Dispelling Myths and Misconceptions Through the Visualization of Quantum Concepts in General and Physical Chemistry

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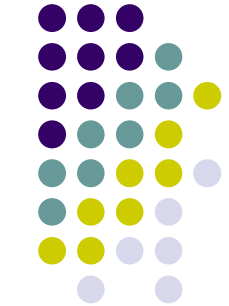
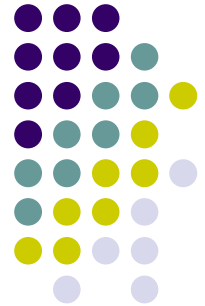
The Problem: Quantum Concepts in General Chemistry



- Quantum concepts are the most challenging and unsatisfying topics for students and instructors.
- The quantum world makes no sense to our everyday intuition.
- Failure to reconcile this intuition with quantum behavior results in deeply seated myths and misconceptions.

Myths and Misconceptions



- The electron “waves” as it moves.

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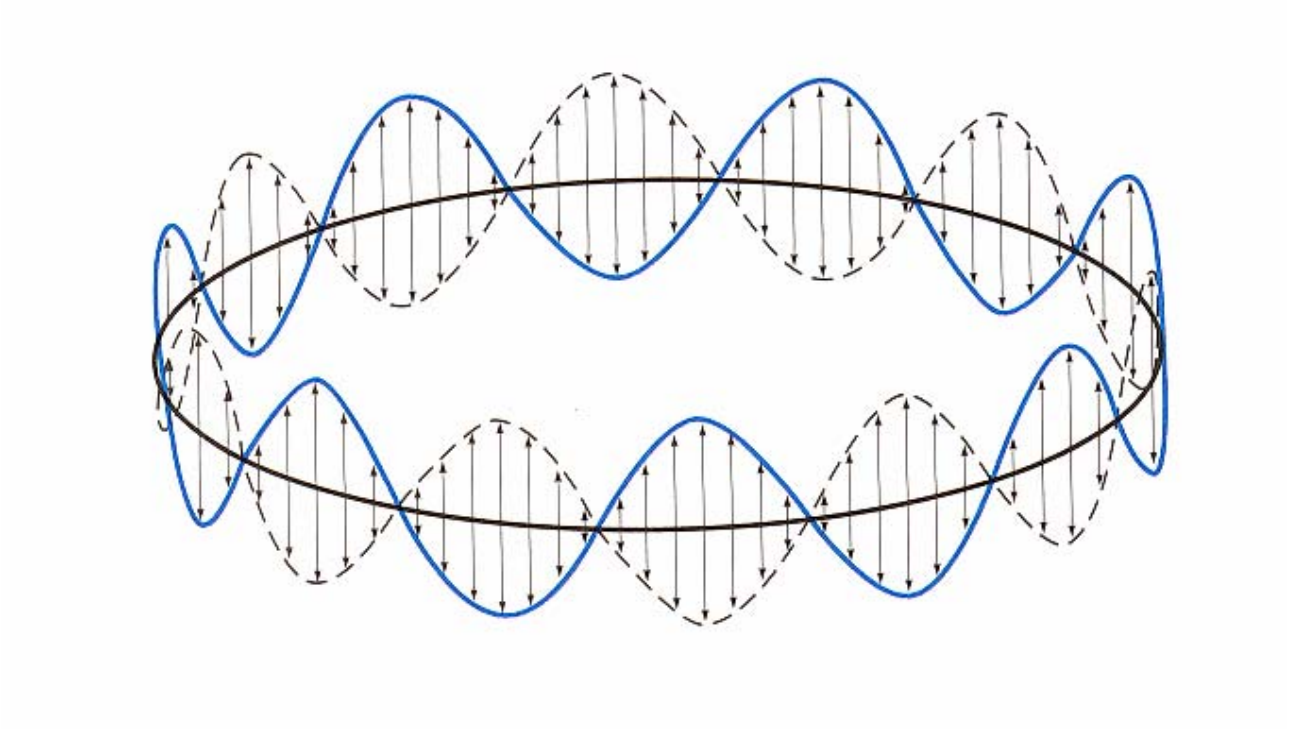
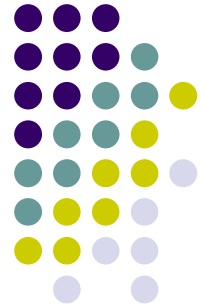


Figure 15.21, p. 528 in "Principles of Modern Chemistry," Fifth Edition, by David W. Oxtoby, H.P. Gillis, and Norman H. Nachtrieb, London: Thomson Learning, 2002. ISBN 0-03-035373-4

Myths and Misconceptions



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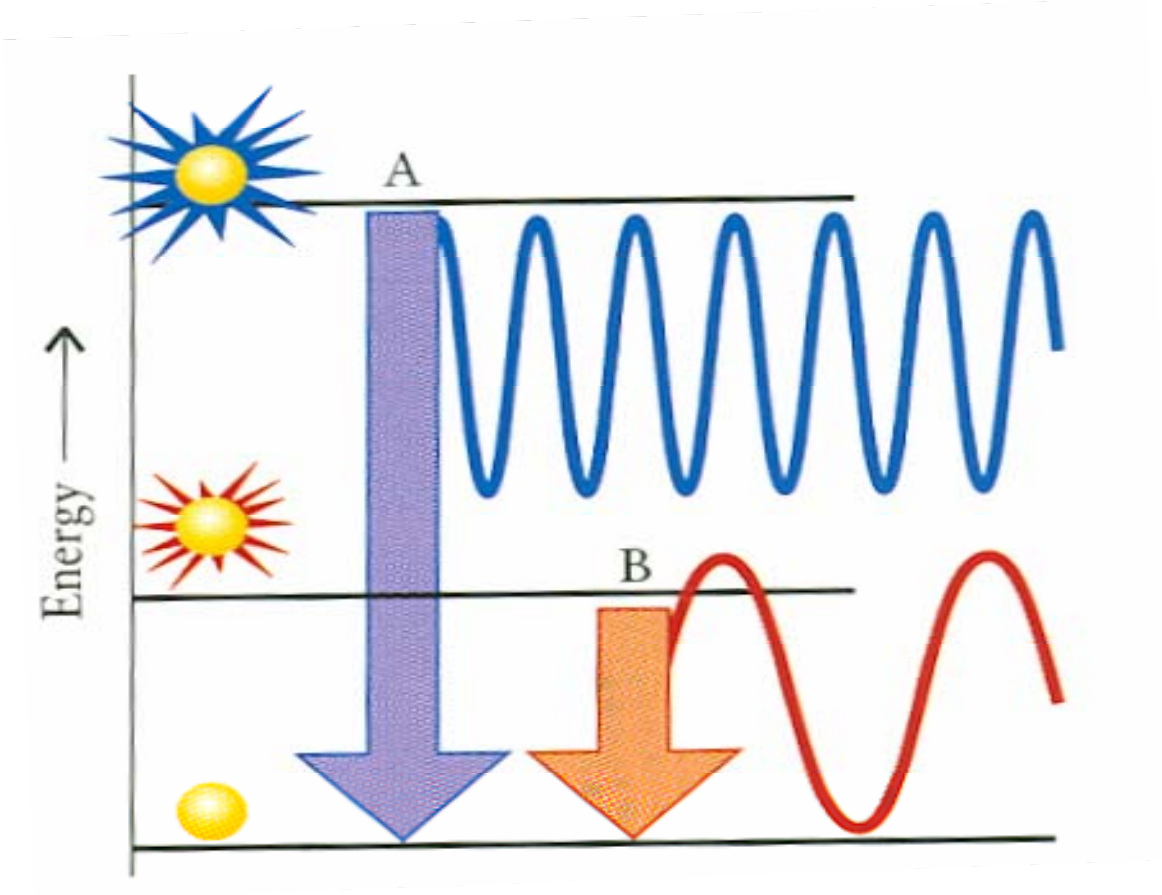

Figure 1.20, p. 17 in "Chemical Principles, The Quest for Insight," Third Edition, by Peter Atkins and Loretta Jones, New York: W.H. Freeman and Company, 2005. ISBN 0-7167-5701-X

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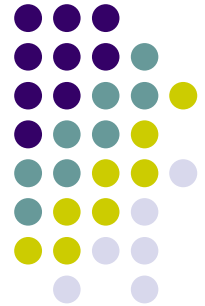
Myths and Misconceptions



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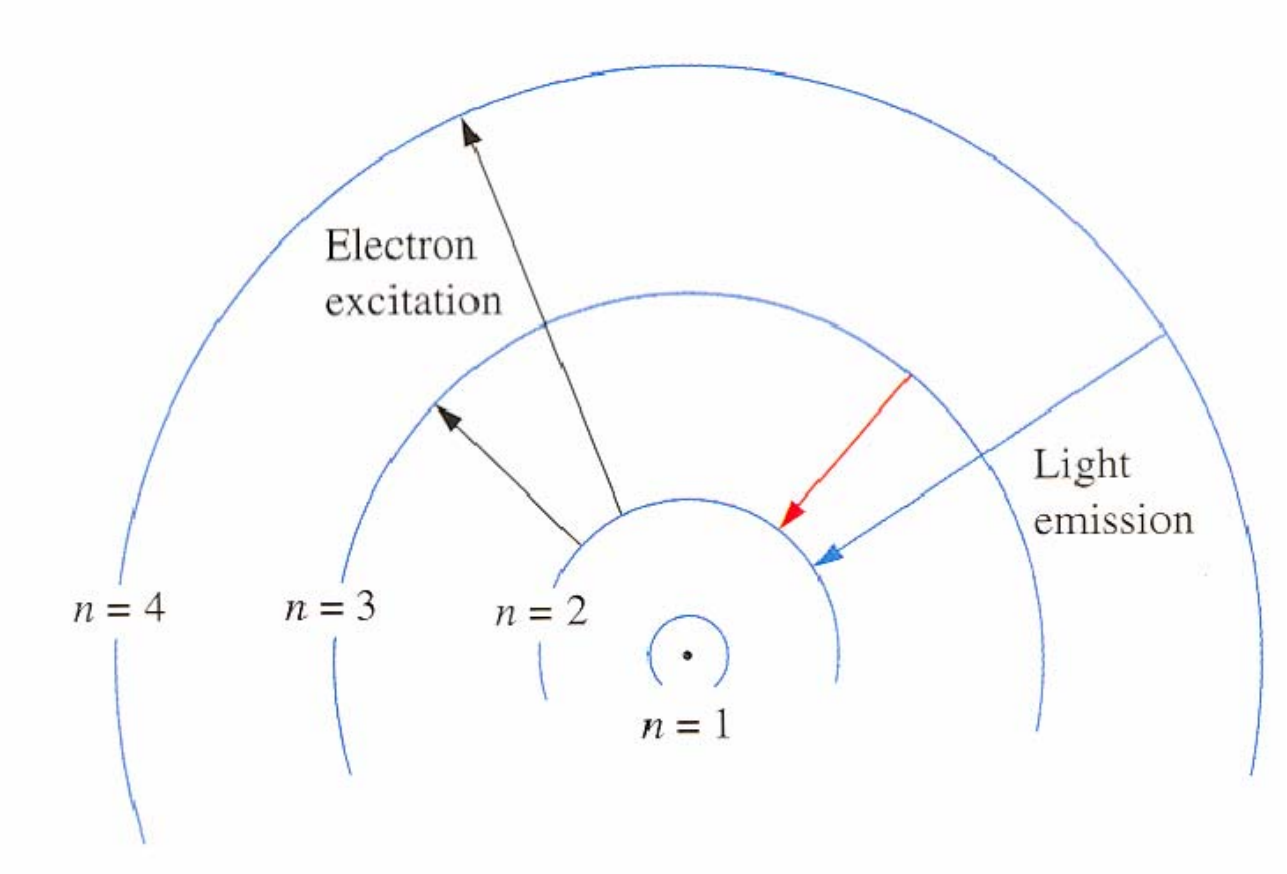

Figure 7.19, p. 295 in "General Chemistry, An Integrated Approach," Second Edition, by John W. Hill and Ralph H. Petrucci, Upper Saddle River, New Jersey: Prentice Hall, 1999. ISBN 0-13-918673-5

Myths and Misconceptions

- The electron “waves” as it moves.
- Electrons “jump” from one quantum level to another.
- Electrons “go around” the atom.
- Spectral lines are “energy levels.”

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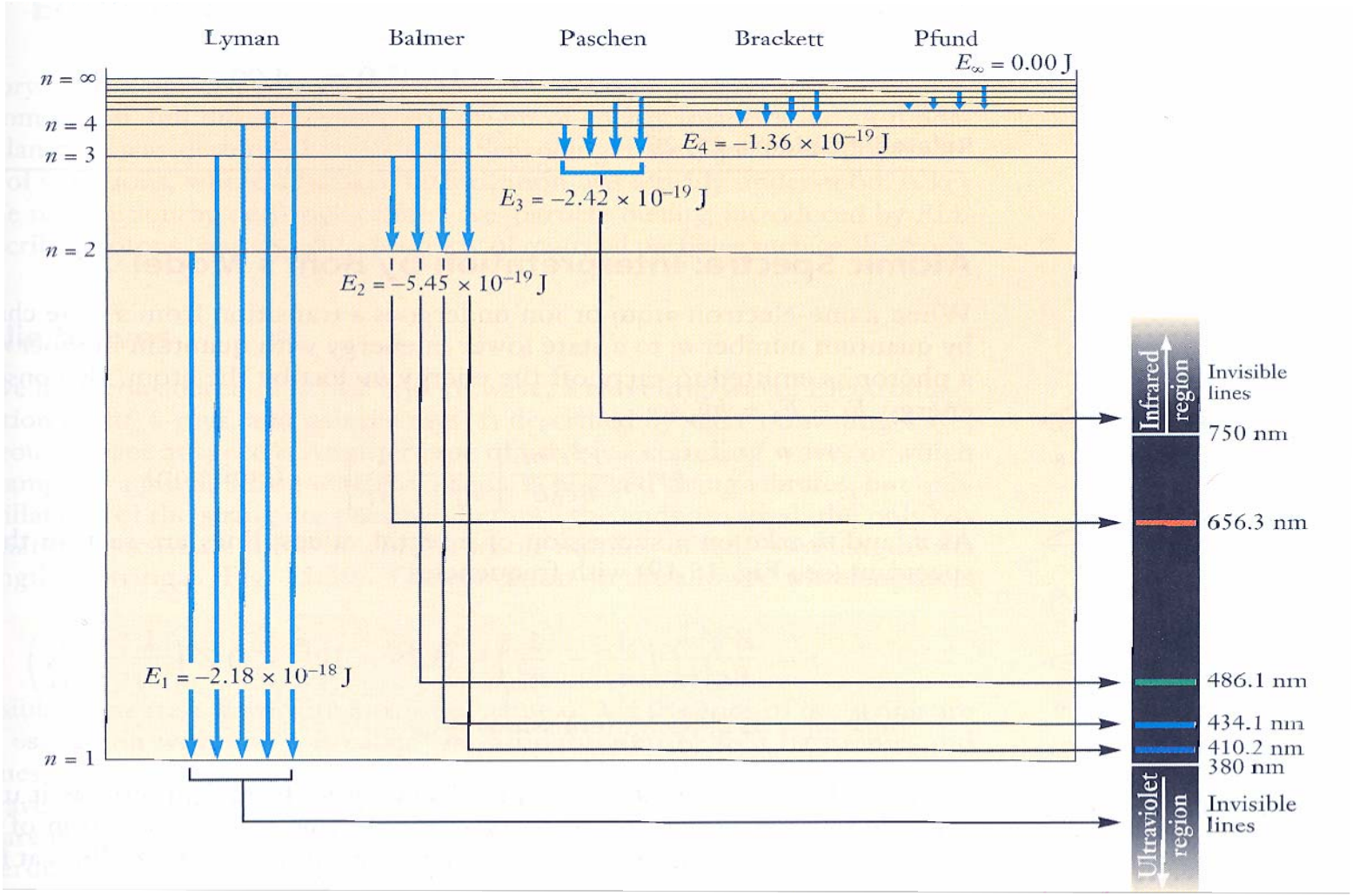

Figure 15.19, p. 525 in "Principles of Modern Chemistry," Fifth Edition, by David W. Oxtoby, H.P. Gillis, and Norman H. Nachtrieb, London:Thomson Learning, 2002. ISBN 0-03-035373-4

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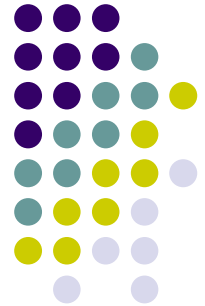
More Myths and Misconceptions



- When a “photon” is absorbed, light vanishes; when a “photon” is emitted, light appears.

