The Hydrogen Atom

Sam McKagan August 29, 2006 Draft 4

Changes in Draft 2

- Get rid of option to fire electrons this option doesn't provide any info you can't get from firing photons, is a lot of work, and may exacerbate cognitive overload.
- Change pull down menu for gun type to radio buttons, so students can always see what the options are.
- Fixed some errors in the discussion of the behavior of alpha particles

Changes in Draft 3

- The format of the slider to switch between models should be changed, but I am leaving the same picture here as a placeholder.
- Replace light switch with a different kind of switch.
- Change light source control to radio buttons.
- Change on button on gun as recommended by Chris. (talk to Sam about making QWI gun consistent)
- Replace "copy spectrometer with camera icon, talk to Sam about doing the same with copy screen in QWI, make copy a little grayer than original and label it.
- Add play/pause/step.
- Remove most of the functionality of solar system model.
- Added directions for behavior of ionized/destroyed atoms.
- Added black boxes for background of all models to be consistent with the idea that black is a vacuum.

Changes in Draft 4

- Show about 6 atoms instead of one, through magic hole in box, like coffee cup in Microwaves sim.
- Switch order of "Experiment" and "Prediction" on switch and start with prediction and billiard ball model as default.
- Change label on gun from "photons" to "light."
- Add "Show spectrometer" checkbox off as default.
- Change "solar system" to "classical solar system."
- Change "Models are not to scale" to "Drawings are not to scale."
- Add learning goal "Engage in model building."
- Add directions for calculating Schrodinger model electron distributions.

Learning Goals

- Visualize different models of the hydrogen atom.
- Explain the similarities for each model.
- Explain what experimental predictions each model makes.
- Explain why people believed in each model and why each historical model was inadequate.
- Explain the difference between the physical picture of the orbits and the energy level diagram of an electron.
- Gain a sense for how scientists build models.
- Engage in model building.

Overview

- There is a gun which students can use to perform experiments on the atom, including shooting light (white or single color) or alpha particles at it.
- Students can switch between "experiment" mode, in which they see the outcome of a real experiment on the atom but cannot see inside the atom, and "prediction" mode, in which the model of the atom is explicit, and they can observe what each model would predict for the outcome of an experiment. The only case in which all predictions match the real experiment is for the Schrodinger model.
- Students can change the settings of the gun, but settings (except spectrometer) should not change when switching between models or between experiment and prediction.
- There is a spectrometer like the one in Discharge Lamps that records the number of photons of each color emitted by the atom. Spectrometer should clear when user switches models. The user should be able to copy the spectrometer like the screen in QWI so they can compare the results of two different models. The copied spectrometer, unlike the original, should be a little grayer, moveable, and closeable, but image shouldn't change. It should be labeled with the model in which it was created.

Visualization

- Photons should be represented as little balls with tails as in other sims:
- Electrons should be represented as little blue spheres as in other sims:
- Alpha particles should be represented as a glob of two red spheres (protons) and two gray spheres (neutrons) as in Nuclear Physics:

Gun

- Gun should look like the gun from QWI, with gun controls similar to those in High Intensity panel, but replace the drop down menu with radio buttons.
- Particles should come in a wide beam out of all parts of the wide mouth of the gun.
- There is an on/off button on the gun.
- There is an intensity slider for all particles. At minimum intensity, gun shoots one particle at a time, at maximum it shoots many.
- For photons, there is a wavelength slider and a checkbox for white light. If white light is checked (default), slider control removed from wavelength slider and all colors of photons come out of gun. If unchecked, only the color selected by slider comes out. Wavelength slider should include wavelengths in UV & IR that are part of hydrogen spectrum.
- For alpha particles, no controls other than intensity.

