The Hydrogen Atom

Sam McKagan

December 1, 2006

Draft 5

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.

Changes in Draft 5

- Added directions for calculating states in Schrodinger model
- Added transition strength to Spectral line table.
- Added equations for calculating wavelengths and energies.
- Changed directions for destroying/ionizing atoms. Now atom is reset when model changes.
- Updated energy level diagram requirements

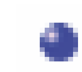
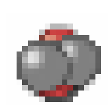
Learning Goals

- 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

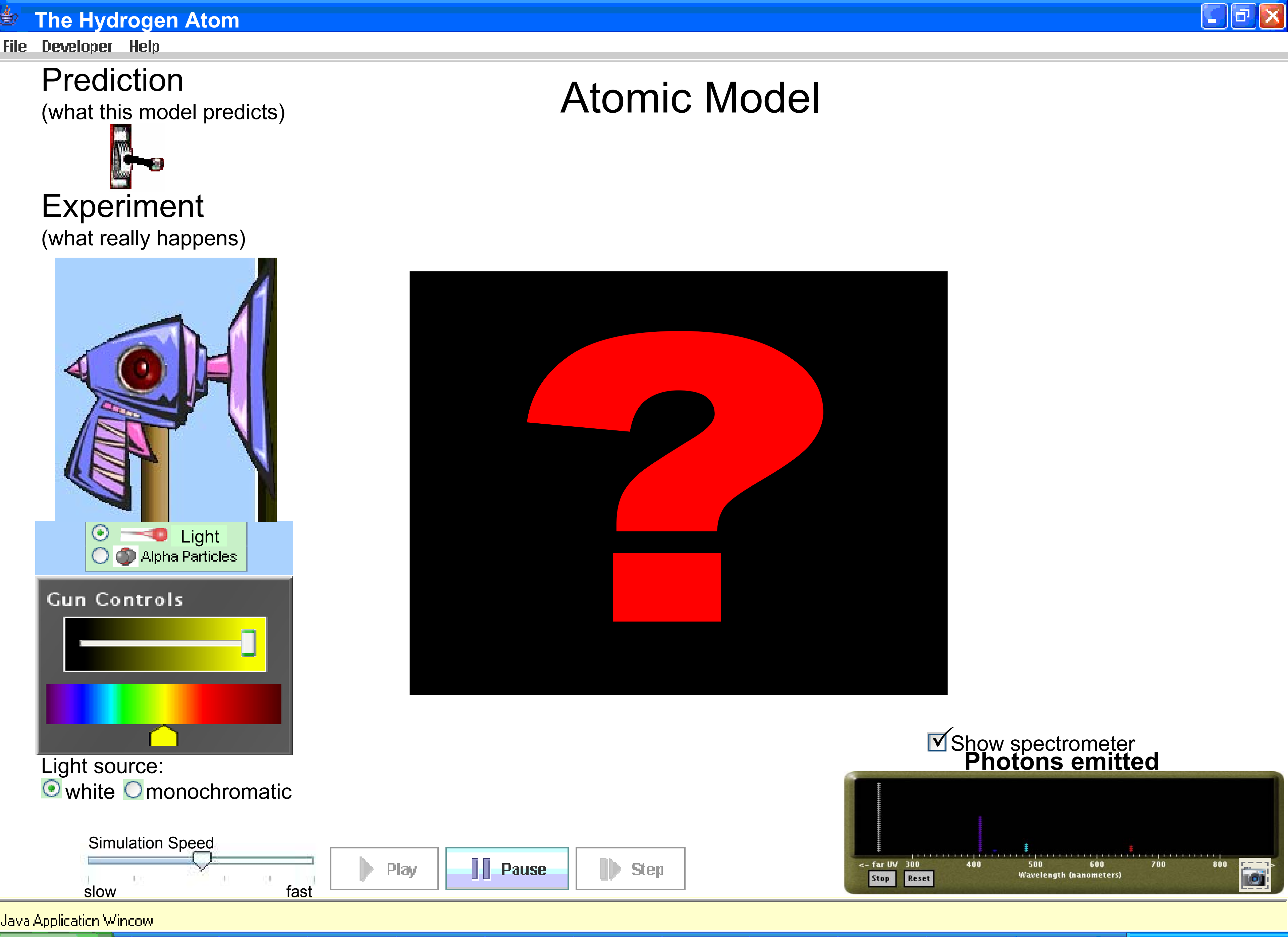
- Photons should be represented as little balls with tails as in other sims: 
- Electrons should be represented as little blue spheres as in other sims: 
- Alpha particles should be represented as a glob of two red spheres (protons) and two gray spheres (neutrons) as in Nuclear Physics: 