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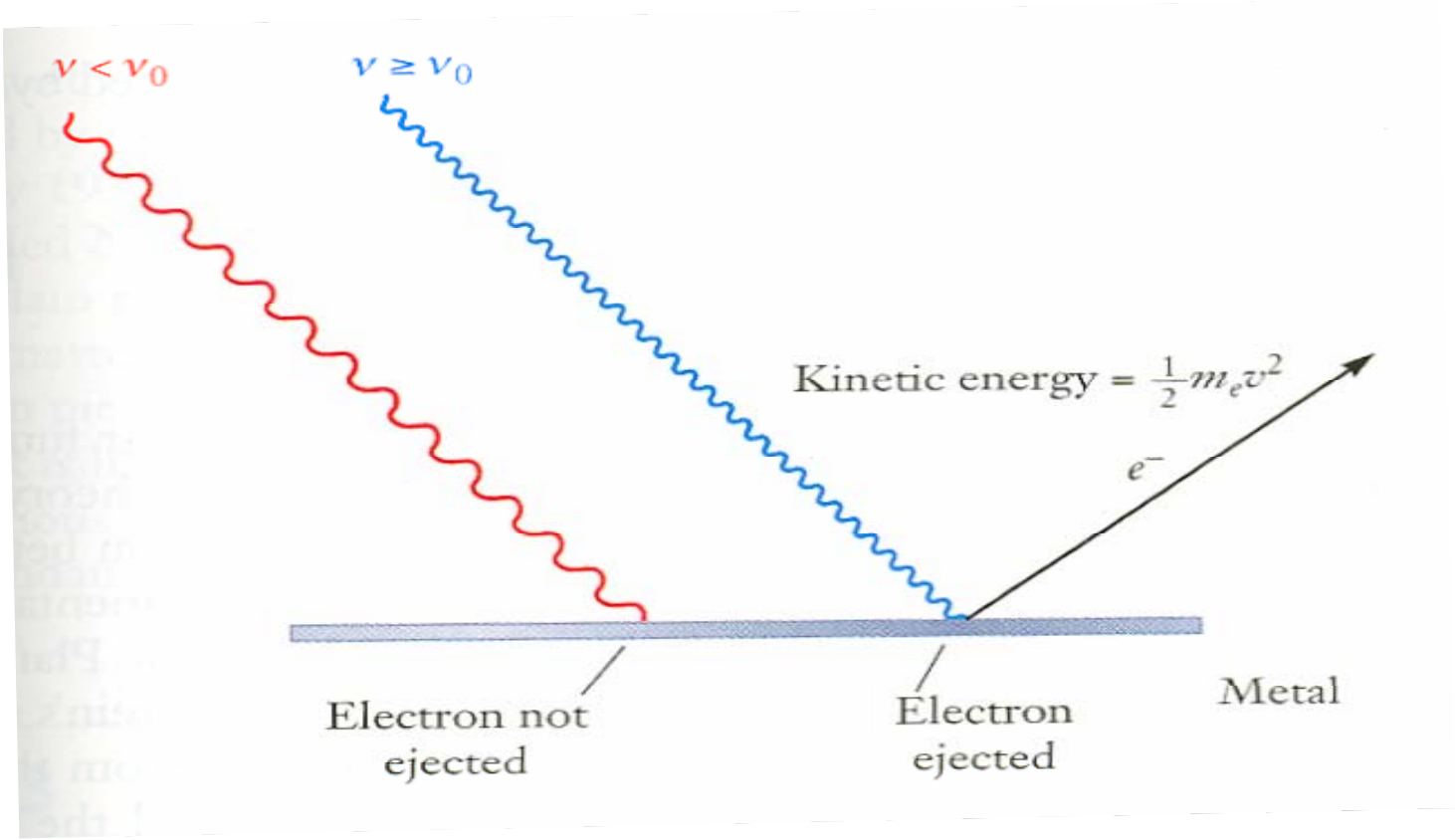

Figure 15.12 (a), p. 515 in "Principles of Modern Chemistry," Fifth Edition, by David W. Oxtoby, H.P. Gillis, and Norman H. Nachtrieb, London: Thomson Learning, 2002. ISBN 0-03-035373-4

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More Myths and Misconceptions

- When a “photon” is absorbed, light vanishes; when a “photon” is emitted, light appears.
- “Orbital” pictures represent electrons in motion.

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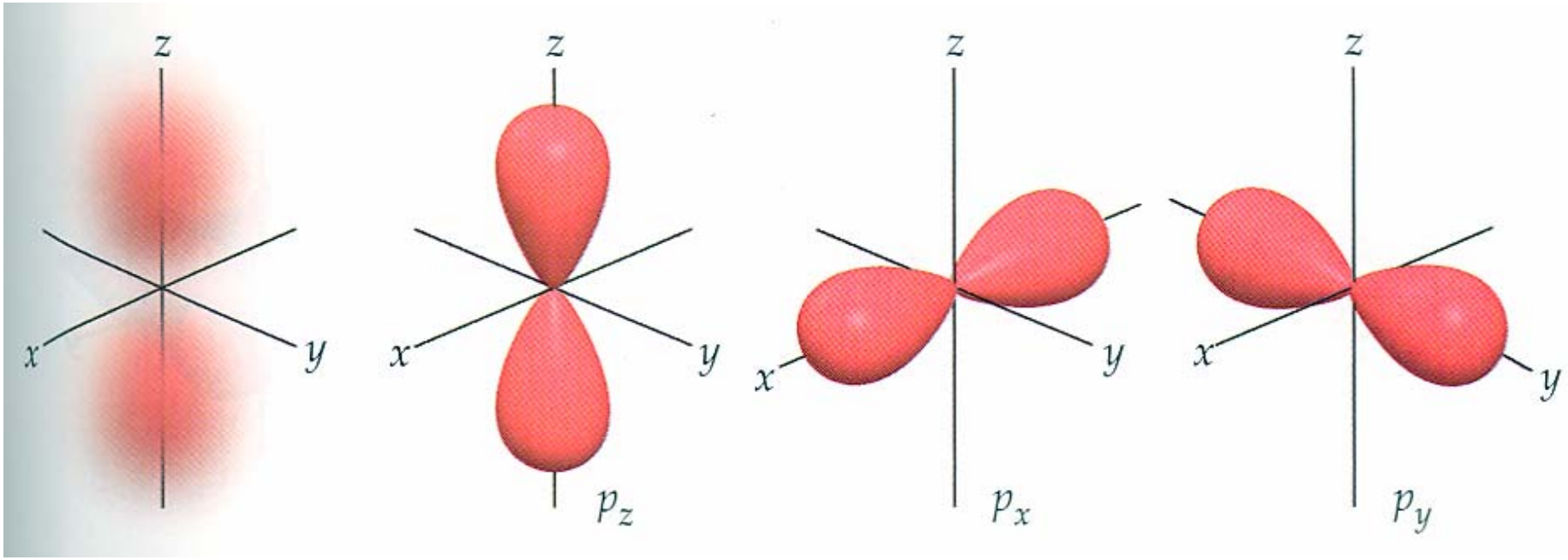

Figure 6.22, p. 205 in "Chemistry, The Central Science," Eighth Edition, by Theodore L. Brown, H. Eugene LeMay, Jr., and Bruce E. Burstein, Upper Saddle River, New Jersey: Prentice Hall, 2000. ISBN 0-13-010310-1

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More Myths and Misconceptions

- When a “photon” is absorbed, light vanishes; when a “photon” is emitted, light appears.
- “Orbital” pictures represent electrons in motion.
- Electrons are described by static “wavefunctions.”

Electrons are described by static "wavefunctions."

TABLE 1.2 Hydrogen Wavefunctions (Atomic Orbitals), $\psi = RY$

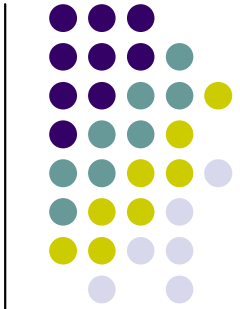
(a) Radial wavefunctions, $R_{nl}(r)$

n	l	$R_{nl}(r)$
1	0	$2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$
2	0	$\frac{1}{2\sqrt{2}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2 - \frac{Zr}{a_0}\right)e^{-Zr/2a_0}$
	1	$\frac{1}{2\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right)e^{-Zr/2a_0}$
3	0	$\frac{1}{9\sqrt{3}}\left(\frac{Z}{a_0}\right)^{3/2}\left(3 - \frac{2Zr}{a_0} + \frac{2Z^2r^2}{9a_0^2}\right)e^{-Zr/3a_0}$
	1	$\frac{2}{27\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2 - \frac{Zr}{3a_0}\right)e^{-Zr/3a_0}$
	2	$\frac{4}{81\sqrt{30}}\left(\frac{Z}{a_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right)^2 e^{-Zr/3a_0}$

(b) Angular wavefunctions, $Y_{lm_l}(\theta,\phi)$

l	"m_l"*	$Y_{lm_l}(\theta,\phi)$
0	0	$\left(\frac{1}{4\pi}\right)^{1/2}$
1	x	$\left(\frac{3}{4\pi}\right)^{1/2} \sin\theta\cos\phi$
	y	$\left(\frac{3}{4\pi}\right)^{1/2} \sin\theta\sin\phi$
	z	$\left(\frac{3}{4\pi}\right)^{1/2} \cos\theta$
2	xy	$\left(\frac{15}{16\pi}\right)^{1/2} \sin^2\theta\cos 2\phi$
	yz	$\left(\frac{15}{4\pi}\right)^{1/2} \cos\theta\sin\theta\sin\phi$
	zx	$\left(\frac{15}{4\pi}\right)^{1/2} \cos\theta\sin\theta\cos\phi$
	$x^2 - y^2$	$\left(\frac{15}{16\pi}\right)^{1/2} \sin^2\theta\sin 2\phi$
	z^2	$\left(\frac{5}{16\pi}\right)^{1/2} (3\cos^2\theta - 1)$

Table 1.2, p. 21 in "Chemical Principles, The Quest for Insight," Third Edition, by Peter Atkins and Loretta Jones, New York: W.H. Freeman and Company, 2005. ISBN 0-7167-5701-X



These myths and misconceptions arise because

time has been left out!

The Resolution:

Include Time!

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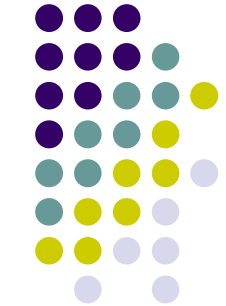
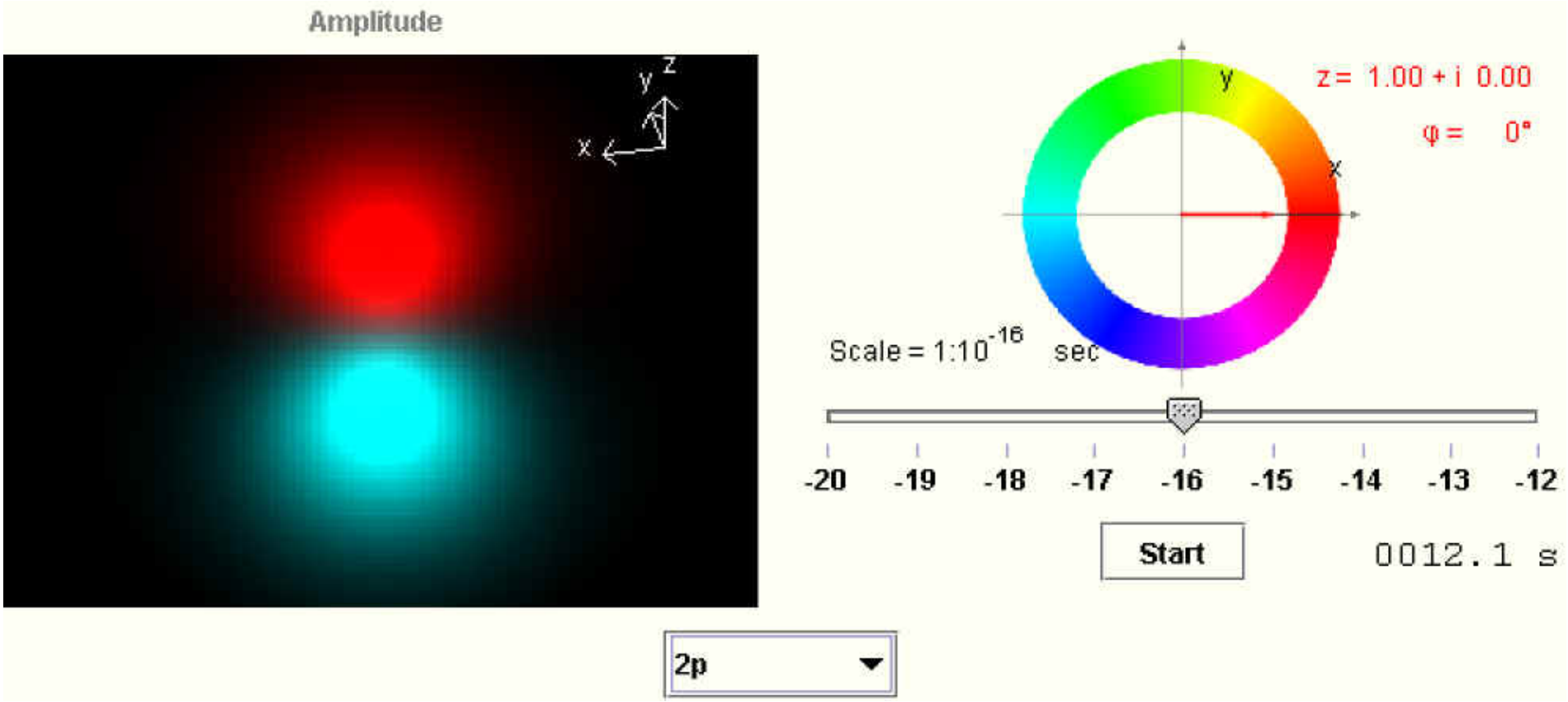
The Resolution: *Include Time!*



When time is properly included, three key concepts emerge:

- The electron wavefunction ***does change with time***.