Models

- Billiard Ball giant solid sphere
- Plum Pudding squishy blob of positive goo with electron jiggling around in it. Should look as gooey and cartoonish as possible, not jagged like the picture here.
- Classical Solar System electron orbiting around tiny nucleus. Electron quickly spirals into the nucleus, emitting a steady stream of photons tangent to its path. When it reaches the nucleus, there is a huge explosion and the atom is destroyed.
- Bohr (see http://hyperphysics.phy-astr.gsu.edu/hbase/hyde.html for details) electron orbiting around nucleus along fixed paths (dotted lines) with radii ~ n², where n=1,2,3... is the number of the level. If electron is in higher orbit, it can spontaneously decay to lower orbit, emitting a photon.
- deBroglie there is no experimental difference between Bohr and deBroglie, but here electrons are represented as waves around a ring rather than electrons orbiting around a ring. The amplitude of the waves is given by sin(nx/r+ft), where x is the position along the circumference, r is the radius, n is the number of the level, and f is the frequency of oscillation. I think f should be proportional to 1/n².
- Schrodinger electrons represented as 3d probability waves.









Prediction

(what this model predicts)



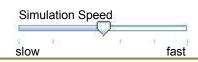
Experiment

(what really happens)



Light source:

white \(\text{\text{\text{monochromatic}}}\)

