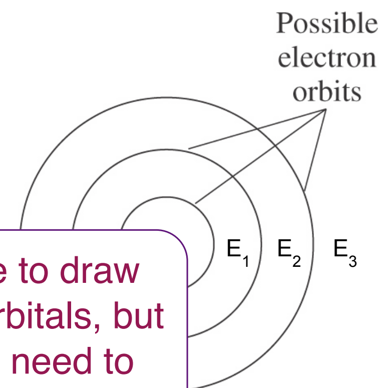

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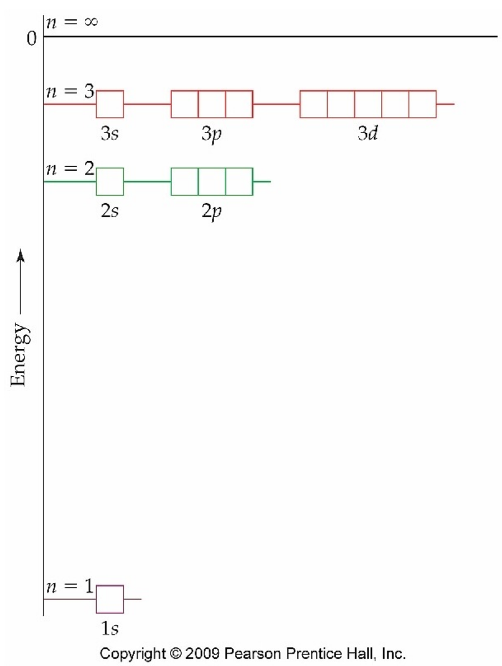
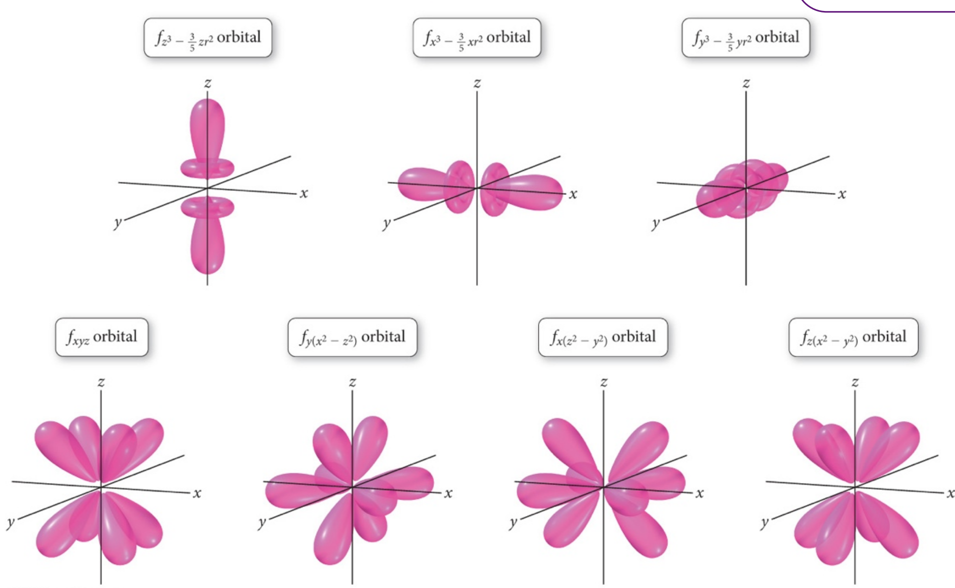
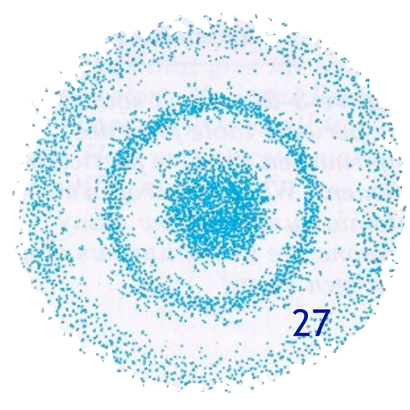