Wavefunctions change with time.



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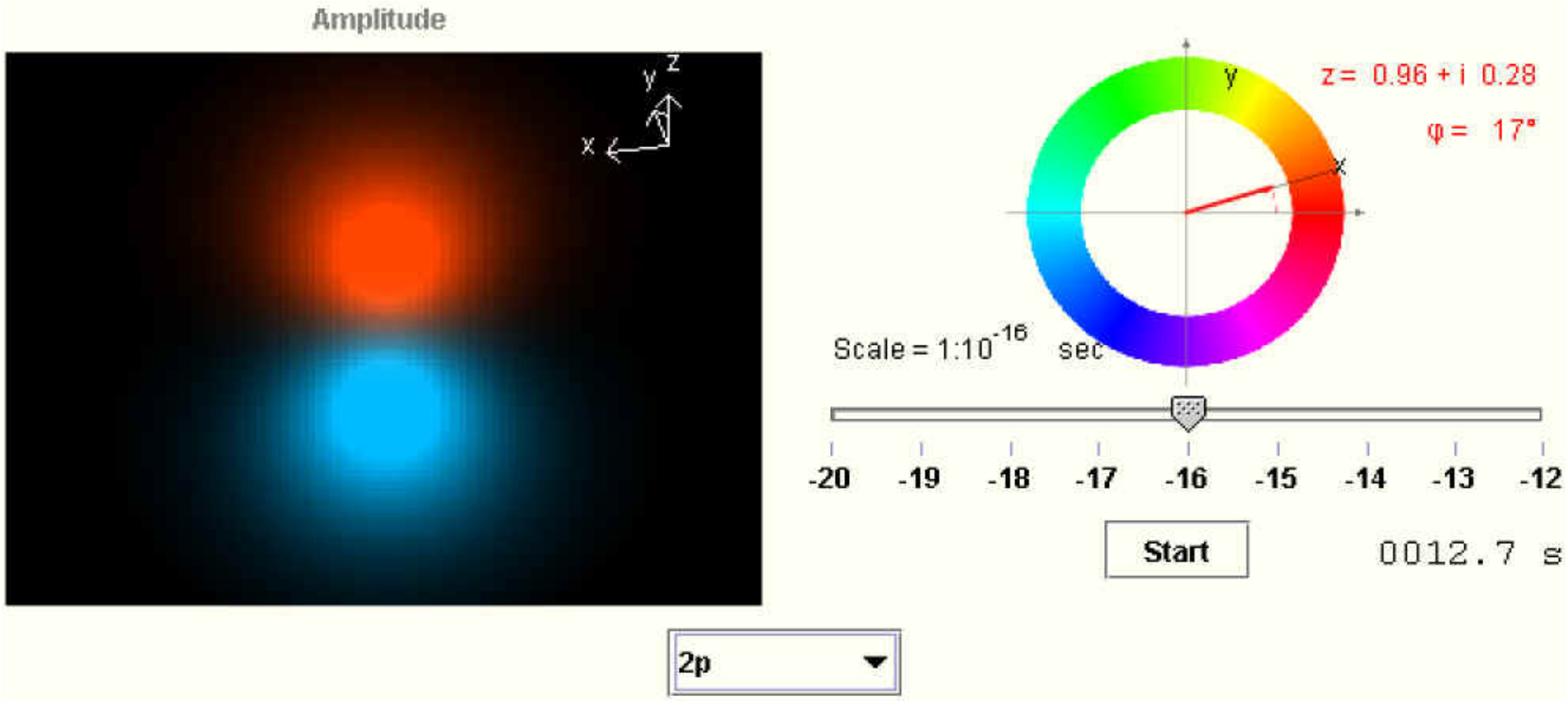

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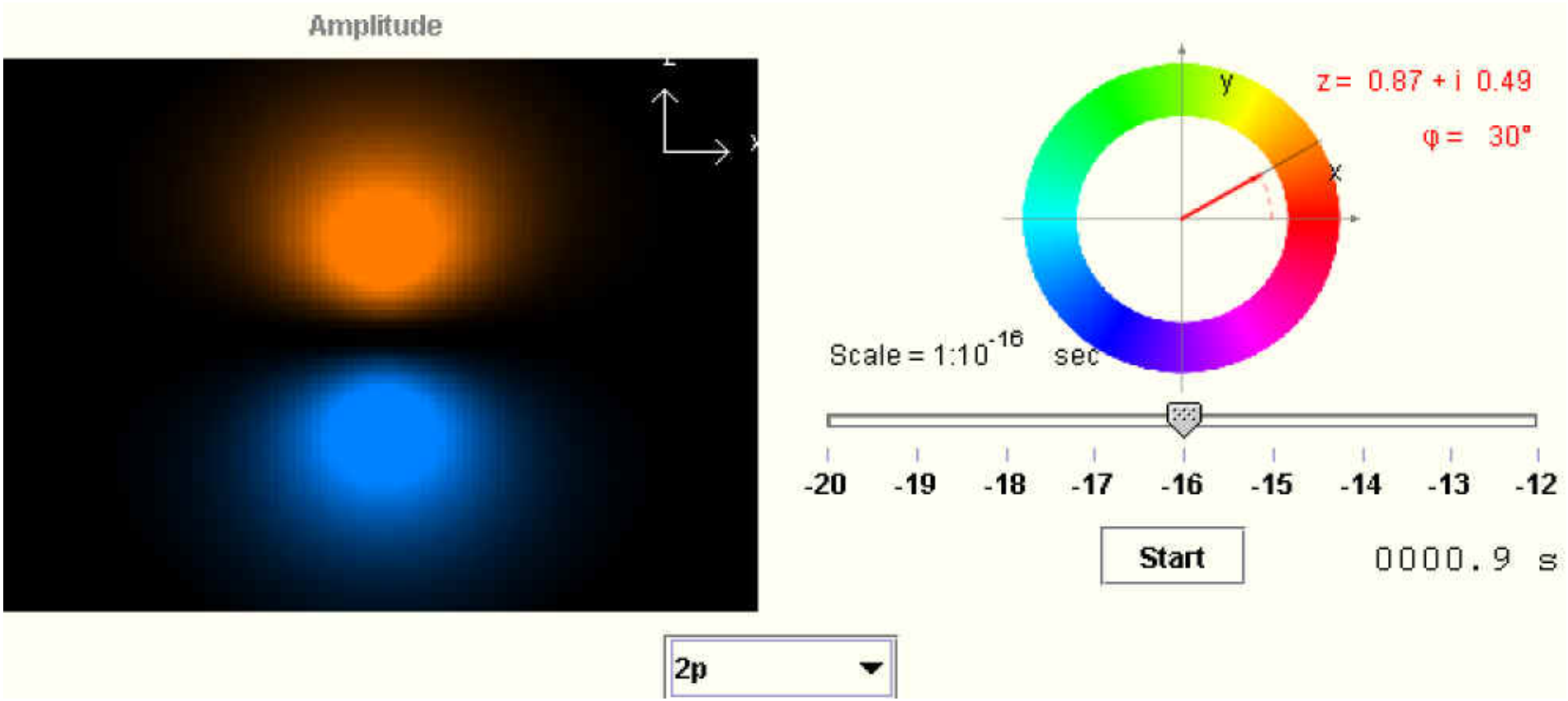

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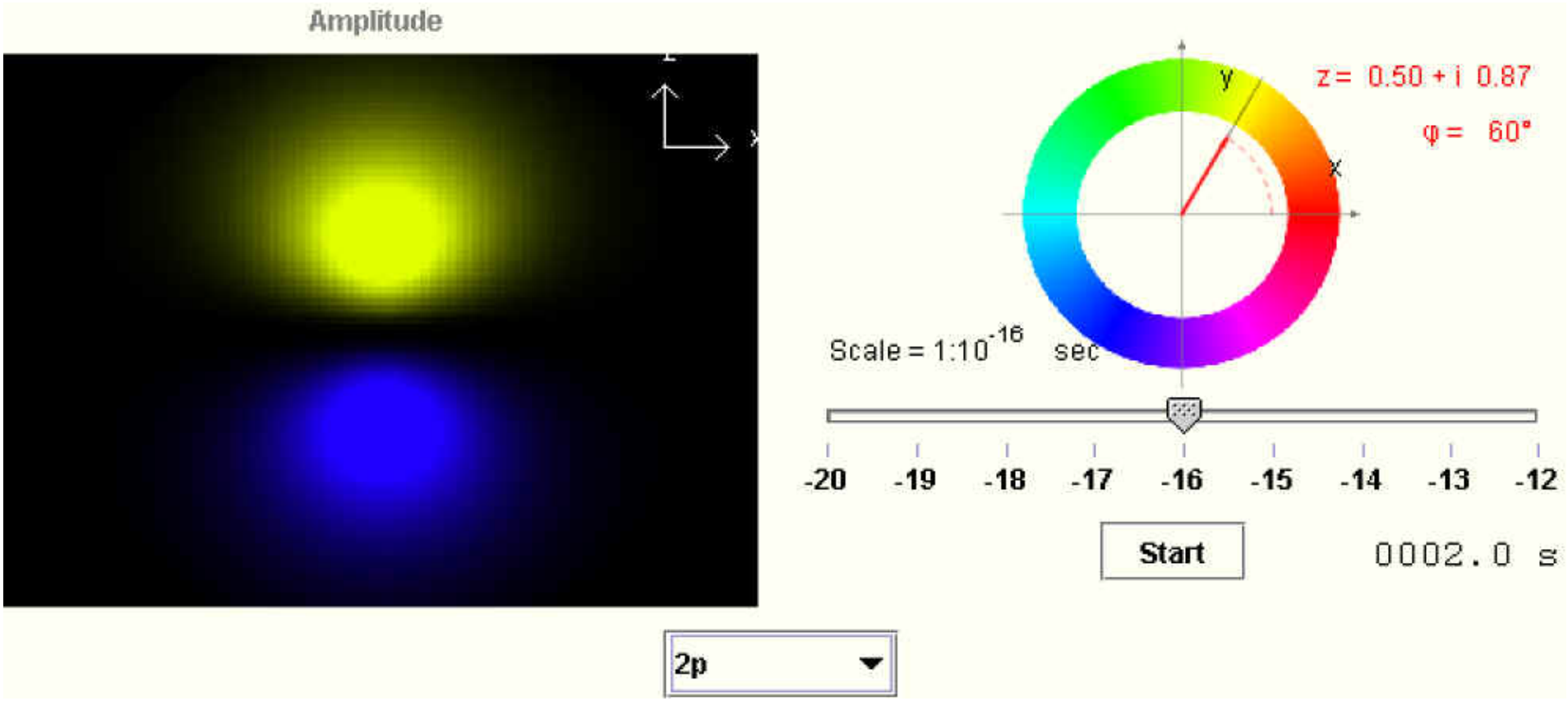

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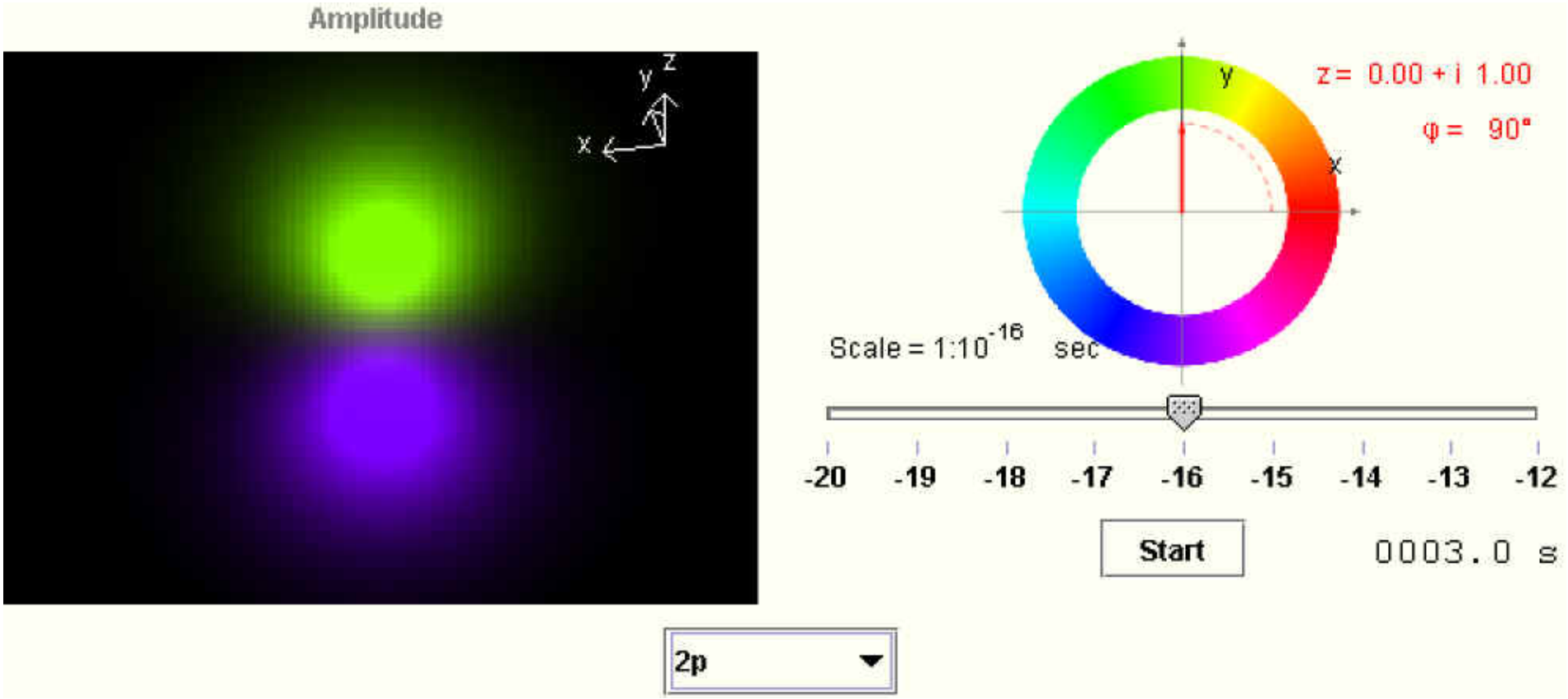