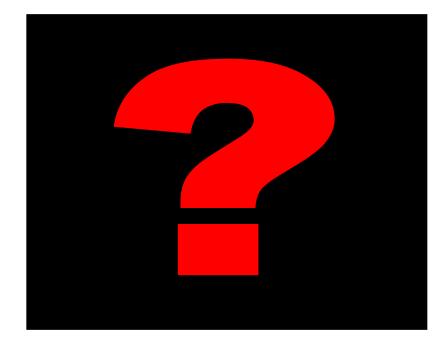


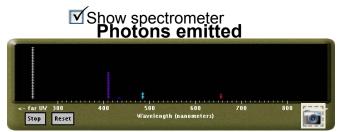


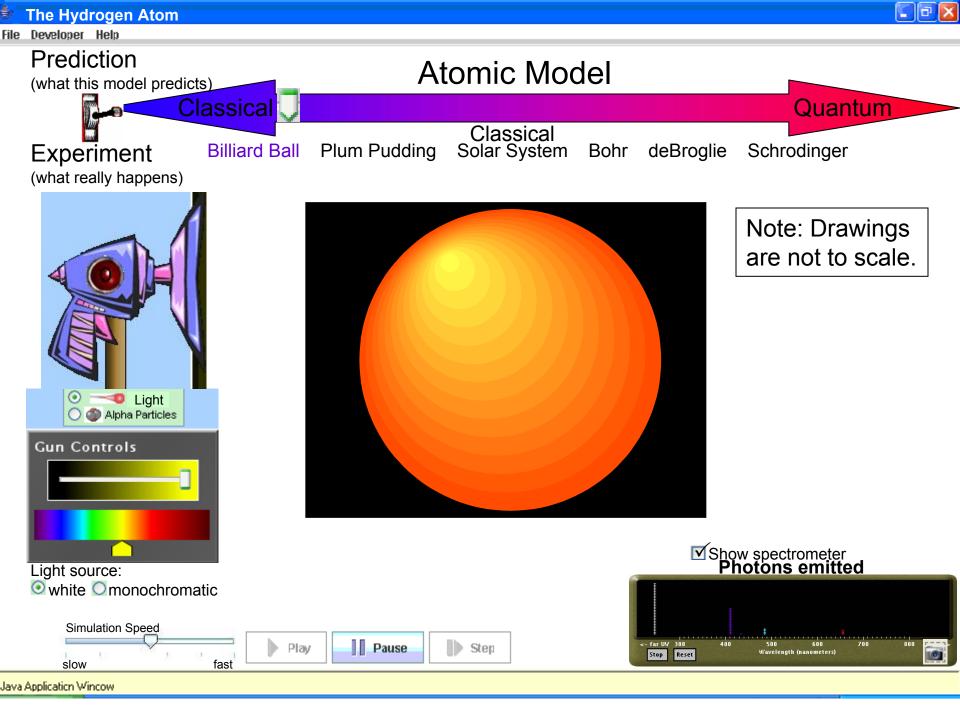


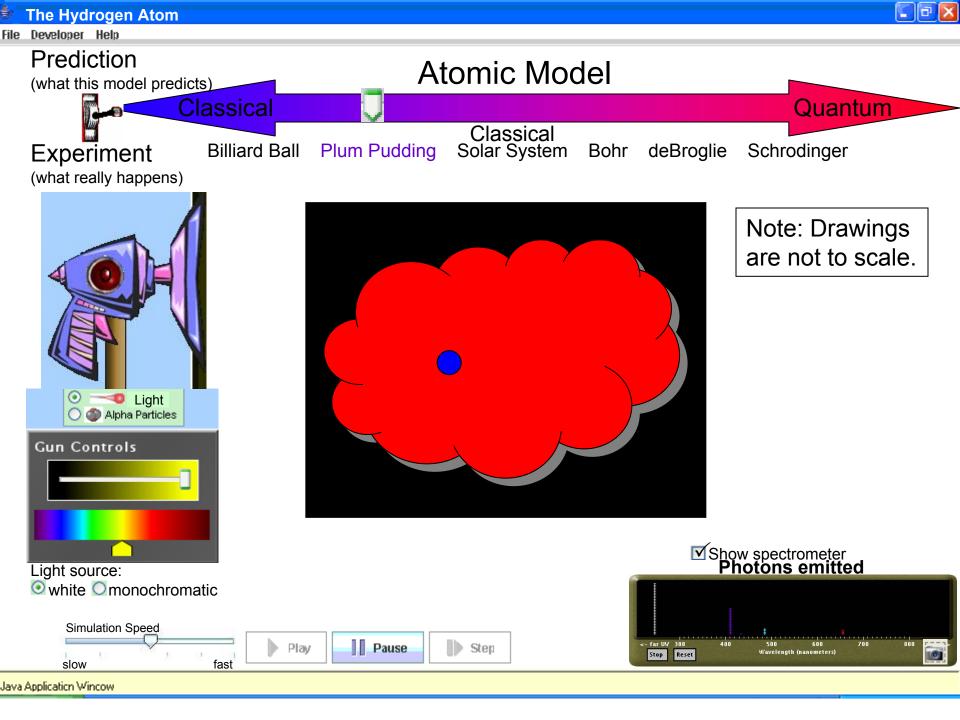