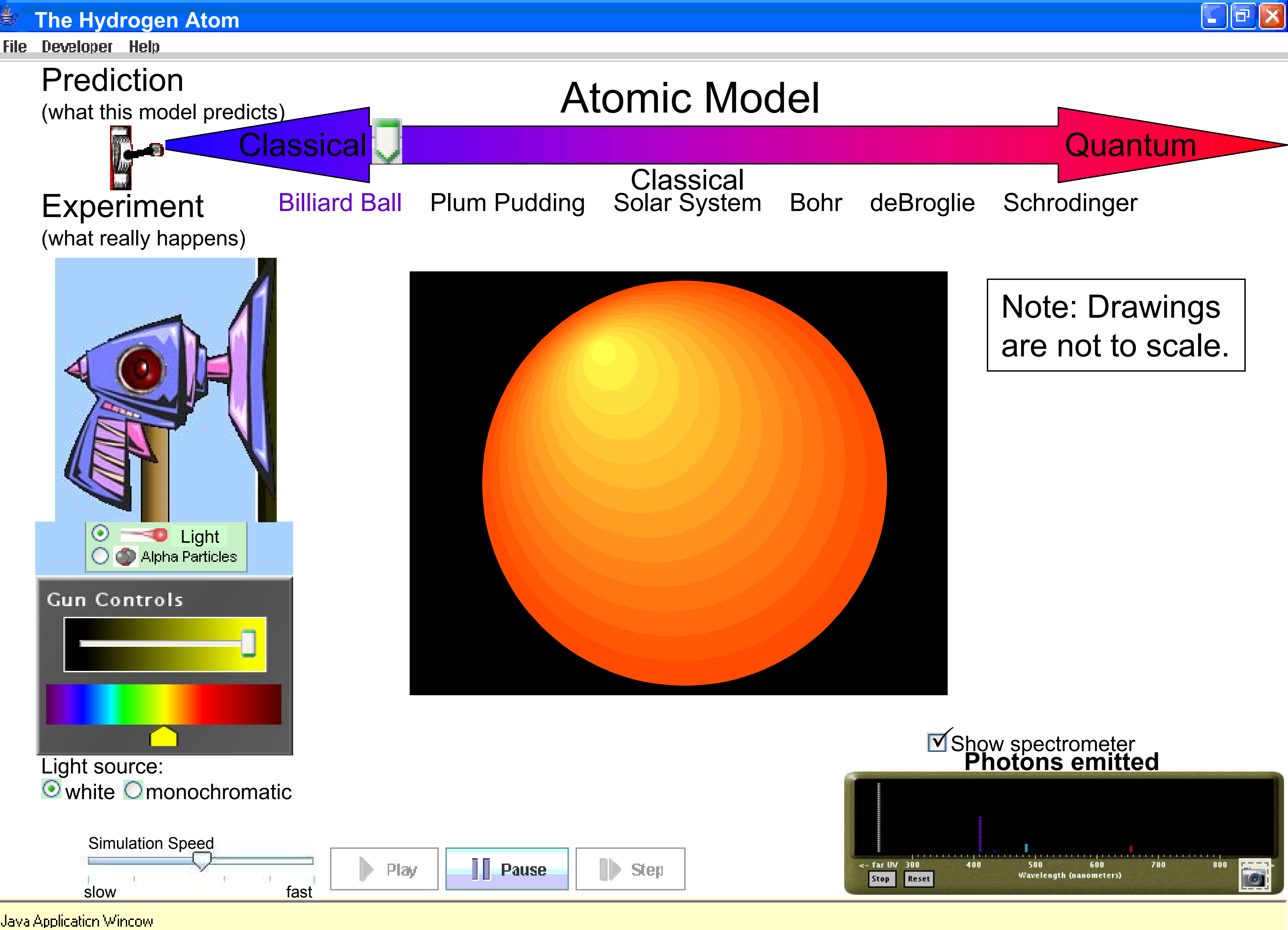
Gun

- 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 ~ n^2, 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)sin(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.
- Schrodinger – electrons represented as 3d probability waves.