F orbitals ... are just weird





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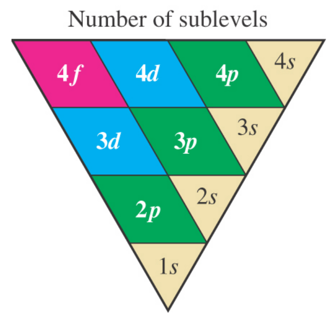
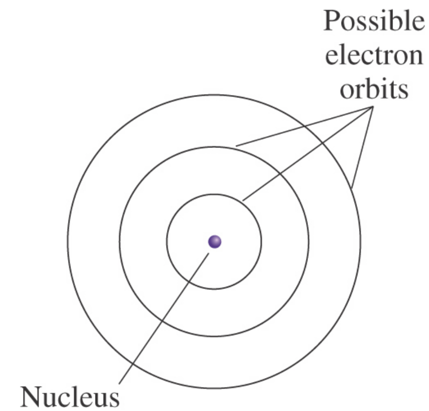
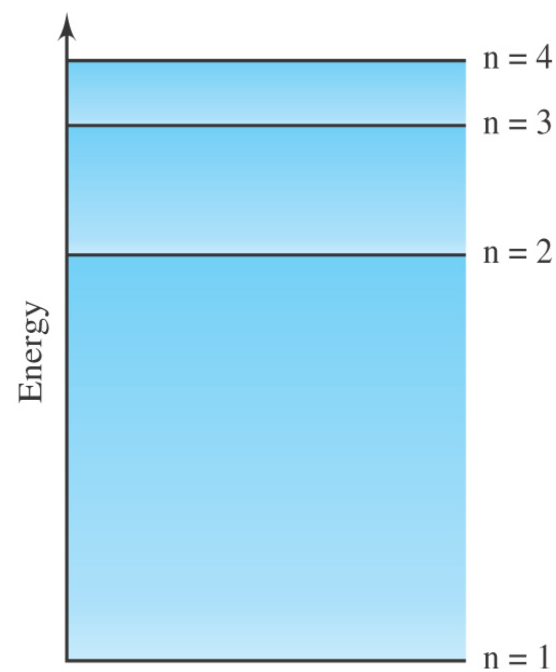
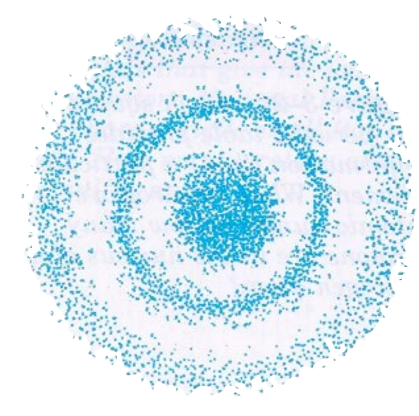


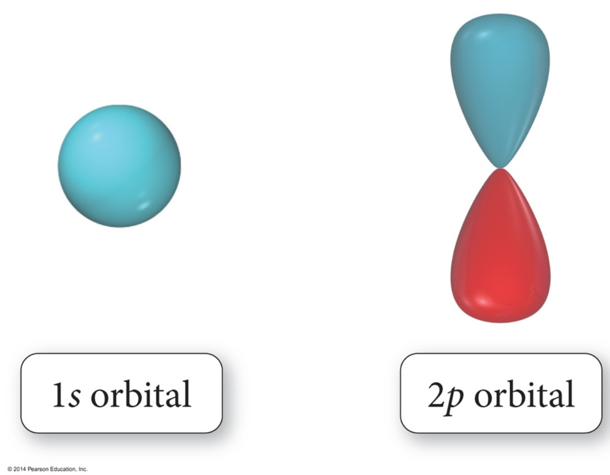


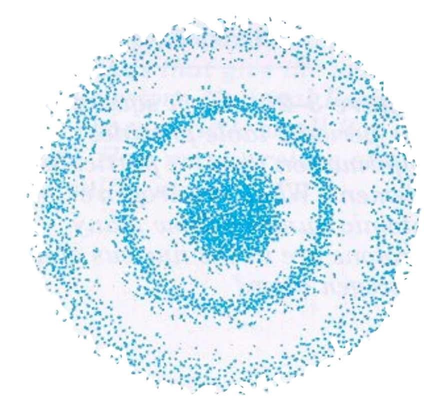




Orbital Phases

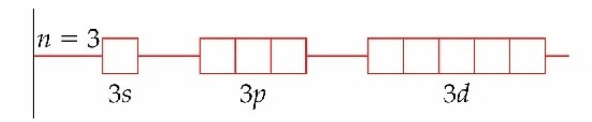
- Orbitals are waves.
- Waves have phases.
- It's important to understand orbitals also have phases.
- Phases are indicated by coloring either side of a node with different colors.