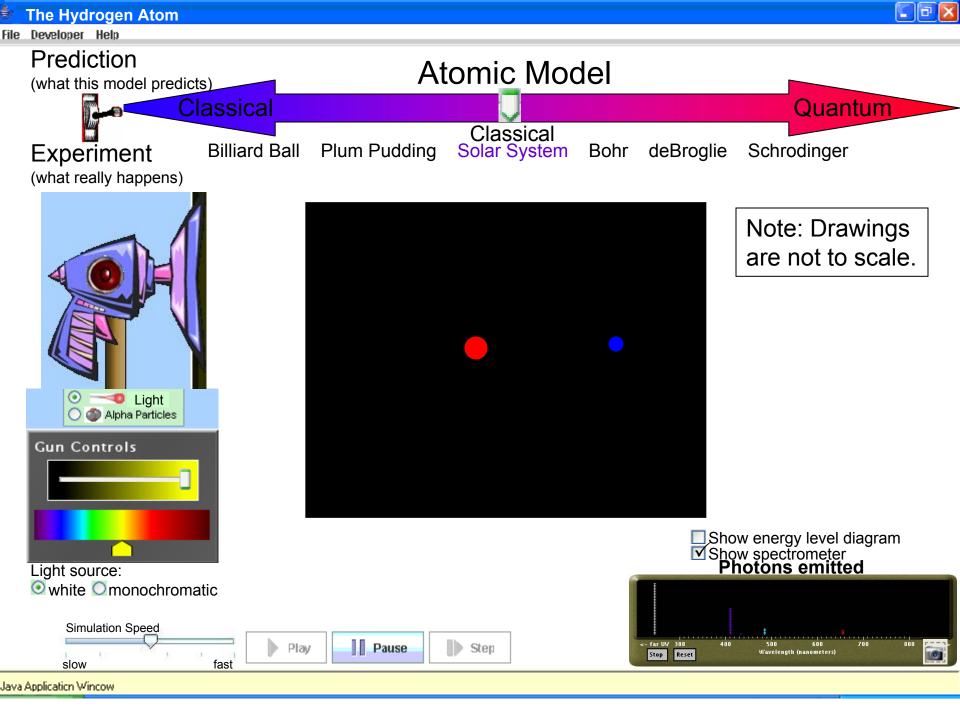
Atomic Model

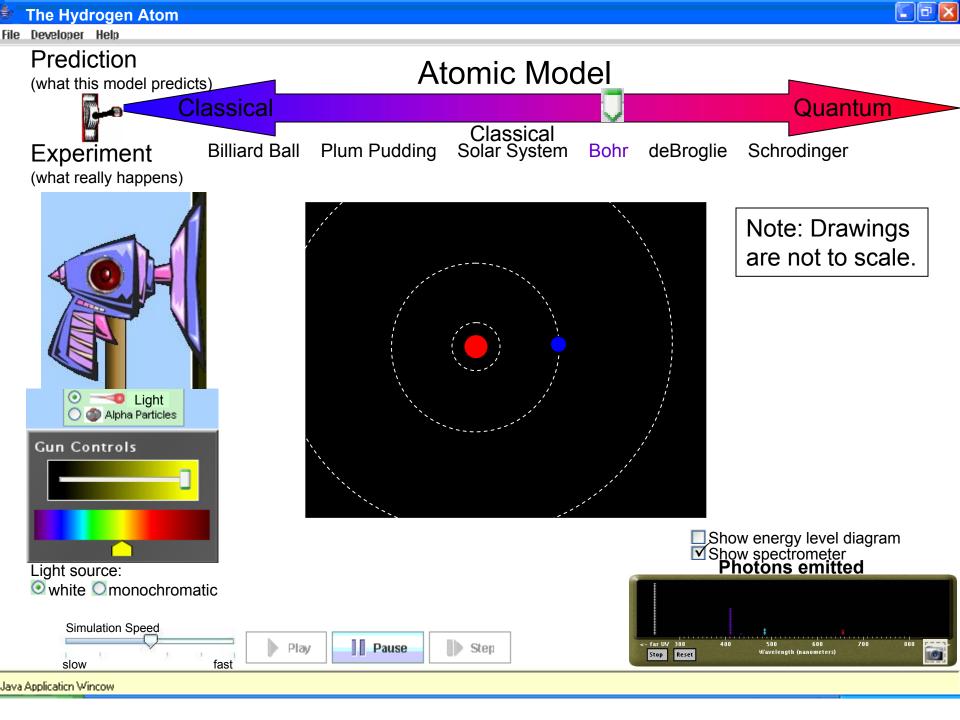


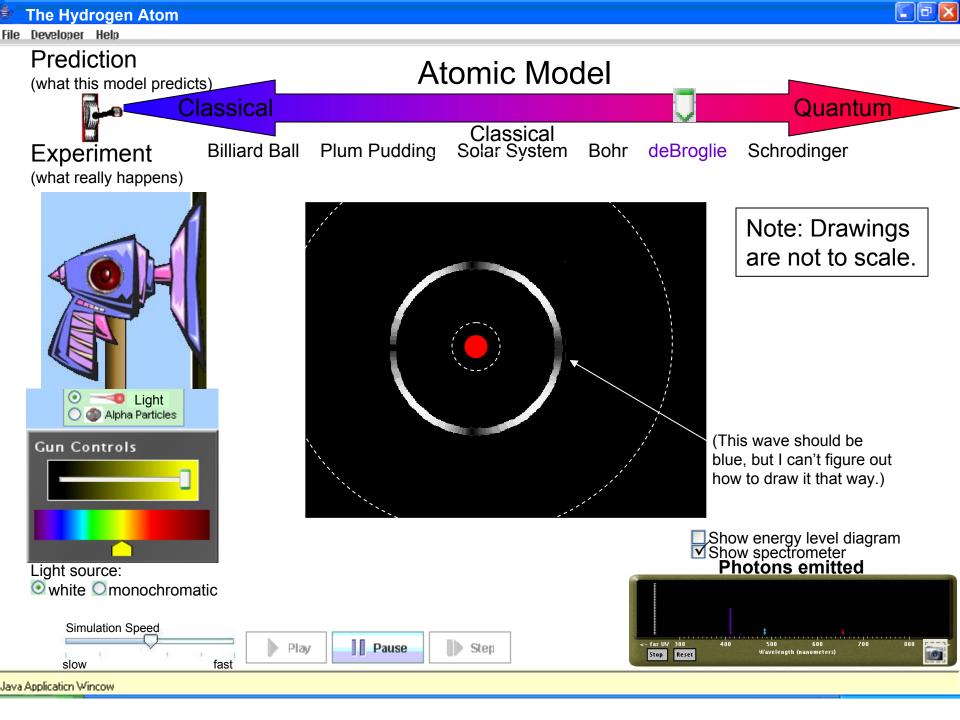