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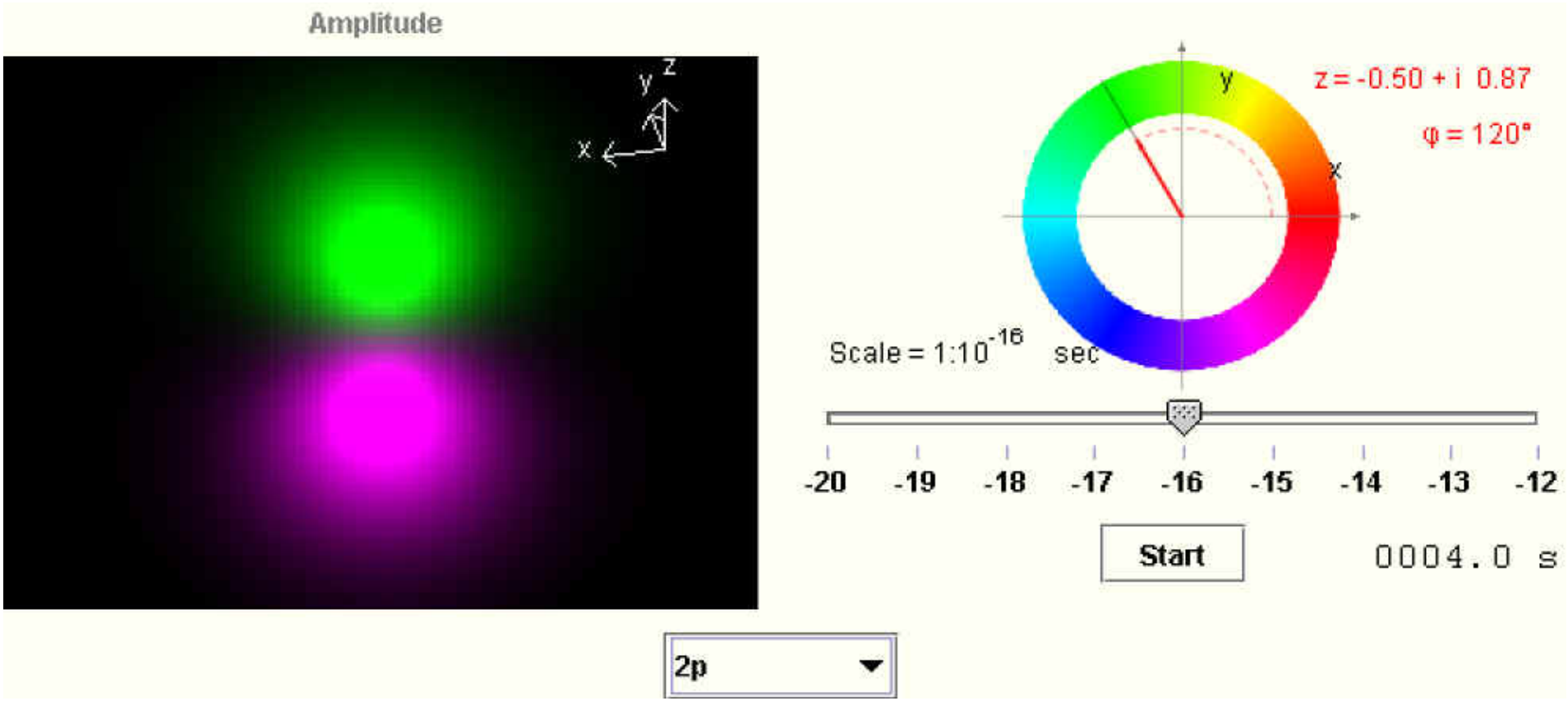

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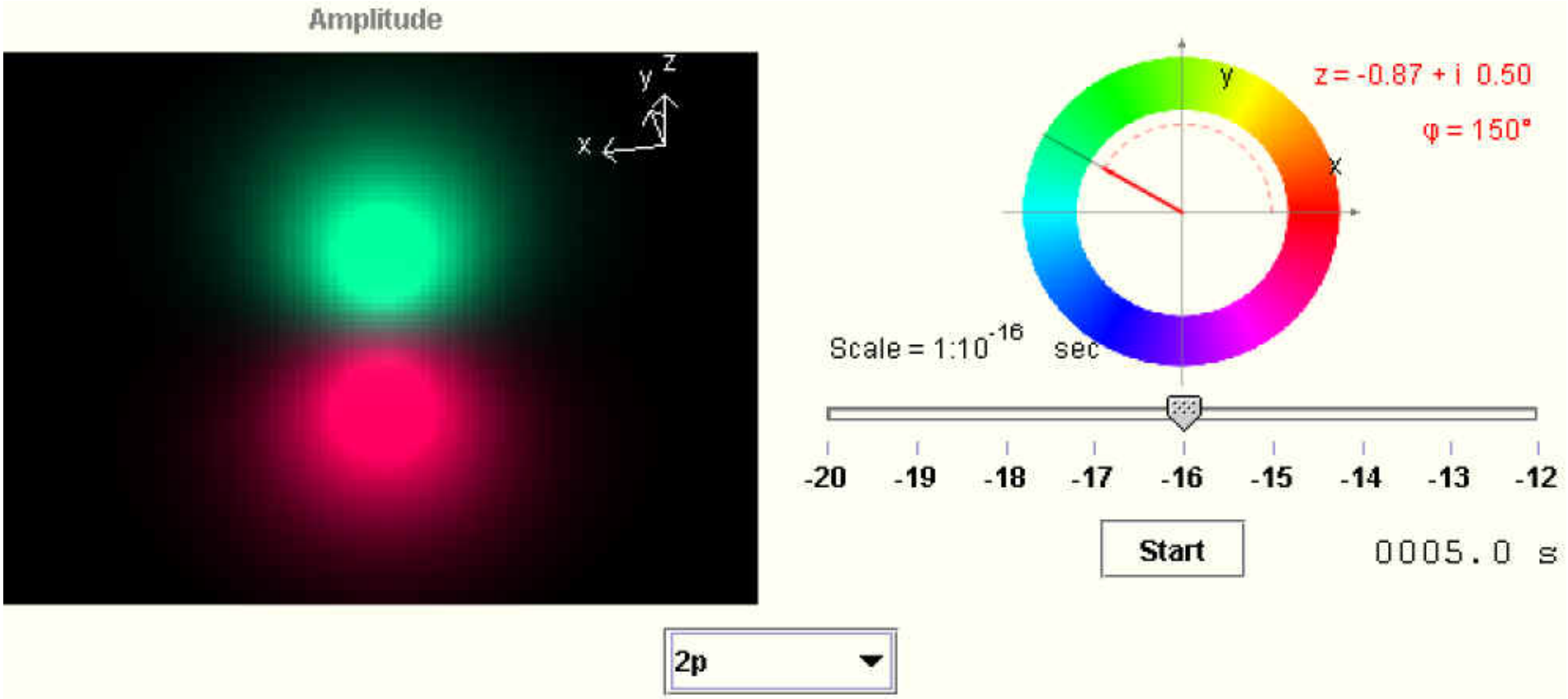

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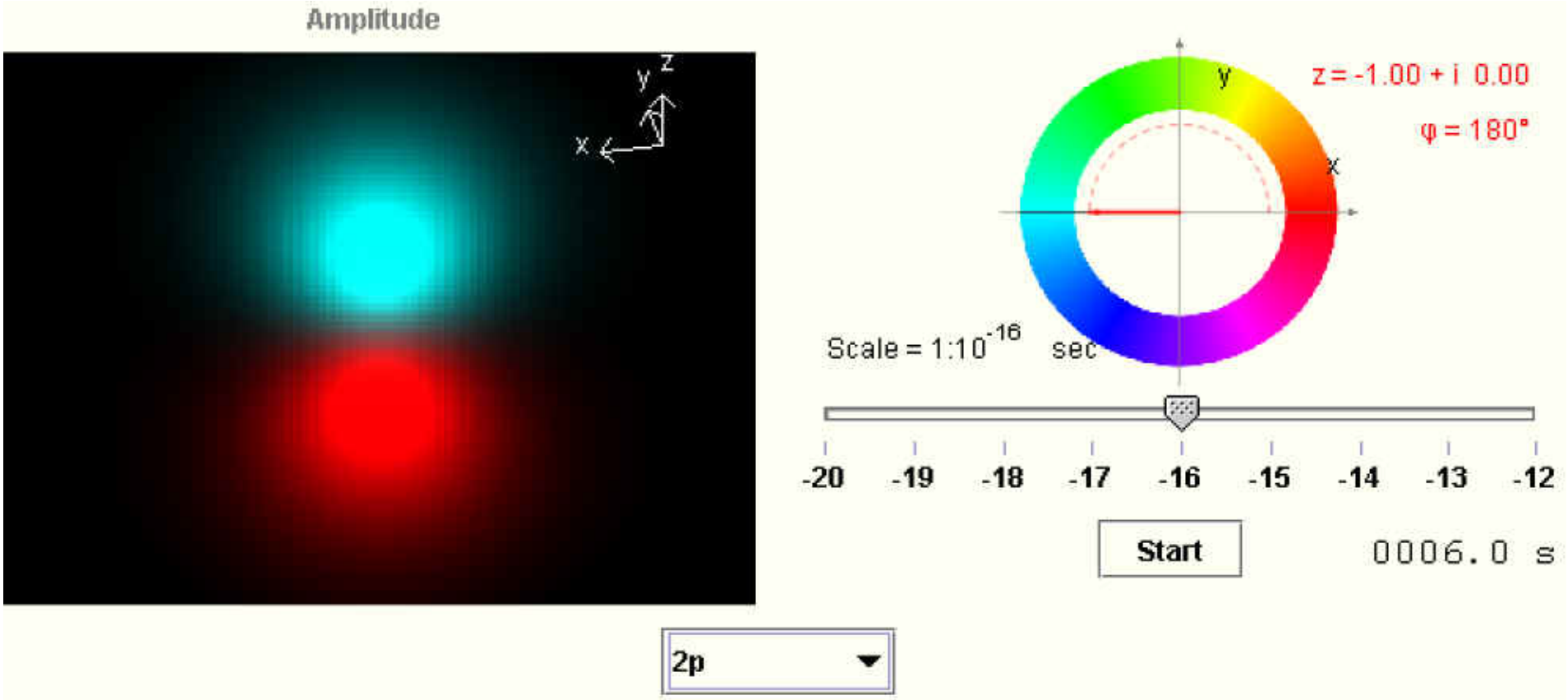

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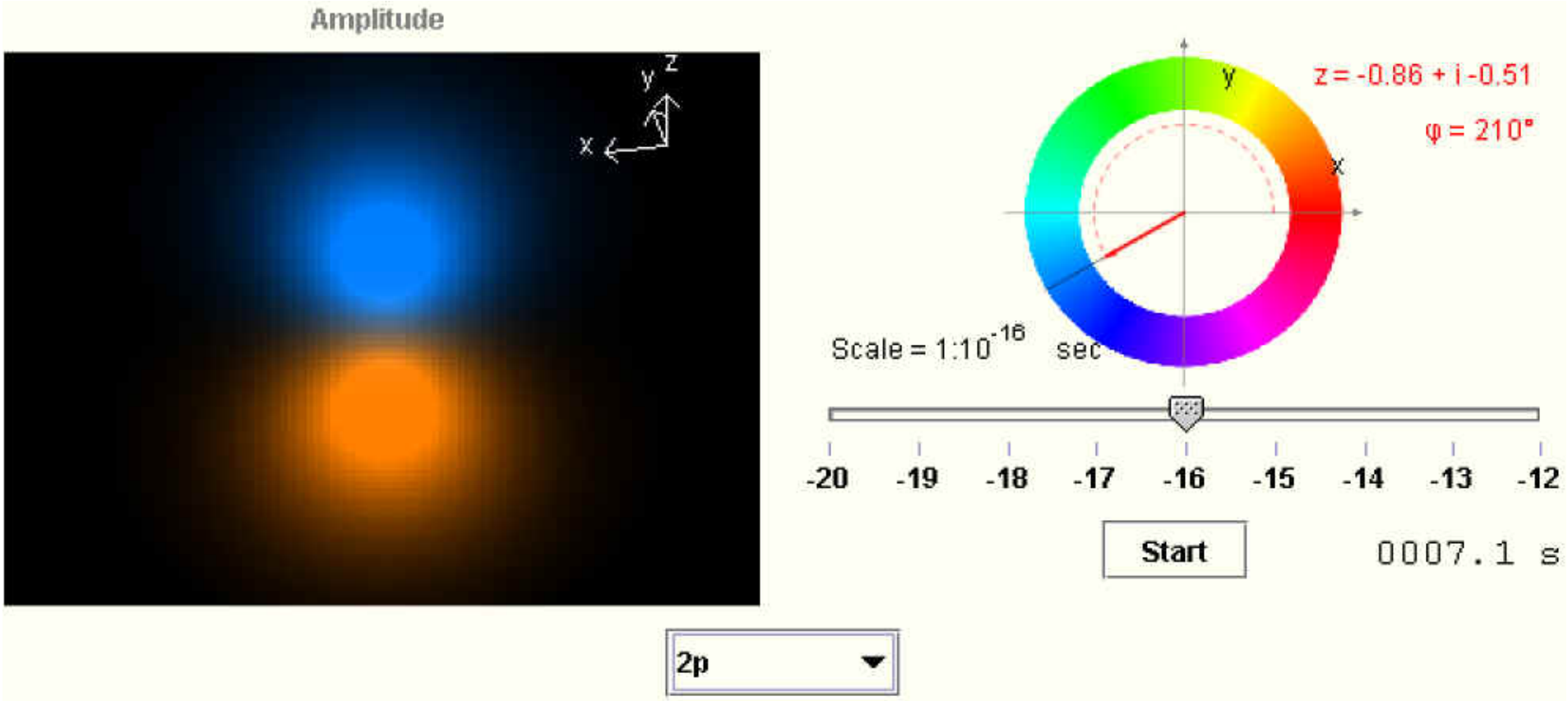