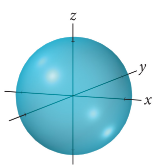


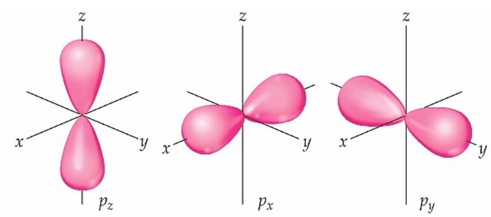


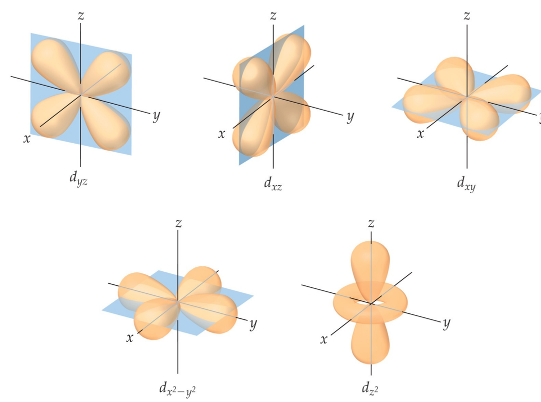
Atomic Shape & Orbital Size

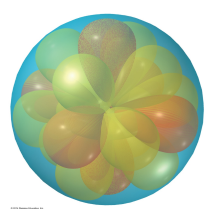
- At any given energy level n, the sum of all the orbitals approximates a sphere.
- This is why we draw atoms as spheres.