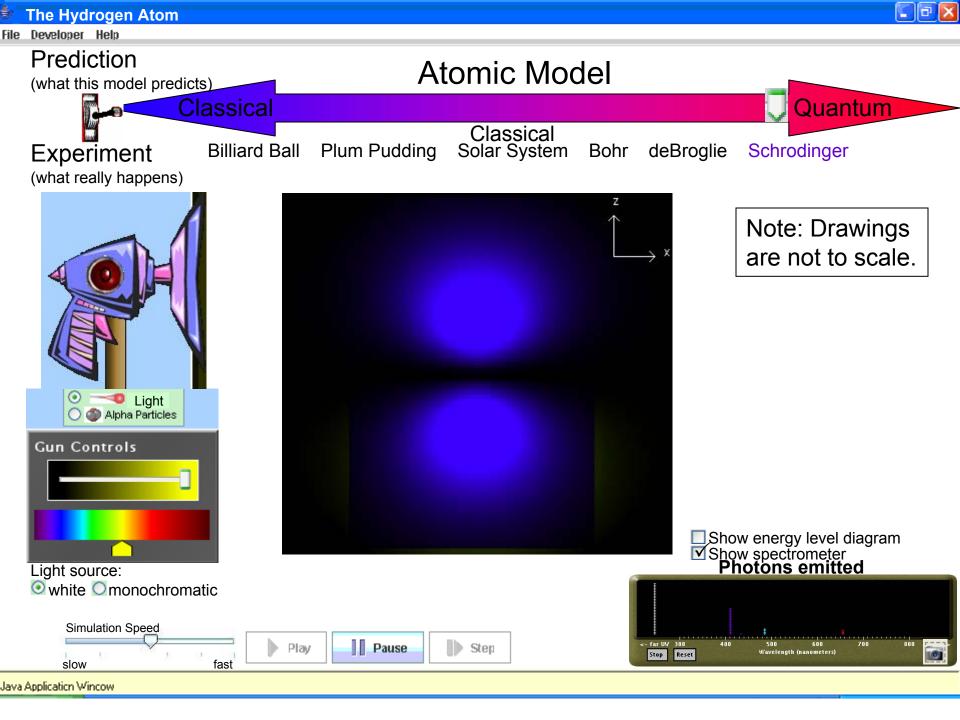








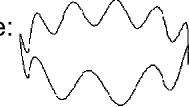




Representation of waves in deBroglie model.