The Hydrogen Atom
File Developer Help
Prediction
(what this model predicts)
Experiment
(what really happens)
Atomic Model
Light
Alpha Particles
Gun Controls
Light source:
white monochromatic
Simulation Speed
slow
fast
Play
Pause
Step
Show spectrometer
Photons emitted
<- far UV 300 400 500 600 700 800
Wavelength (nanometers)
Stop
Reset
Java Application Window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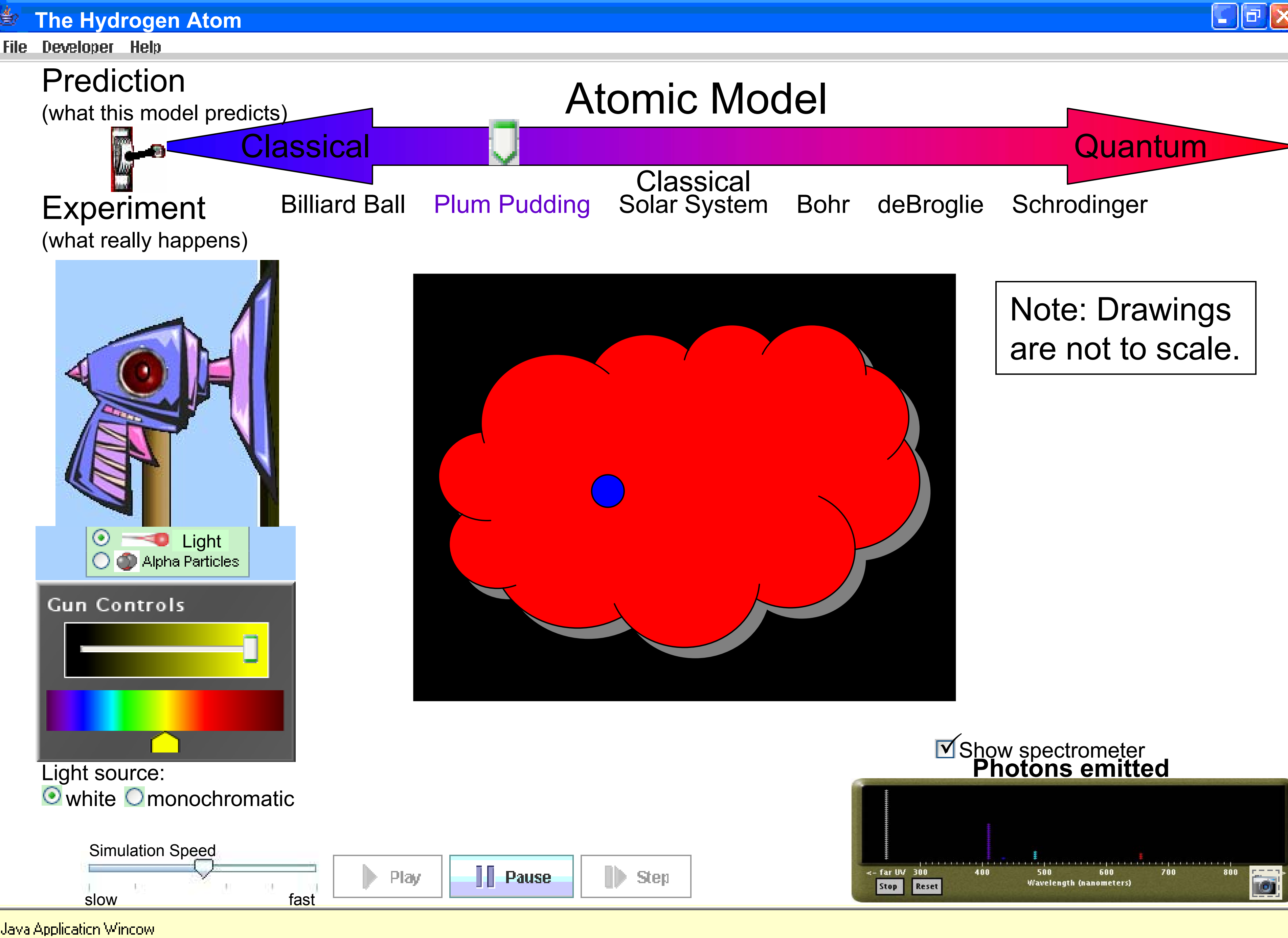
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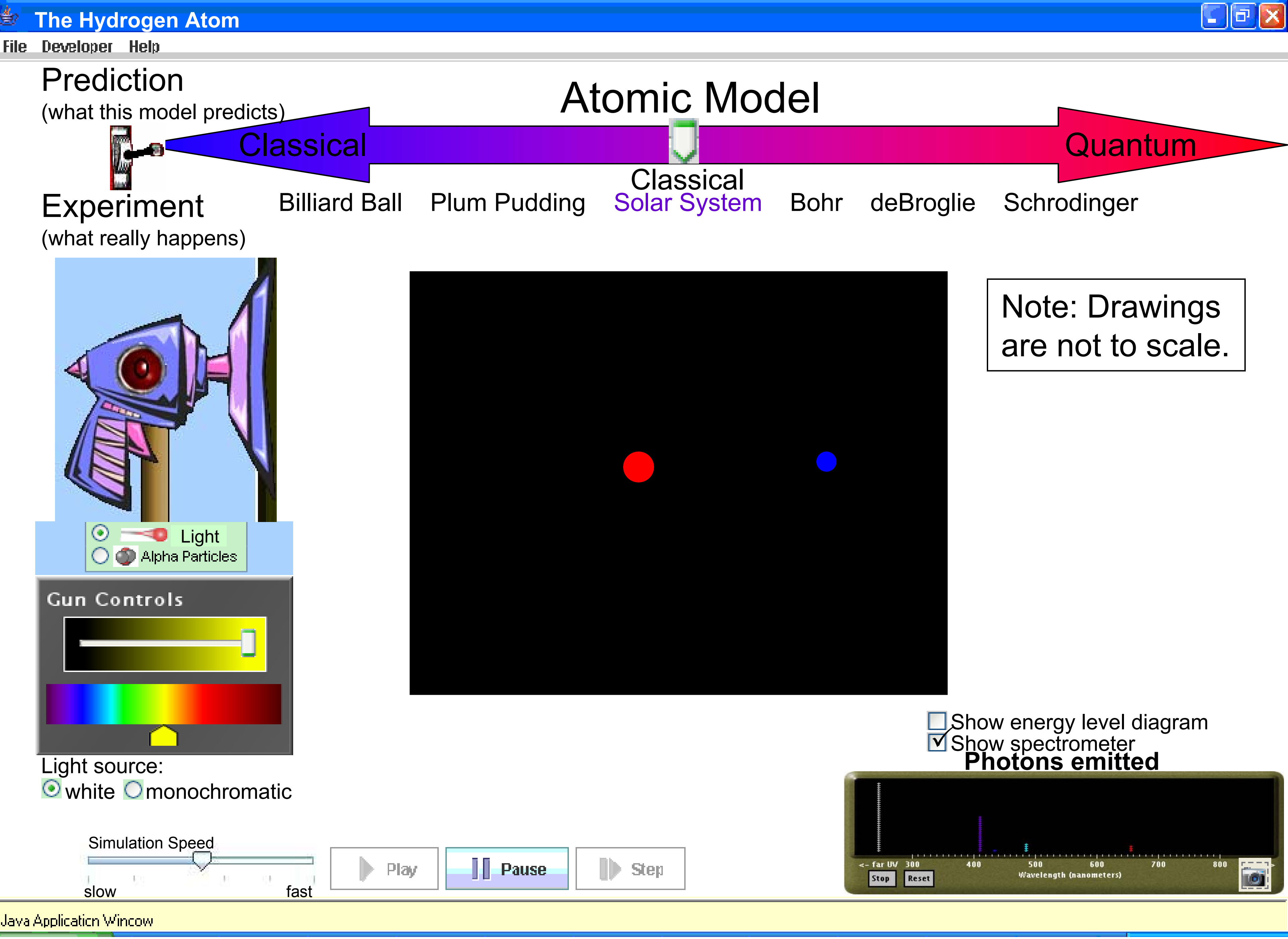
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