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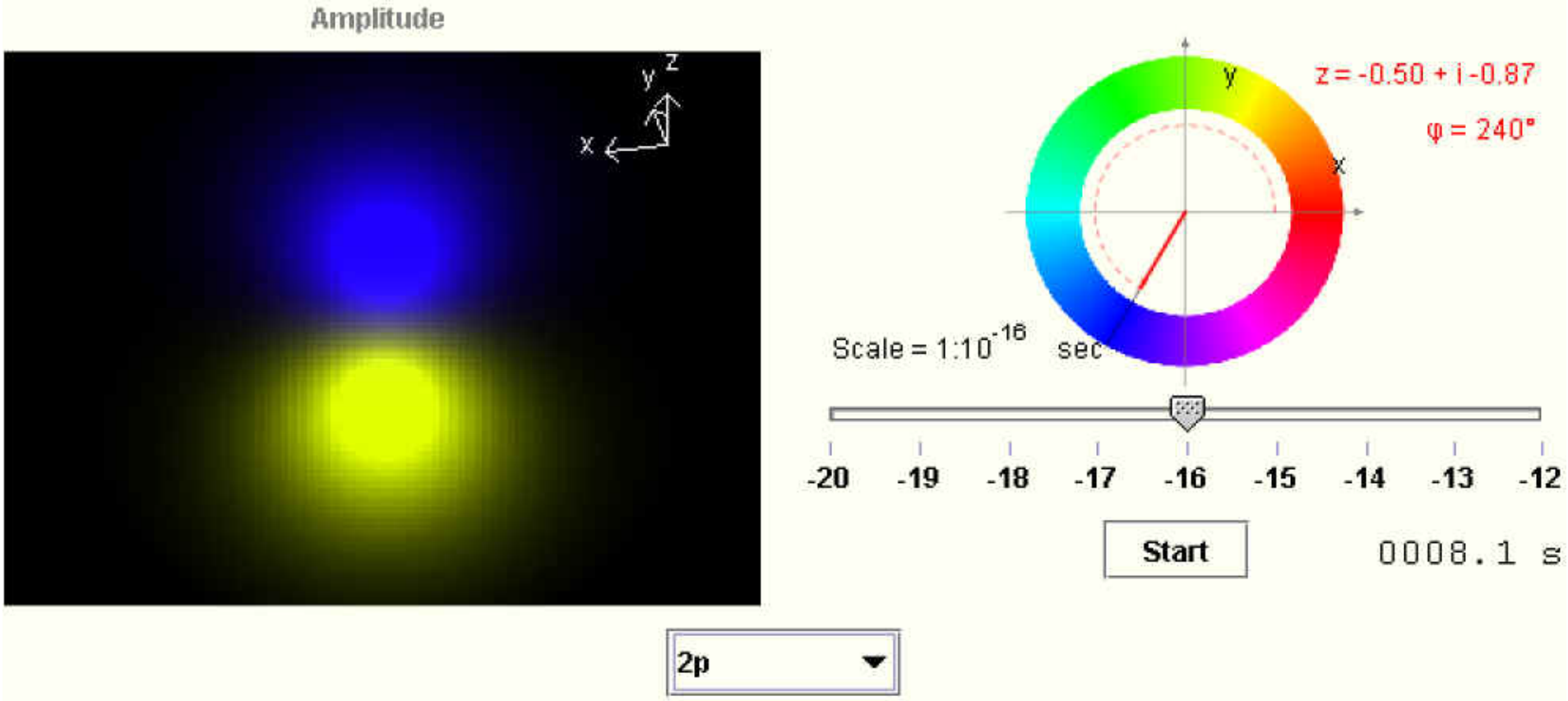

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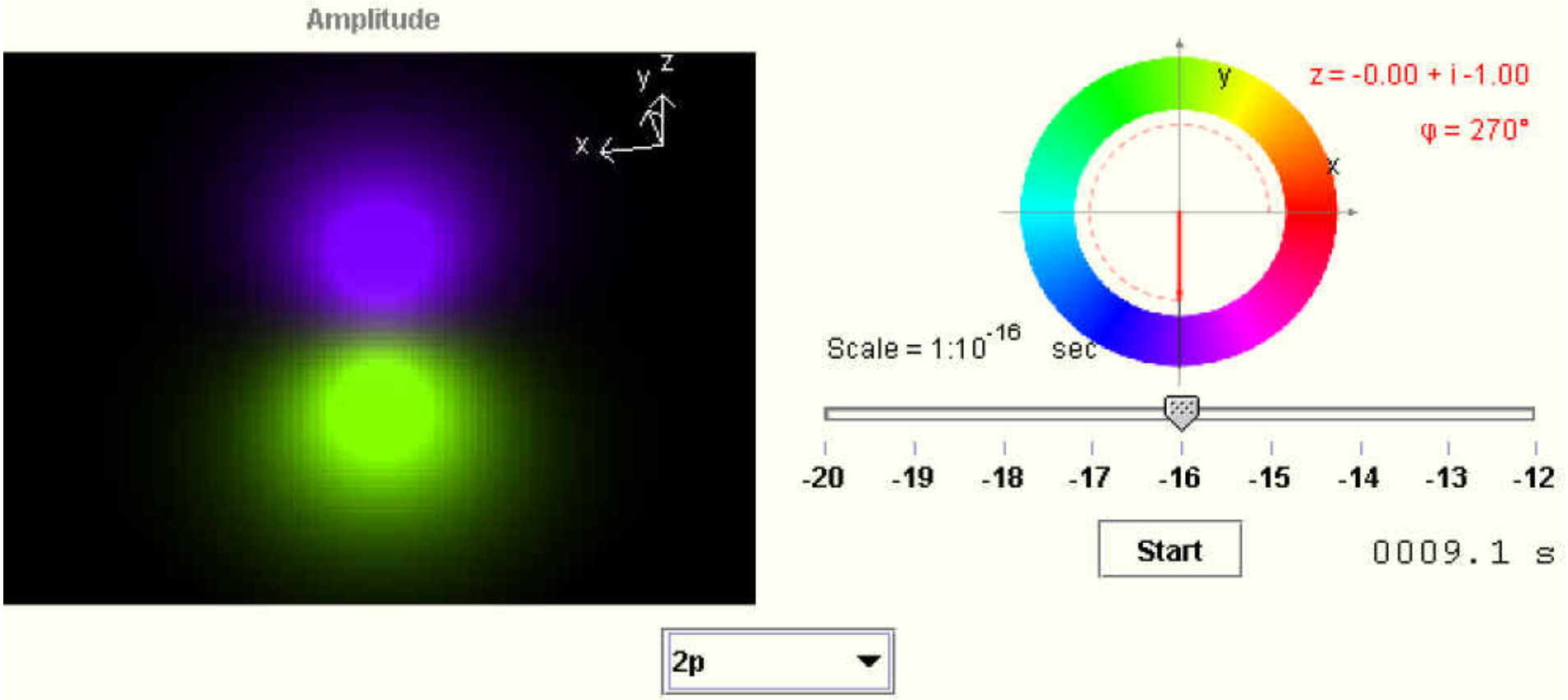

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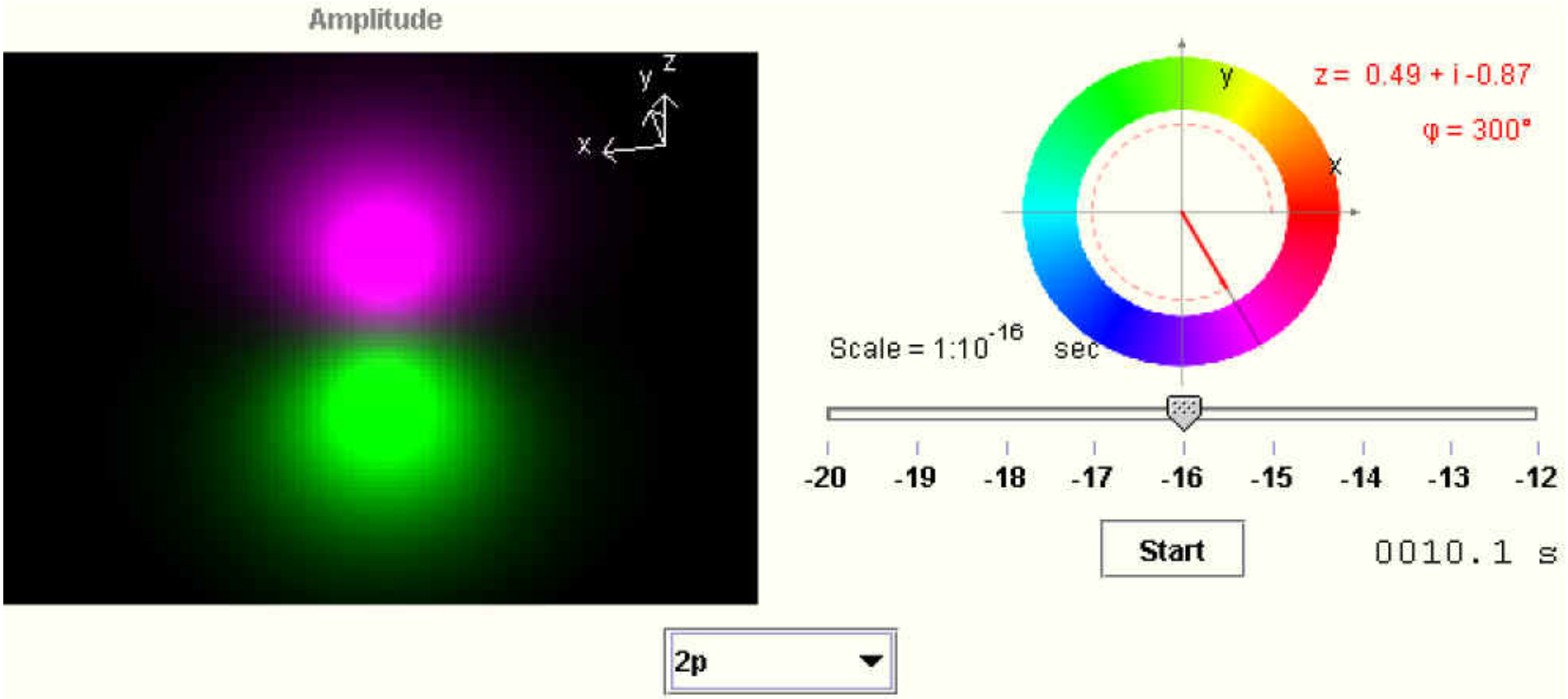

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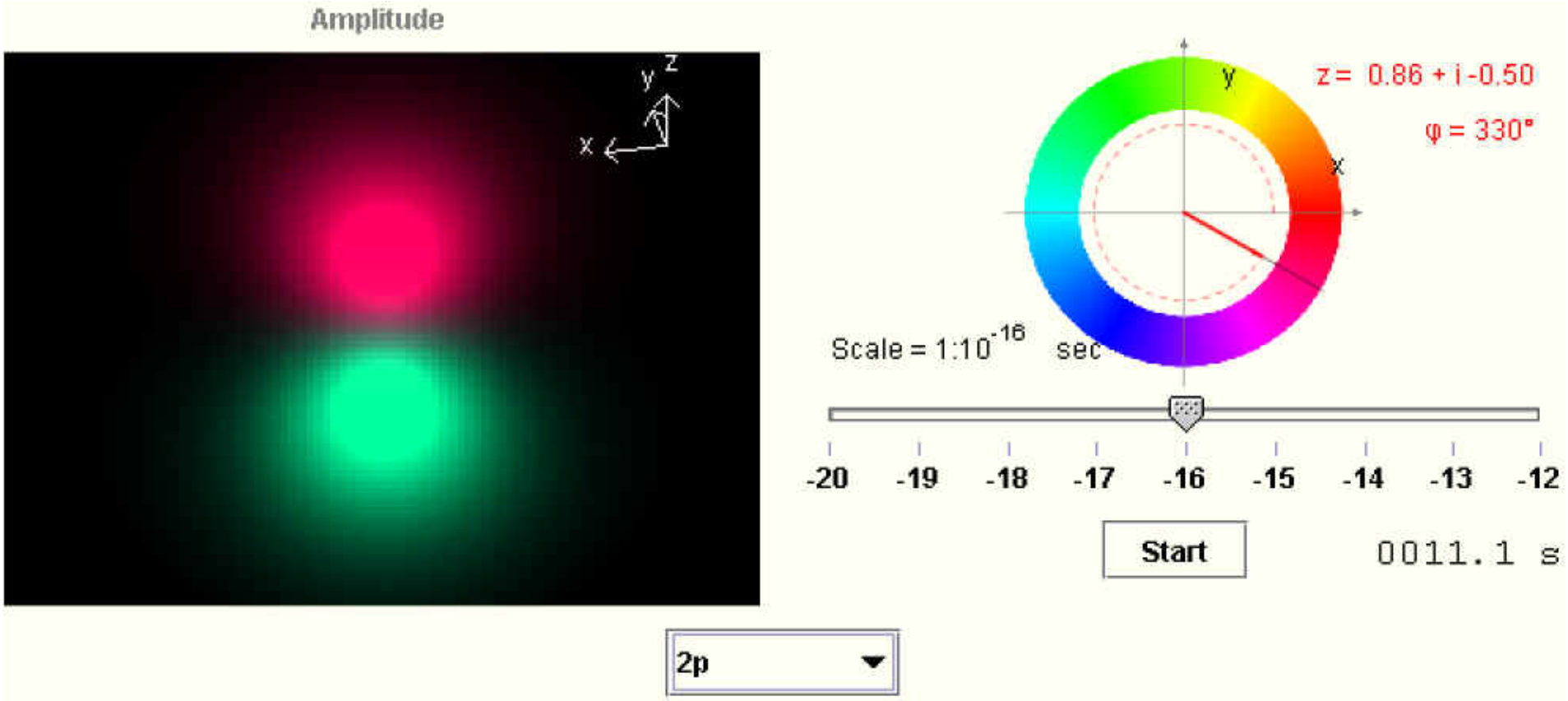