There are several possible ways to represent standing waves on a ring:

- Brightness = mag. of amplitude, bright = large mag (+ or -), dark = 0 (e.g. QWI, radio waves):
- Brightness = amplitude, bright = +, dark = -, grey = 0
 (e.g. wave interference):
- Radial distance = amplitude:
- 3D perspective view, height = amplitude:



One of the brightness representations is probably best, but we have no interview data on how students will react to this representation alone. For now, let's put all 4 representations in a menu in the menu bar called "wave view" and interview on them to see what works best.

Action of Firing Photons

- Billiard Ball all photons bounce off.
- Plum Pudding All photons are absorbed and cause the electron to jiggle around. Speed of jiggling proportional to frequency.
- Solar System All photons go straight through.
- Bohr Only photons with correct energy are absorbed and cause electron to jump to higher level. (see table) Other photons go right through. All transitions are equally likely so spectrometer will show all colors that can be emitted building up equally.
- deBroglie same as Bohr
- Schrodinger same as Bohr, except that not all photons are absorbed even
 if they have the correct energy. Probability of photons being emitted is
 different for each color, so spectrometer builds up unevenly. (see table –
 relative intensity ~ probability of being absorbed)

Note: for all models with an electron, if the photons give the electron sufficient energy, it can be removed from atom. If this happens, electron should fly off and a note should come up that says "Your atom has been ionized. Hit OK to capture another electron."

Spectral Line Table

From:

http://hyperphysics. phyastr.gsu.edu/hbase/t ables/hydspec.html #c1

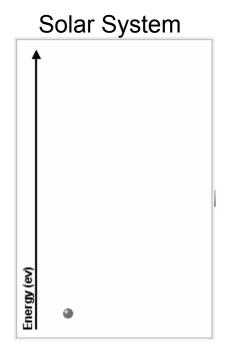
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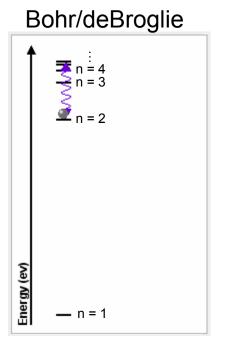
http://physics.nist.go v/PhysRefData/Han dbook/Tables/hydro gentable2.htm

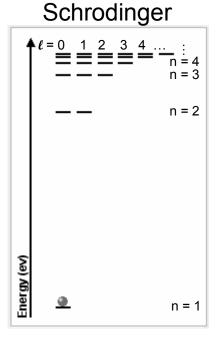
	Wavelength	Relative		Color or region	
	(nm)	Intensity	Transition	of EM spectrum	
ſ	Lymann Series				
	93.782	30	6 -> 1	UV	
	94.976	50	5 -> 1	UV	
	97.254	100	4 -> 1	UV	
	102.583	300	3 -> 1	UV	
	121.566	1500	2 -> 1	UV	
	Balmer Series				
	383.5384	5	9 -> 2	Violet	
	388.9049	6	8 -> 2	Violet	
	397.0072	8	7 -> 2	Violet	
	410.174	15	6 -> 2	Violet	
	434.047	30	5 -> 2	Violet	
	486.133	100	4 -> 2	Bluegreen (cyan)	
	656.272	120	3 -> 2	Red	
	656.2852	180	3 -> 2	Red	
	Paschen Series				
	954.62	5	8 -> 3	IR	
	1004.98	7	7 -> 3	IR	
	1093.8	12	6 -> 3	IR	
	1281.81	20	5 -> 3	IR	
ſ	1875.01	40	4 -> 3	IR	
ſ	Brackett Series				
ſ	2630	8	6 -> 4	IR	
ſ	4050	15	5 -> 4	IR	
ſ		Pfund Series			
Ī	7400	6	6 -> 5	IR	

Energy Level Diagrams

 For last 4 models, when "show electron energy level diagram" is checked, a diagram should appear to the right of the atom. For Bohr/deBroglie, this diagram is identical to the one in Discharge Lamps. For Schrodinger, there are additional states corresponding to different angular momentum, For Solar System, electron energy will start at the top of the diagram and move straight down continuously as the electron spirals into the nucleus.