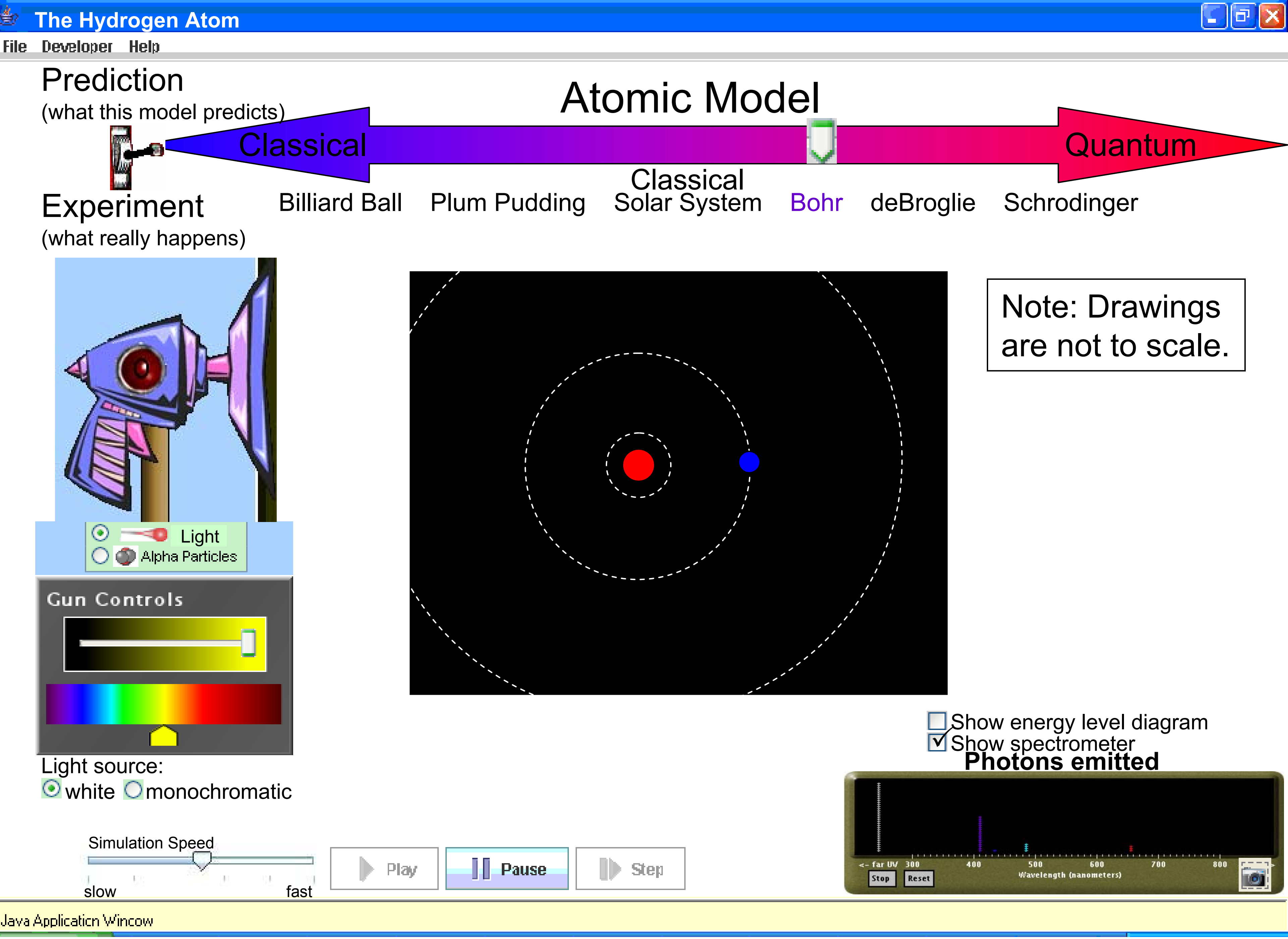
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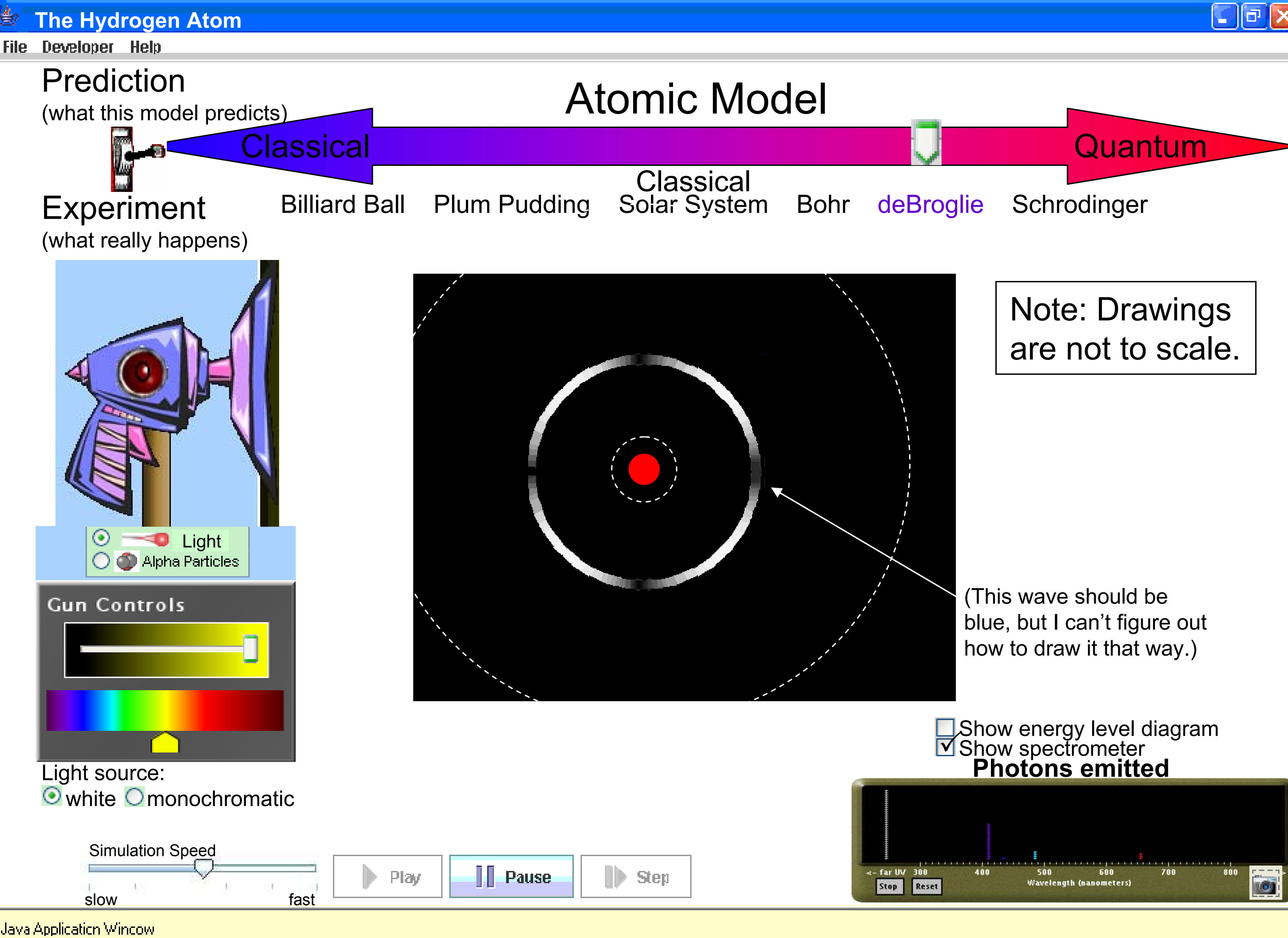
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Schrodinger
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Light
Alpha Particles
Gun Controls