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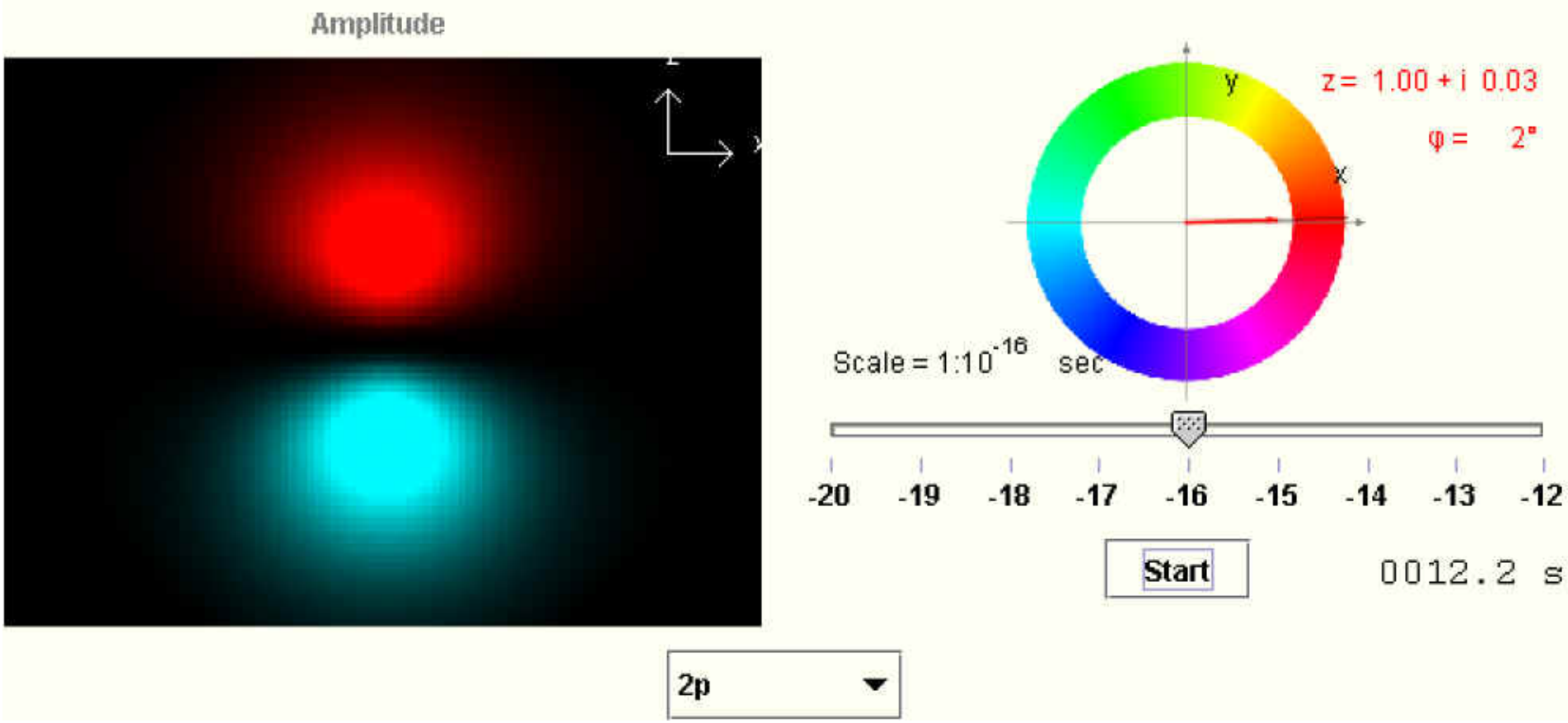

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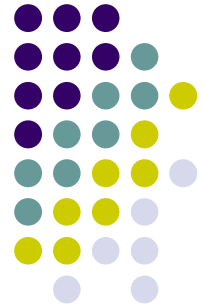
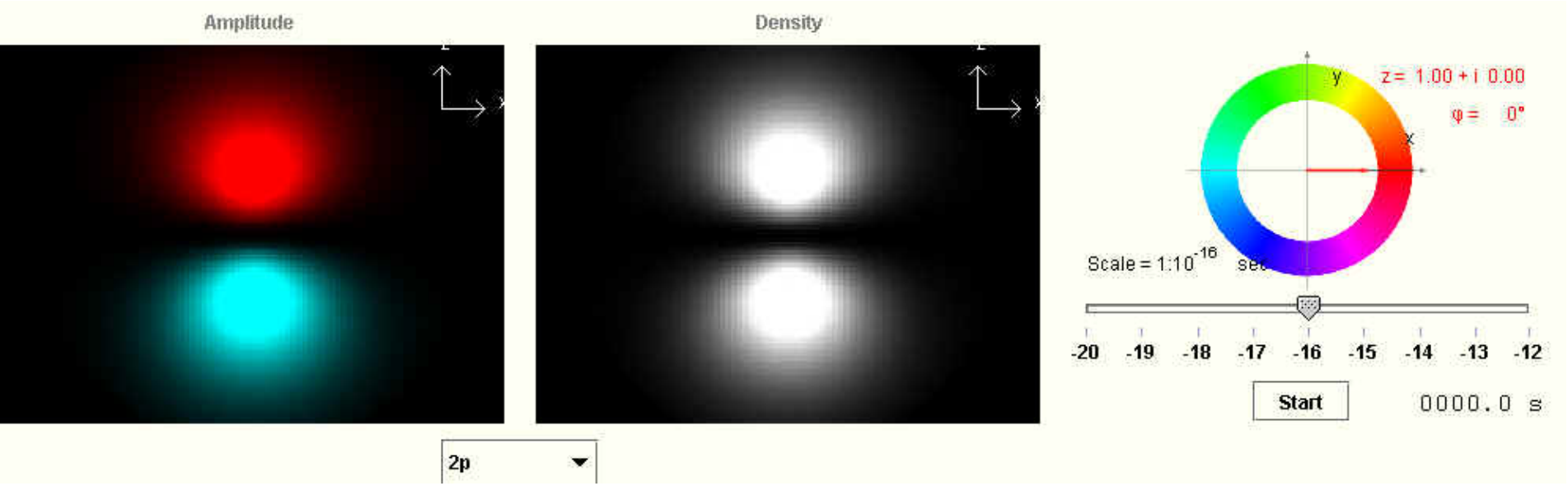
The Resolution: *Include Time!*



When time is properly included, three key concepts emerge.

- The electron wavefunction *does change with time*.
- Electron density in a specific energy state *is nevertheless static*: nothing moves, nothing evolves, nothing changes.

Electron density is *static.*



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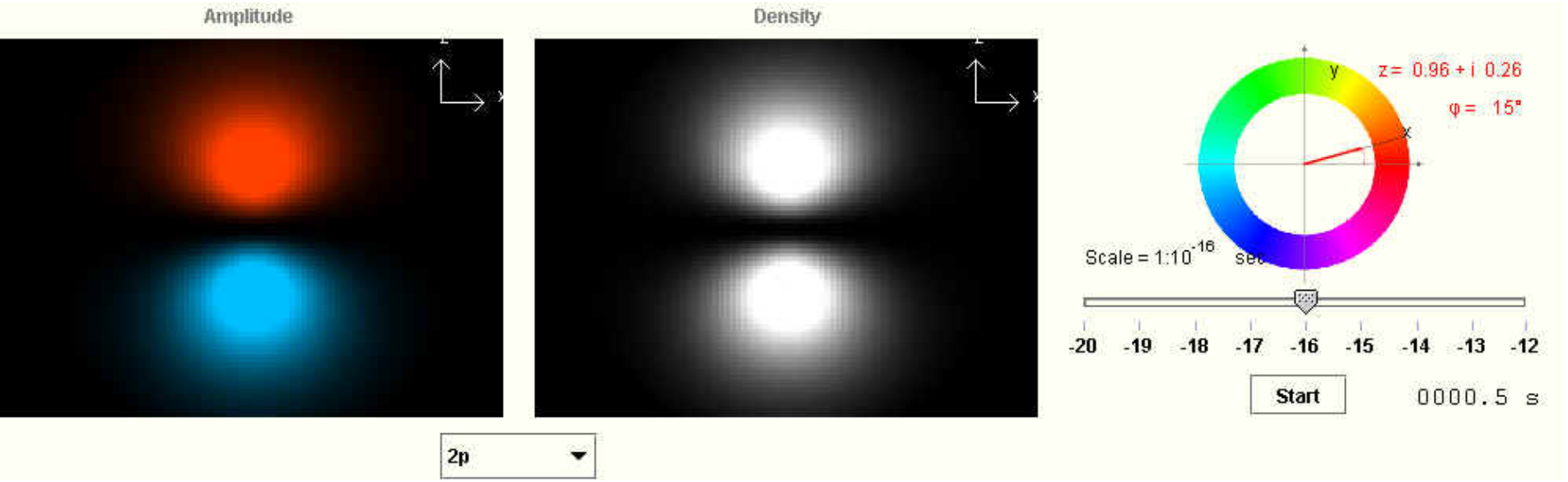

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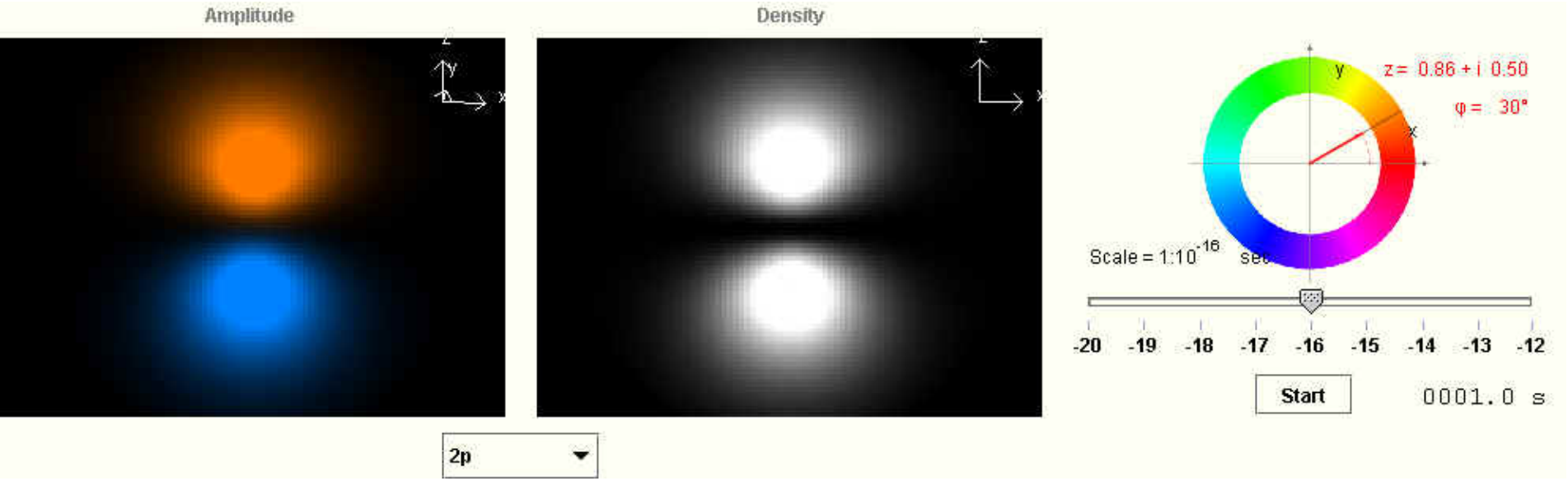

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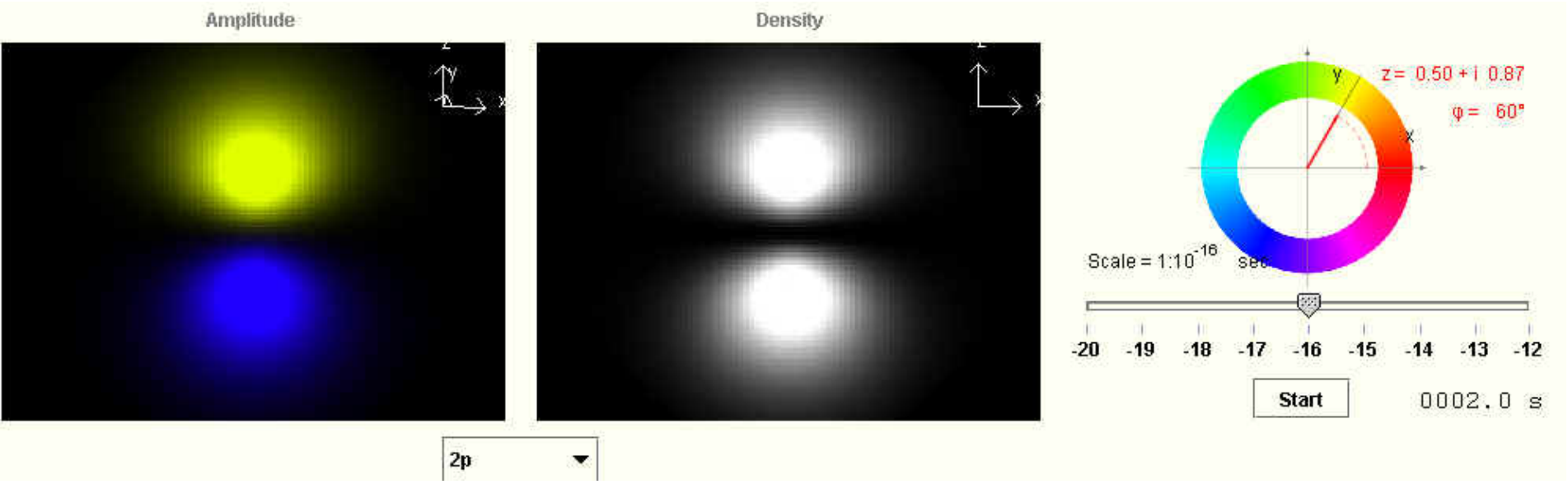

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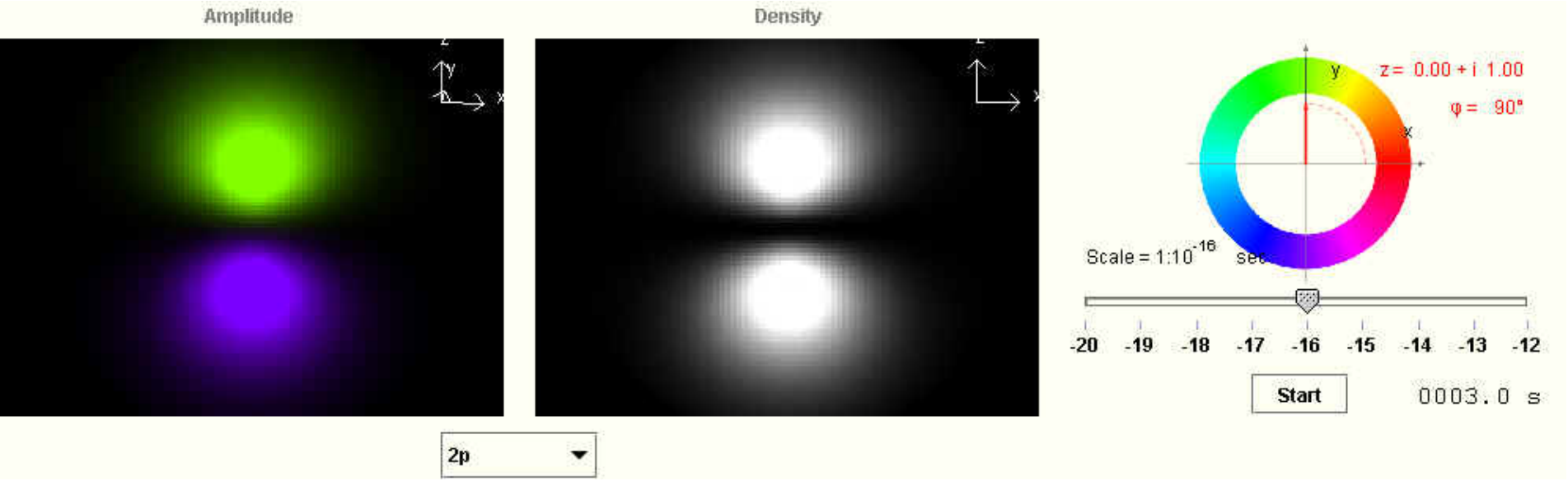