Action of Firing Alpha Particles

- Billiard Ball Alpha particles bounce off atoms at all different angles.
- Plum Pudding Alpha particles go through positive goo and are slightly deflected, but still go through.
- Solar System If an alpha particle hits the nucleus before the atom is destroyed, it would behave like Bohr, but this should never happen because it should be destroyed before the particle arrives.
- Bohr Most alpha particles go straight through. A few hit the nucleus and bounce back at sharp angles. Below is the exact equation for the number of alpha particles reflected at each angle θ:
- deBroglie same as Bohr
- Schrodinger same as Bohr

$$N(\theta) = \frac{N_i n L Z^2 k^2 e^4}{4r^2 K E^2 \sin^4(\theta/2)}$$

 N_i = number of incident alpha particles

n = atoms per unit volume in target

L = thickness of target

Z = atomic number of target

e = electron charge

k = Coulomb's constant

r = target-to-detector distance

KE = kinetic energy of alpha

 θ = scattering angle

Directions for destroyed atoms

 After electron spirals into nucleus in solar system model, a note appears in its place that says "Your atom has been destroyed. Press 'reset' to create a new atom," along with a reset button. This note should stay there even if the user changes models. Until students hit reset, all photons and alpha particles just go straight through.

Directions for ionized atoms

 Atoms can be ionized by supplying sufficiently high energy photons to atoms in the plum pudding, Bohr, deBroglie, and Schrödinger models. When this happens, the electron flies off and a note comes up that says "Your atom has been ionized. Press 'OK' to capture another electron," and an OK button. If you hit OK, an electron flies in and is captured, resetting the atom to the ground state. Ionizing an atom does not change the behavior of alpha particles, but until user hits OK, photons should just go straight through (except for billiard balls). This note should stay there even if the user switches models, unléss the user switches to billiard ball, in which case it should be replaced by a note that says, "You can't ionize a billiard ball." and an OK button (on top of the billiard ball). For the billiard ball, the behavior of photons and alpha particles is unchanged if atom is "ionized." If you switch from a billiard ball with the "you can't ionize a billiard ball" note, it goes back to saying "your atom has been ionized..." until you hit OK.

where:

$$|\psi_{n\ell m}(r,\cos\theta)| = R_{nl}(r)P_{\ell}^{m}(\cos\theta)$$

 $|\psi_{n\ell m}(r,\cos\theta)|^2$

Laguerre Polynomials:

$$R_{nl}(r) = r^l e^{-r/na} \sum_{j=0}^{n-l-1} b_j r^j$$

where

$$a = \hbar^2 / (mke^2)$$

$$b_0 = 2(na)^{-3/2}$$

$$b_j = \frac{2}{na} \frac{j+l-n}{(j)(j+2l+1)} b_{j-1}$$

Associated Legendre Polynomial:

$$P_{\ell}^{m}(\cos\theta) = \frac{1}{\Gamma(-\ell)\Gamma(\ell+1)} \left[\frac{1+\cos\theta}{1-\cos\theta} \right]^{m/2} \sum_{n=0}^{\infty} \frac{\Gamma(n-\ell)\Gamma(n+\ell+1)}{\Gamma(n+1-m)n!} \left(\frac{1-\cos\theta}{2} \right)^{n}$$

Gamma Function:

$$\Gamma(\cos\theta) = \frac{e^{-\gamma\cos\theta}}{\cos\theta} \prod_{n=0}^{\infty} (1 + \cos\theta/n)^{-1} e^{\cos\theta/n}$$

Euler-Mascheroni constant:

$$\gamma = 0.57721566490153286060$$

To convert everything to cartesian coordinates, use:

$$r = \sqrt{x^2 + y^2 + z^2}$$

$$\cos \theta = z/r = z/\sqrt{x^2 + y^2 + z^2}$$