(This wave should be blue, but I can't figure out how to draw it that way.)
Light source:
white
monochromatic
Show energy level diagram
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Photons emitted
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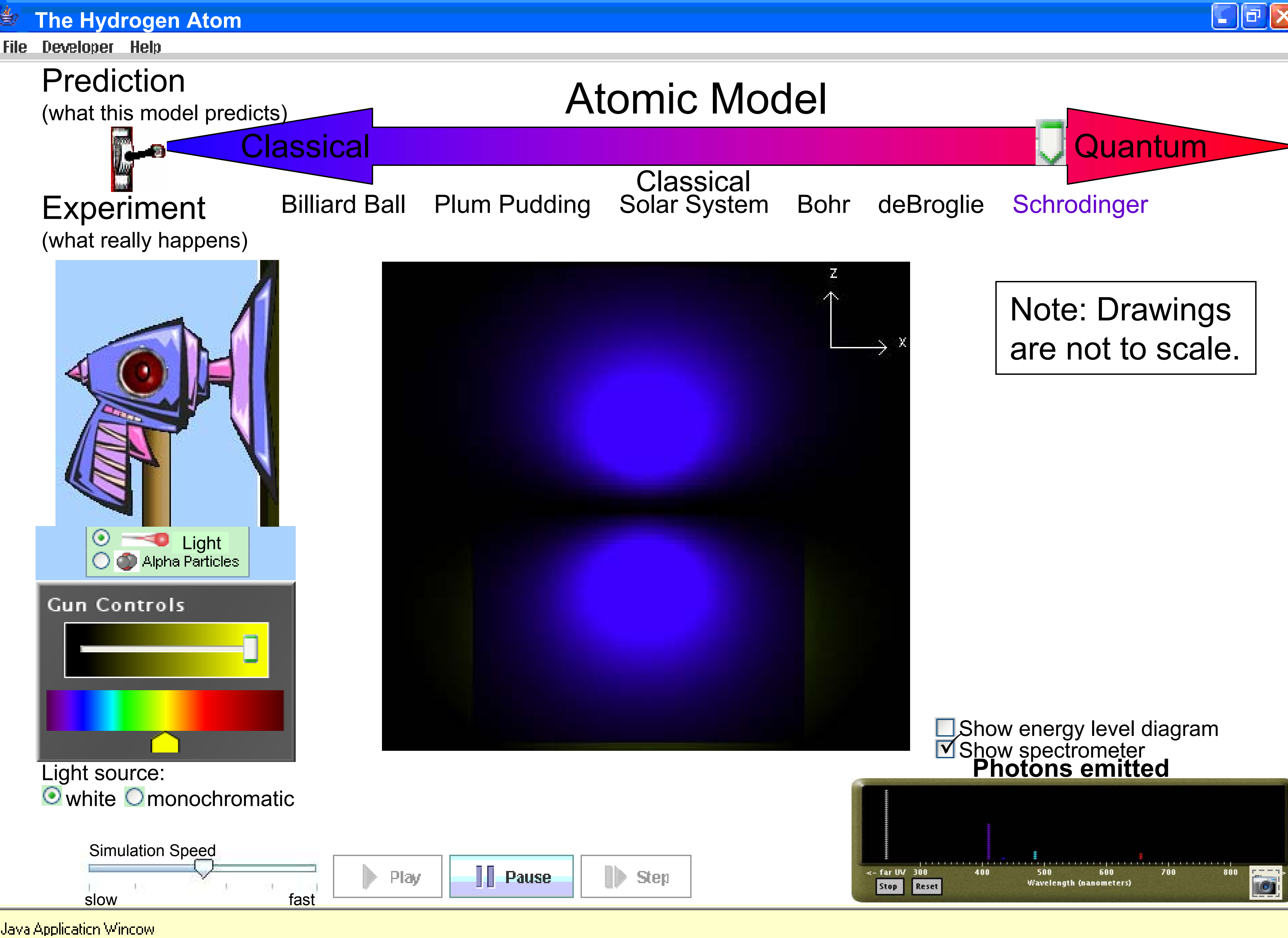