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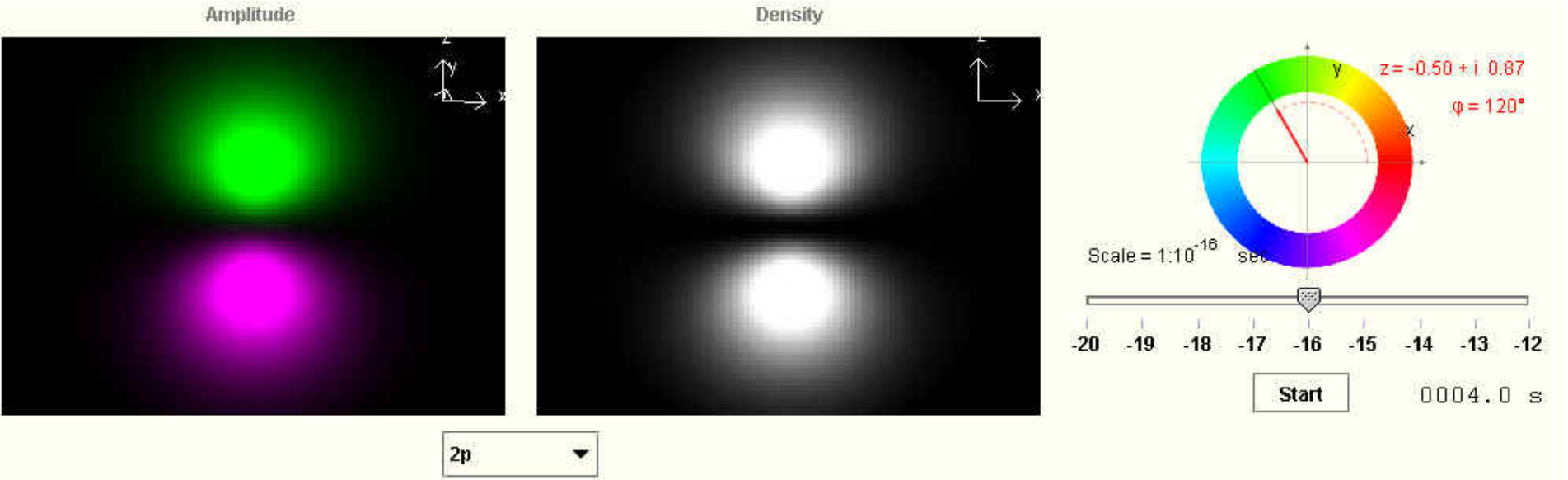

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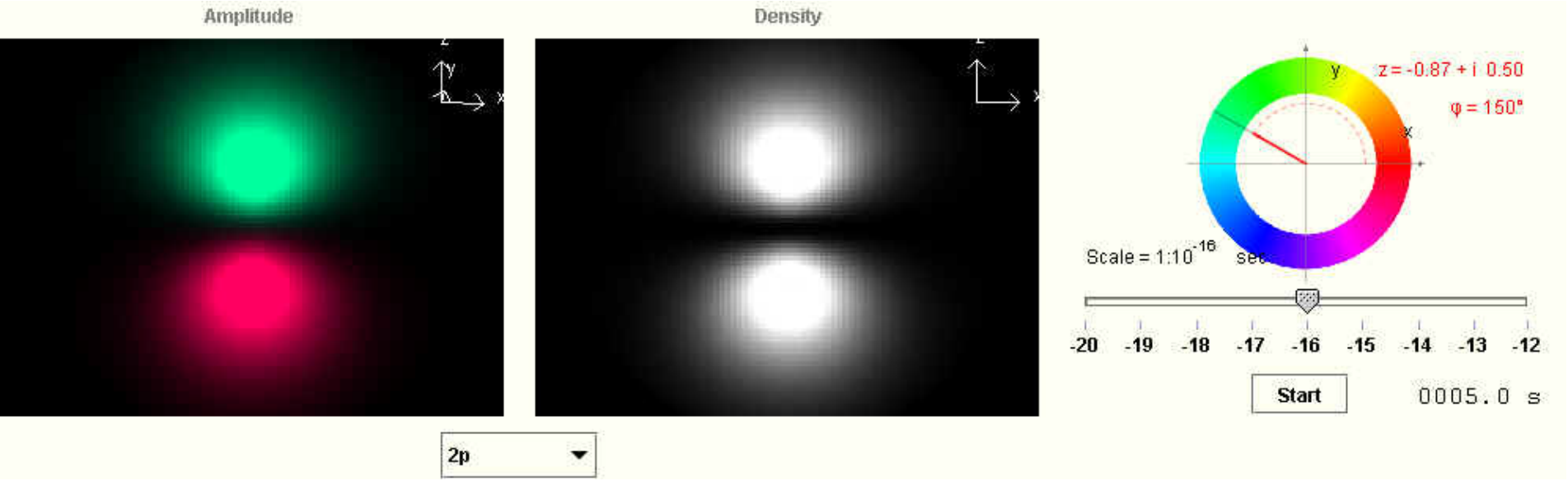

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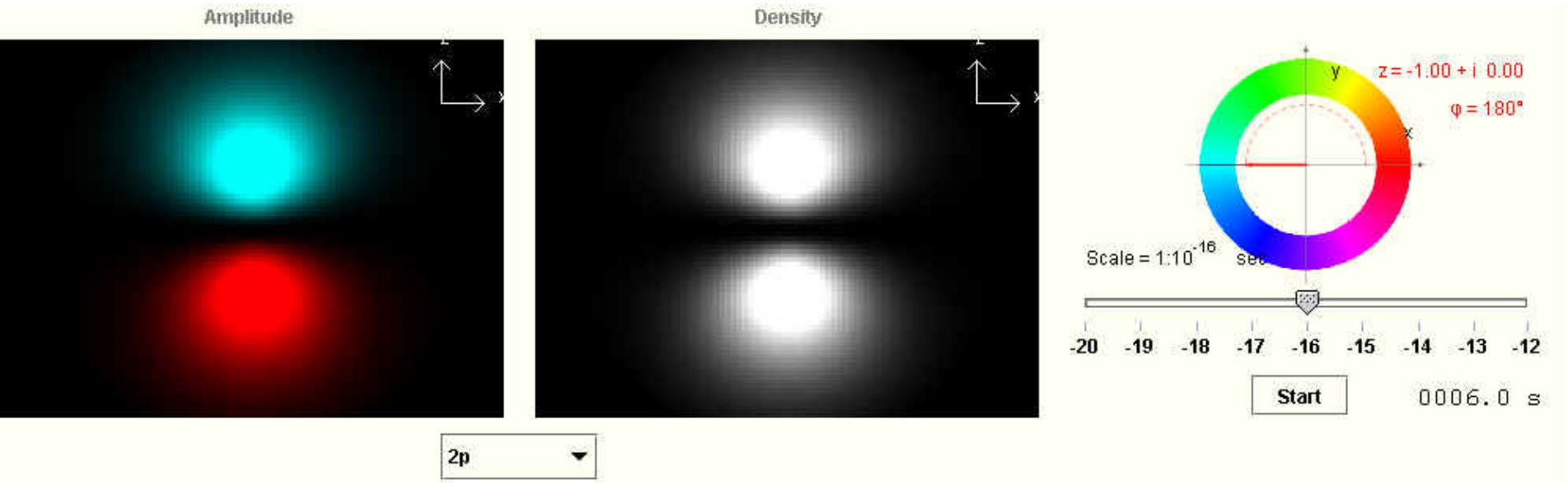

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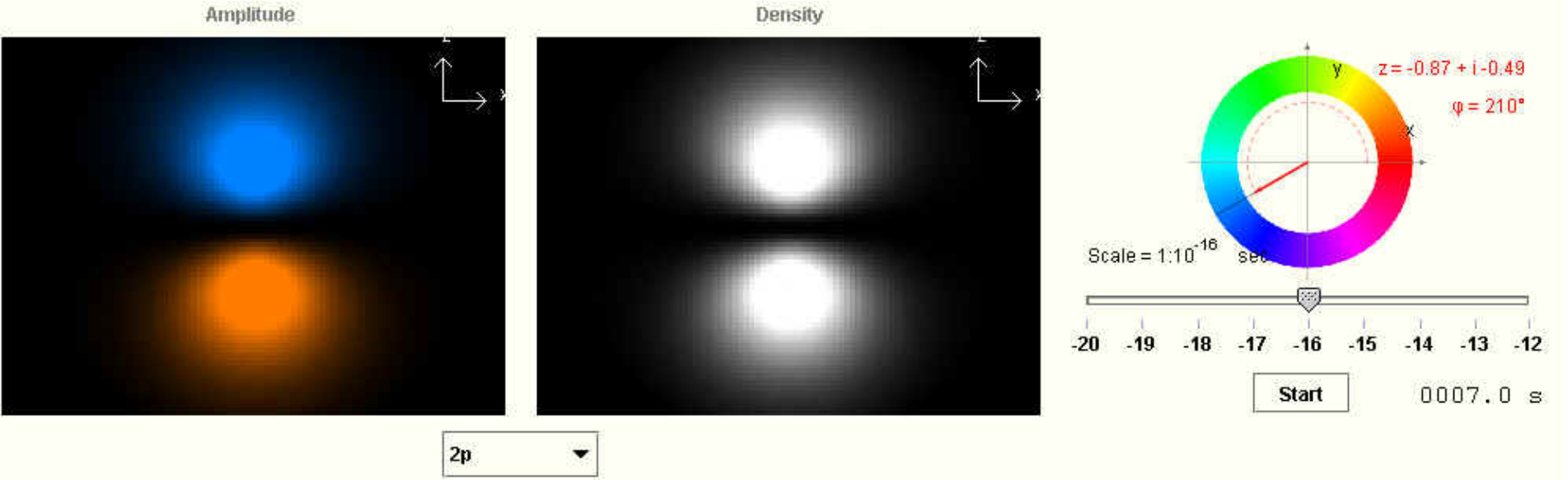

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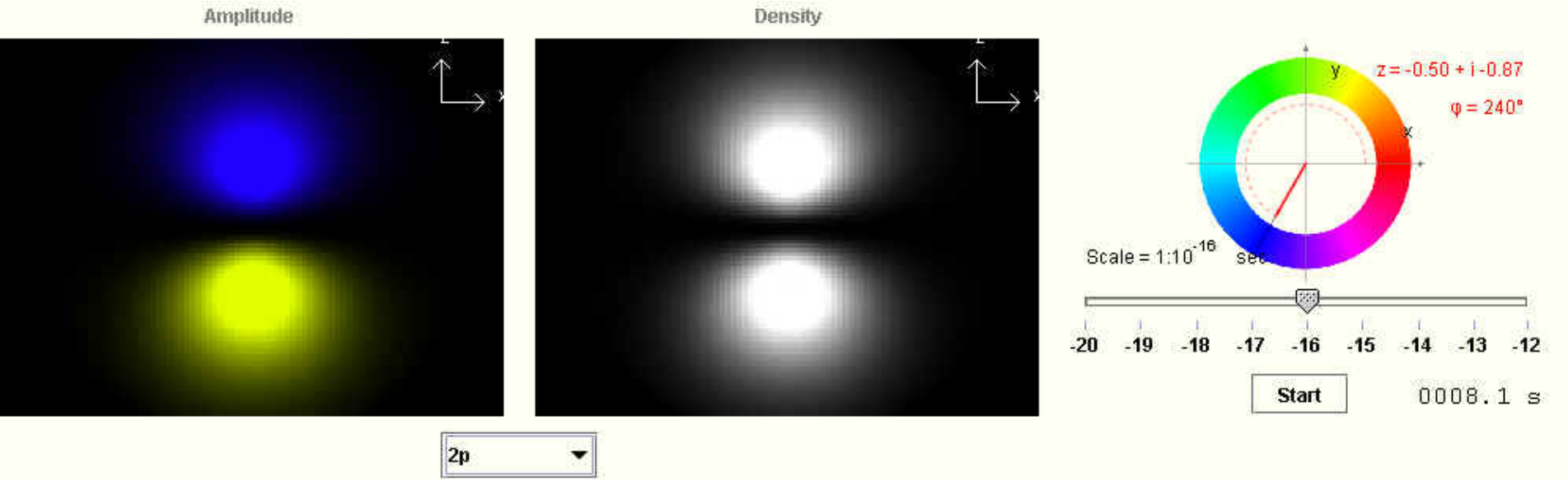

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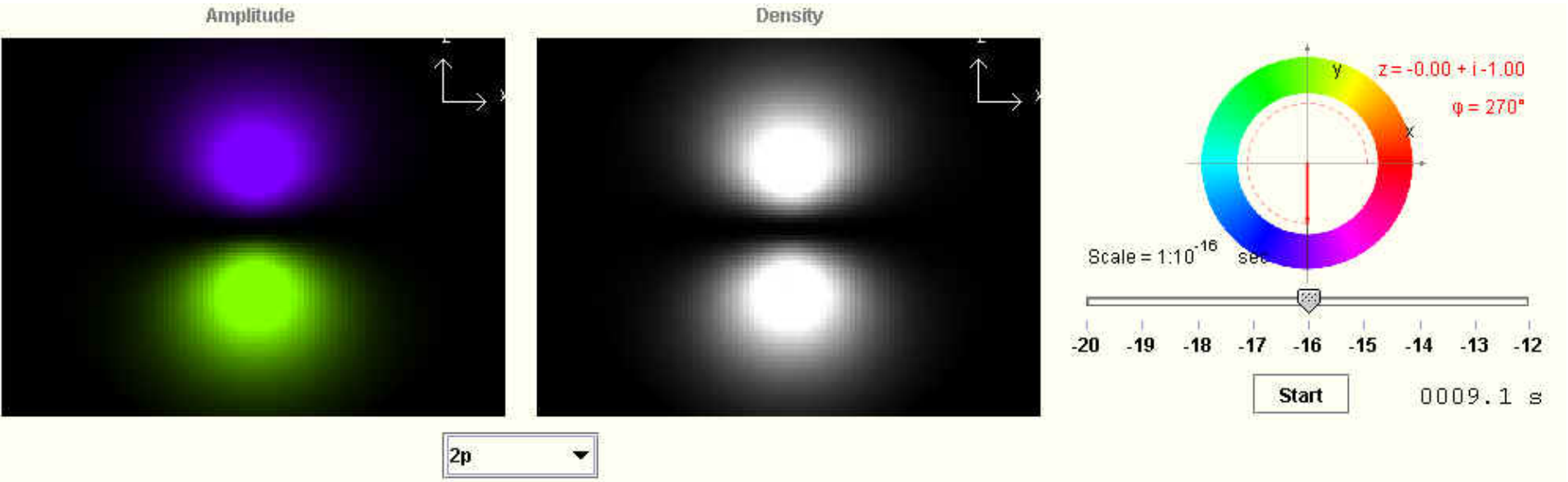