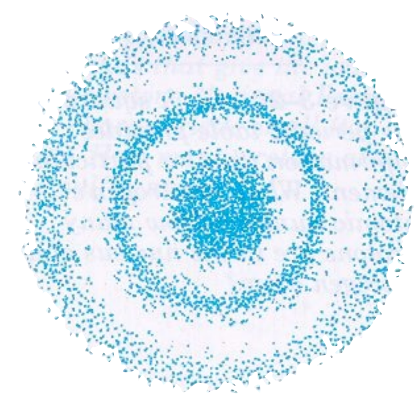




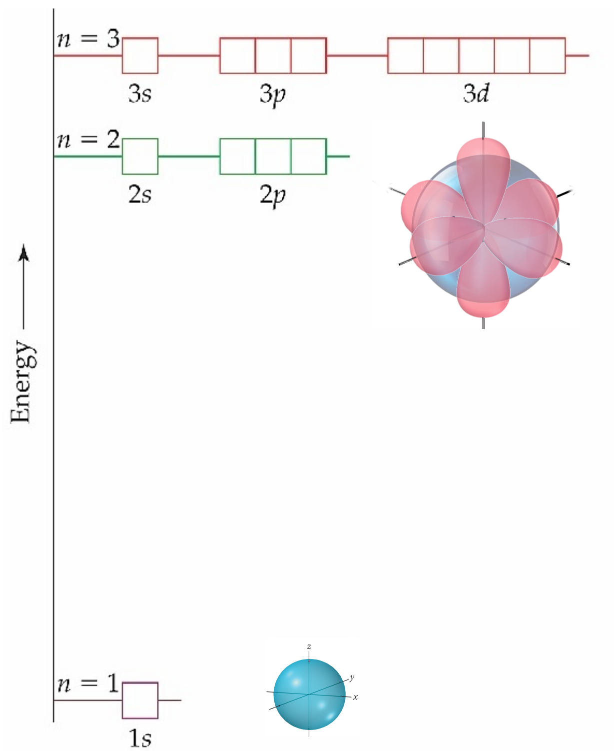


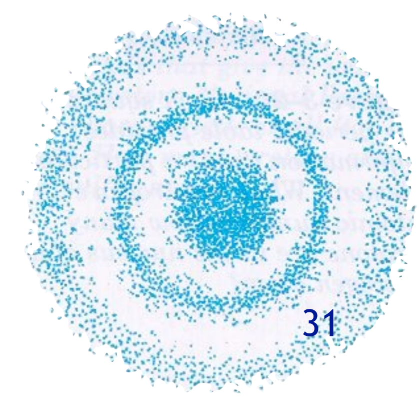






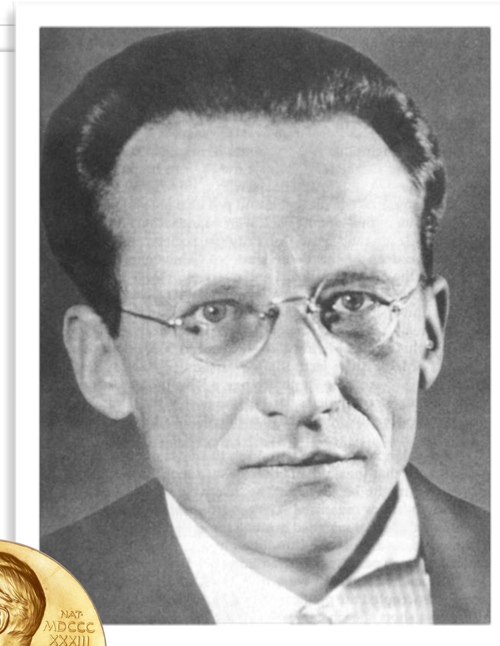
- All orbitals of a given type are identical in shape, but larger in size depending on the value of n.