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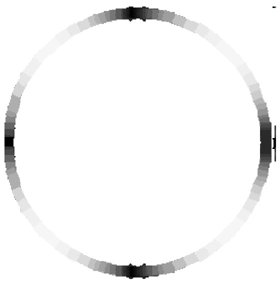
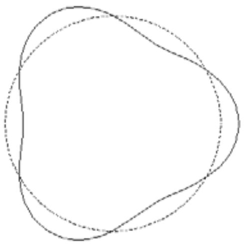
Representation of waves in deBroglie model.

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

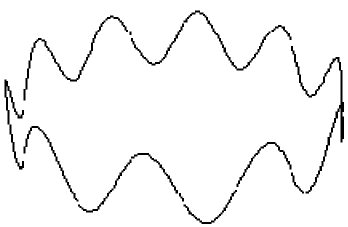
- Brightness = mag. of amplitude, bright = large mag (+ or -), dark = 0 (e.g. QWI, radio waves):
- Brightness = amplitude, bright = +, dark = -, grey = 0 (e.g. wave interference):



- 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

Energy of level n:

$E_n = E_1/n^2$

Wavelength of transition:

$$\lambda = \frac{hc/|E_1|}{\left|\frac{1}{n^2} - \frac{1}{n'^2}\right|}$$

Where:

$E_1 = -13.6$ eV

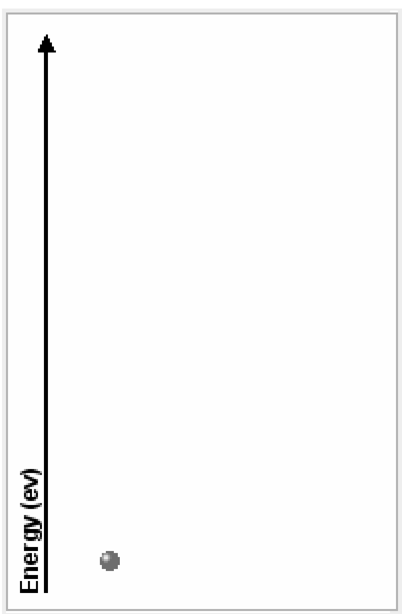
hc = 1240 eV nm

Wavelength (nm)	Transition Strength	Transition	Color
Lymann Series			
93.782	0.39	6 -> 1	UV
94.976	0.69	5 -> 1	UV
97.254	1.36	4 -> 1	UV
102.583	3.34	3 -> 1	UV
121.566	12.53	2 -> 1	UV
Balmer Series			
410.174	0.06	6 -> 2	Violet
434.047	0.11	5 -> 2	Violet
486.133	0.24	4 -> 2	Cyan
656.272	0.87	3 -> 2	Red
Paschen Series			
1093.8	0.02	6 -> 3	IR
1281.81	0	5 -> 3	IR
1875.01	0.07	4 -> 3	IR
Brackett Series			
2630	0	6 -> 4	IR
4050	0.04	5 -> 4	IR
Pfund Series			
7400	0	6 -> 5	IR

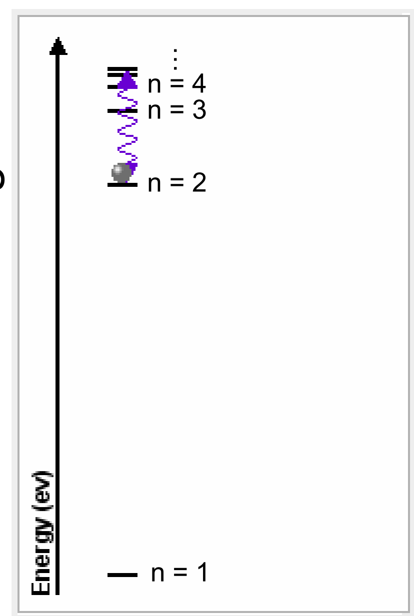
Energy Level Diagrams

- 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, states corresponding to different values of l should be indicated by lines that aligned horizontally. There can be a note on the side that indicates the value of m, but let’s not have separate lines for different values of m. 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.
- The color of the gun is indicated by a squiggle pointing up (located on the left side) that behaves as in Lasers. The color of the emitted photon is indicated by a squiggle pointing down (from original energy level to new energy level) that behaves as in Discharge Lamps.