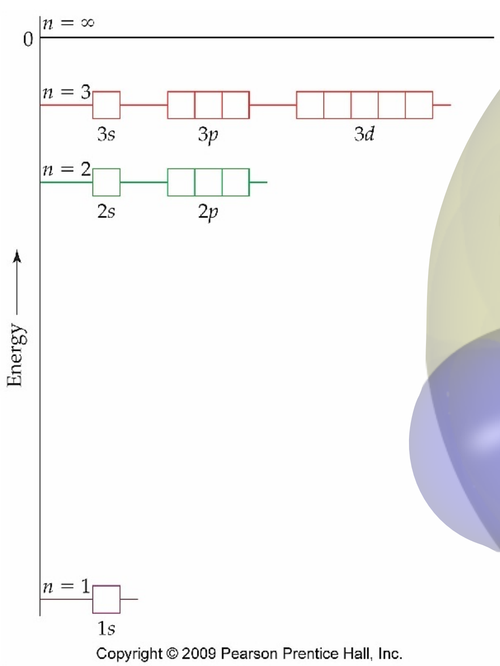


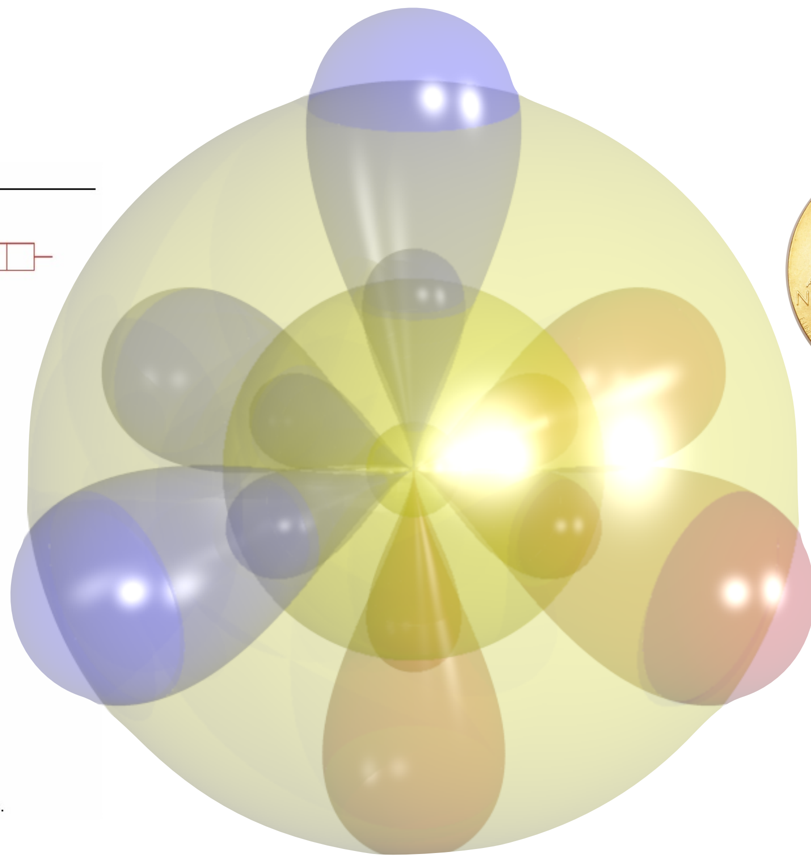


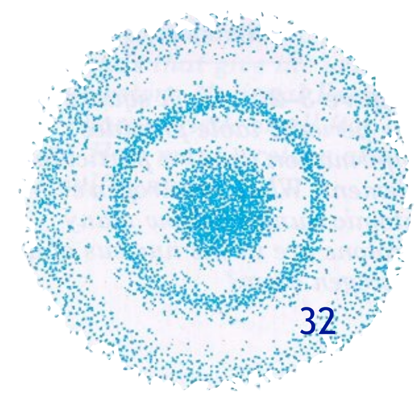
Erwin Schrödinger

- Erwin Schrödinger produced a model of the Bohr atom that described electrons not as particles, but as waves.
- The Nobel Prize in Physics 1933 was awarded jointly to Erwin Schrödinger and Paul Adrien Maurice Dirac "for the discovery of new productive forms of atomic theory."
- Schrödinger produced the quantum model of the atom.

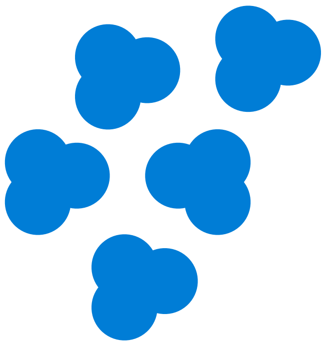




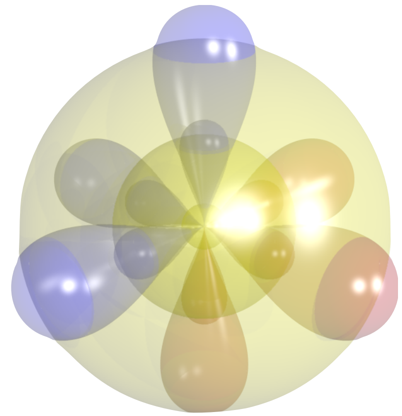




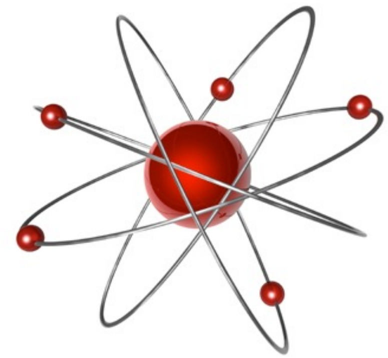
Evolution of the atom.



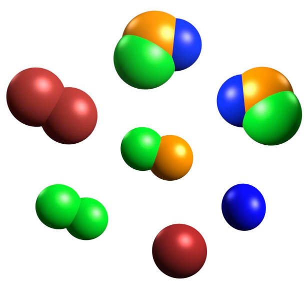
Atomos.



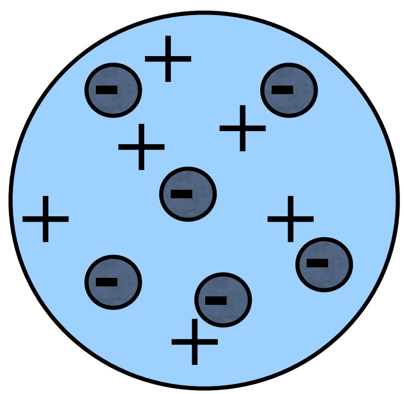
The quantum atom.



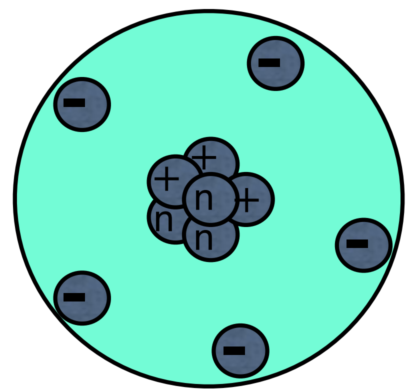
The planetary model.



Molecules & Compounds.
Elements, flavors of the atom.



The plum pudding model.

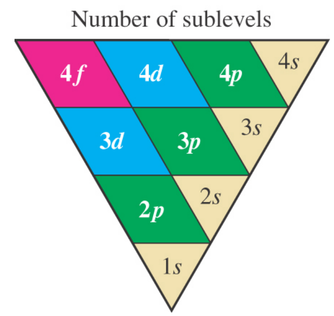


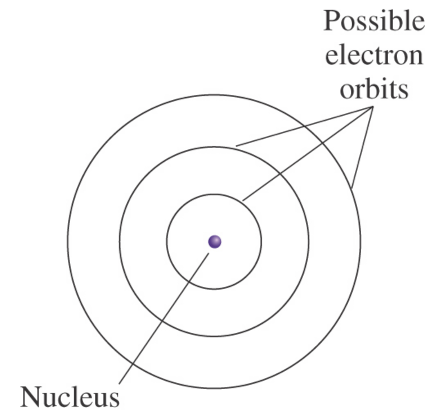
The nuclear atom.

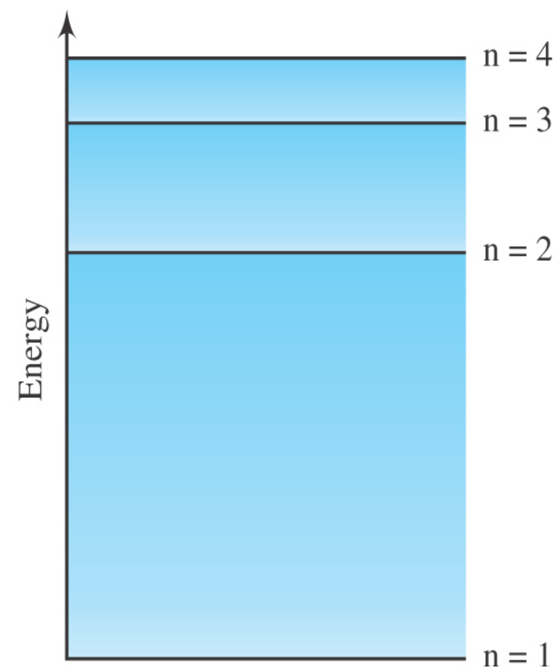
Ch07

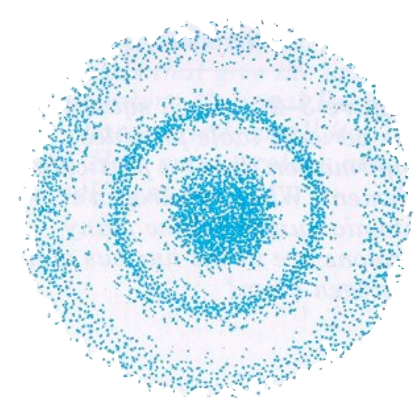
The Wave Nature of Matter

- Problems with the Bohr Model
- New Math & the Wave nature of Matter
  - The de Broglie Hypothesis
    - Davisson-Thomson Experiment
  - Heisenberg & Uncertainty
- The Schrödinger Equation
  - Energy Levels
    - Allowed States
    - Quantum Numbers
      - n, l, m_l, m_s
  - Orbitals replace Orbits
    - Probability Fields
  - Sub Levels Exist
    - s orbitals
    - p orbitals
    - d orbitals
    - f orbitals
  - Orbital Phases
  - Atomic Shape & Orbital Size









Questions?