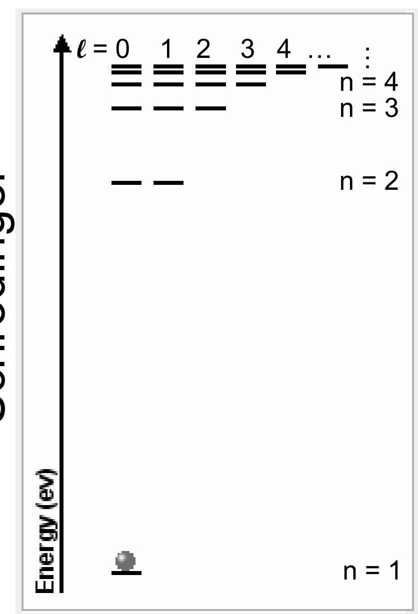
Solar System



Bohr/deBroglie



Schrodinger



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.
- deBroglie – same as Bohr
- Schrodinger – same as Bohr

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. 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 ($\lambda > hc/E_1$) to atoms in the plum pudding, Bohr, deBroglie, and Schrodinger 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.

States and Transitions in Schrodinger model

- States determined by n, l, m
- Rules for allowed nlm values:
  1. n = 1,2,3,4,5,6
  2. l = 0,1,2,…n-1
  3. m = -l, -l+1,… -1, 0, 1,… l-1, l
- Examples:
  - For n=1, only l=0, m=0 allowed
  - For n=2, can have l=1, m=1 or l=1, m=0 or l=1, m=-1 or l=0, m=0.
- For atom in state n,l,m to make transition to state n',l',m':
  - If n'>n, must be hit with photon with right wavelength (same as in Bohr/deBroglie)
  - If n'<n, can have stimulated emission (same as in Bohr/deBroglie), or spontaneous emission. Probability of spontaneous emission from n to n' is given by normalized transition strength.
- Determine values of l' and m' after deciding that transition to n' will occur. Must obey the following transition rules:
  A. l-l' = 1 or -1 (choose randomly between these options)
  B. m-m' = 1 or 0 or -1

Examples of transitions

- Always start in state n=1,l=0,m=0.
- Suppose 103nm photon comes in. This will excite it to a state with n=3. For this n, the possible values of l are 0, 1, and 2 (from rule 2). However, only l=1 obeys the transition rule A, so this is our new value of l. For this l, the possible values of m are -1, 0, and 1 (from rule 3). All of these are allowed by transition rule B, so we choose randomly among these three options to determine our value of m. Suppose we get m=0.
- Now we are in the state n=3, l=1, m=0. This state can undergo spontaneous emission to n=1 or n=2. From the spectral line table, we see that the transition strength is 3.34 for 3->1 and 0.87 for 3->2. Normalizing these gives probabilities of 3.34/(3.34+0.87) = 0.79 for 3->1 and 0.87/(3.34+0.87) = 0.21 for 3->2. Suppose the random number generator decides it will go to state n=2. Then the possible values of l are 0 and 1 (from rule 2). But only l=0 satisfies transition rule A. For this l, the only possible value of m is 0 (from rule 3). So the new state is n=2, l=0, m=0.

Drawing probability densities in Schrodinger model:

- Once you've decided what n, l, and m are, you need to draw the probability density $|\psi_{nlm}|^2 = \psi_{nlm} \times \psi_{nlm}^*$. The wave function ψ_{nlm} is a function of r, θ, and ϕ, which you can convert to a function of x, y, z. You then need to average over y to get a function of x and z, which can be plotted in the box, with z as vertical and x as horizontal.
- The probability density is mapped onto brightness, with bright blue as the maximum and black as zero.

Formulae for calculating Schrodinger model electron distributions

The probability density is given by:

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

where:

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

Laguerre Polynomials:

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

where

$$\cancel{a = \hbar^2/(mke^2)} \rightarrow$$ See next page for definition of a

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

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

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:

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

Euler-Mascheroni constant:

$$\gamma = 0.5772156649015328606$$

To convert everything to cartesian coordinates, use:

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

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

A few notes about calculating wave functions.

- Normally, a, the “Bohr radius,” is equal to the radius of the smallest Bohr orbit. Since we’ve rescaled the Bohr orbits, we need to rescale a too. For a given value of n, set $a=r/n^2$, where r is the radius of the Bohr orbit for that n.
- Note that the probability density will always be the same for +m and –m.
- For large n, the probability density will extend beyond the edge of the box. I think this is OK.

To look at sample Schrodinger wave functions…

- Go to http://falstad.com/qmatom/
- If you can, go to the “view” menu and uncheck “Phase as color.” This may not work on a Mac. If it doesn’t, just ignore the colors.
- In the first pull-down menu on the right, switch from “Real Orbitals (chem.)” to “Complex Orbitals (phys.)”
- Use the pull-down menus to select any values of n, l, and m you want to view.
- Note that this simulation autoscales, so all states will appear to be about the same size, even though states with lower n are actually smaller.
- Aside from the autoscaling and the color, these are what our Schrodinger wave functions should look like.