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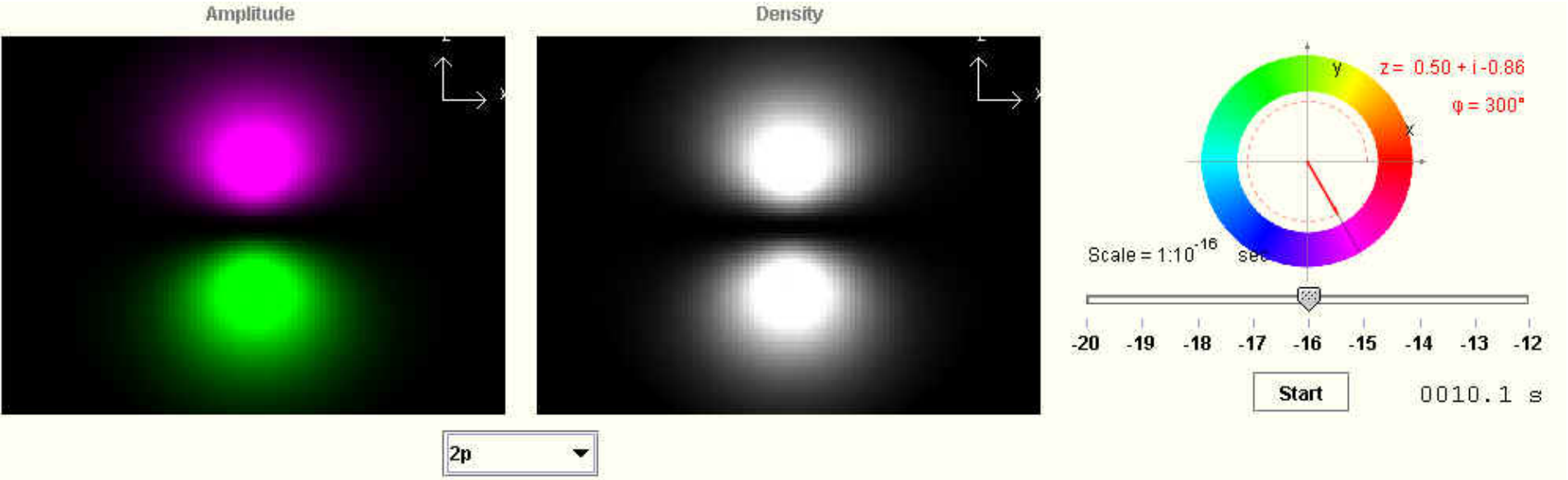

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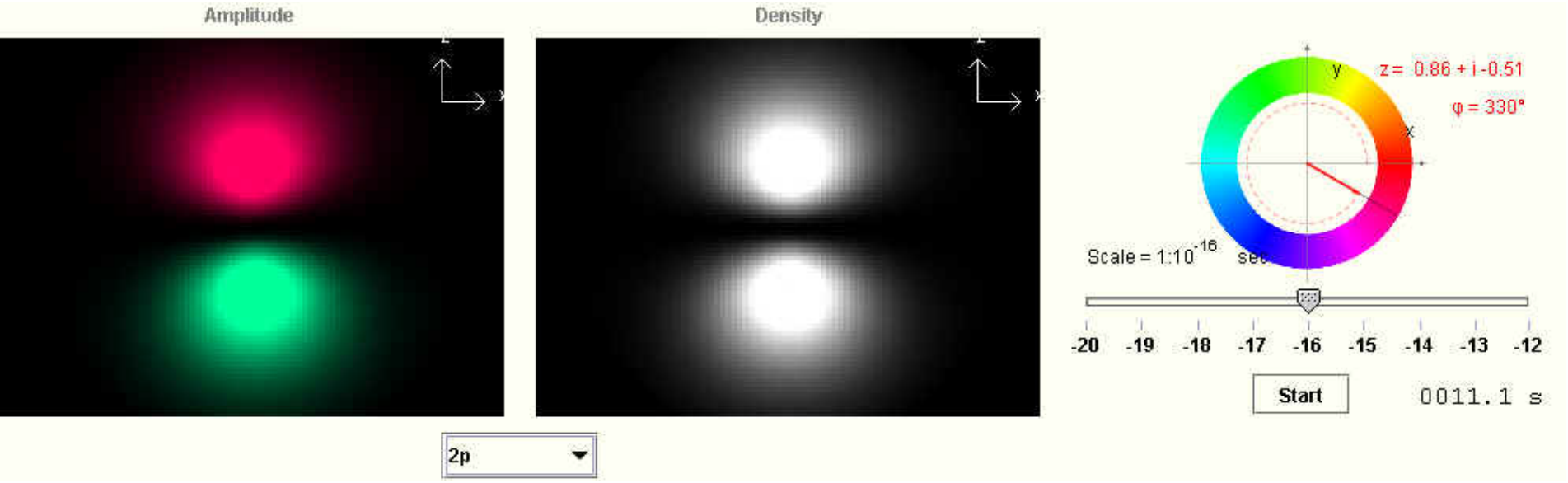

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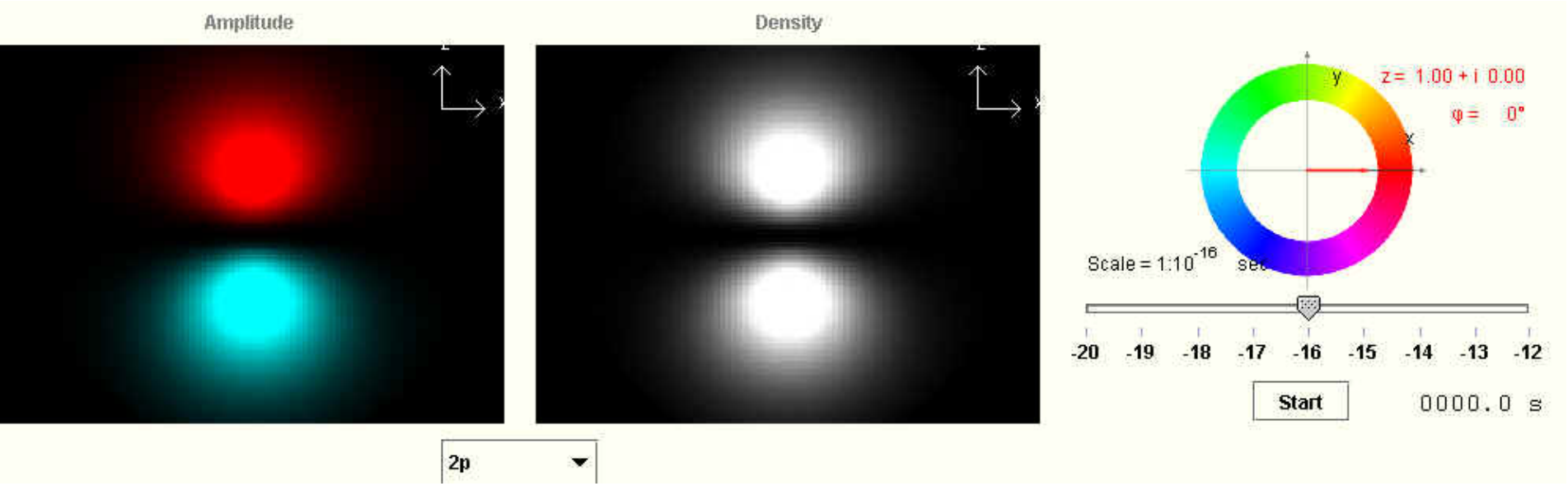

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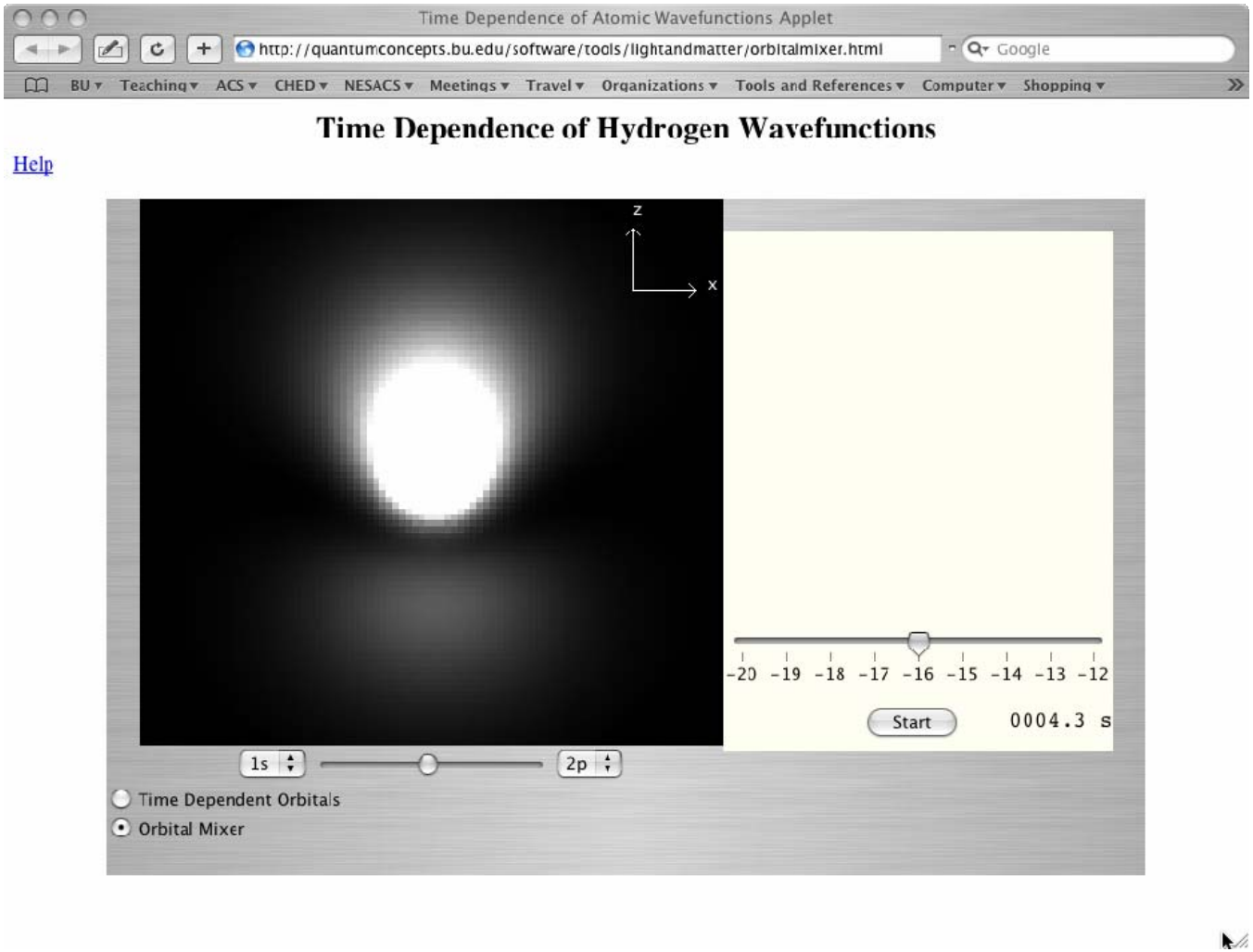
The Resolution: *Include Time!*

When time is properly included, three key concepts emerge.

- The electron wavefunction *does change with time*.
- Electron density in a specific energy state *is nevertheless static*: nothing moves, nothing evolves, nothing changes.
- The ***mixing*** of energy states accounts for ***all*** motion, evolution, and change.

Mixing accounts for motion.



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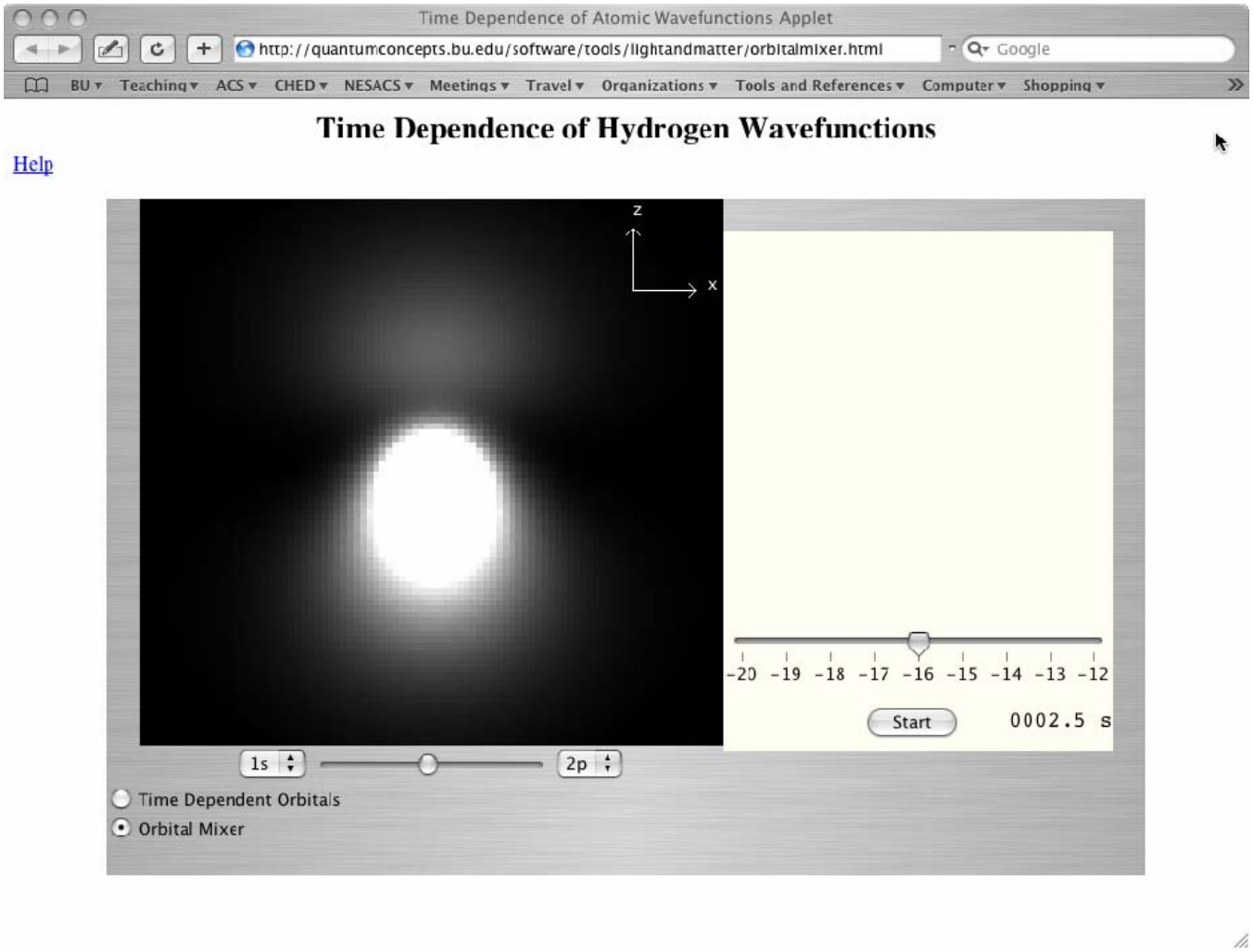
Mixing accounts for motion.



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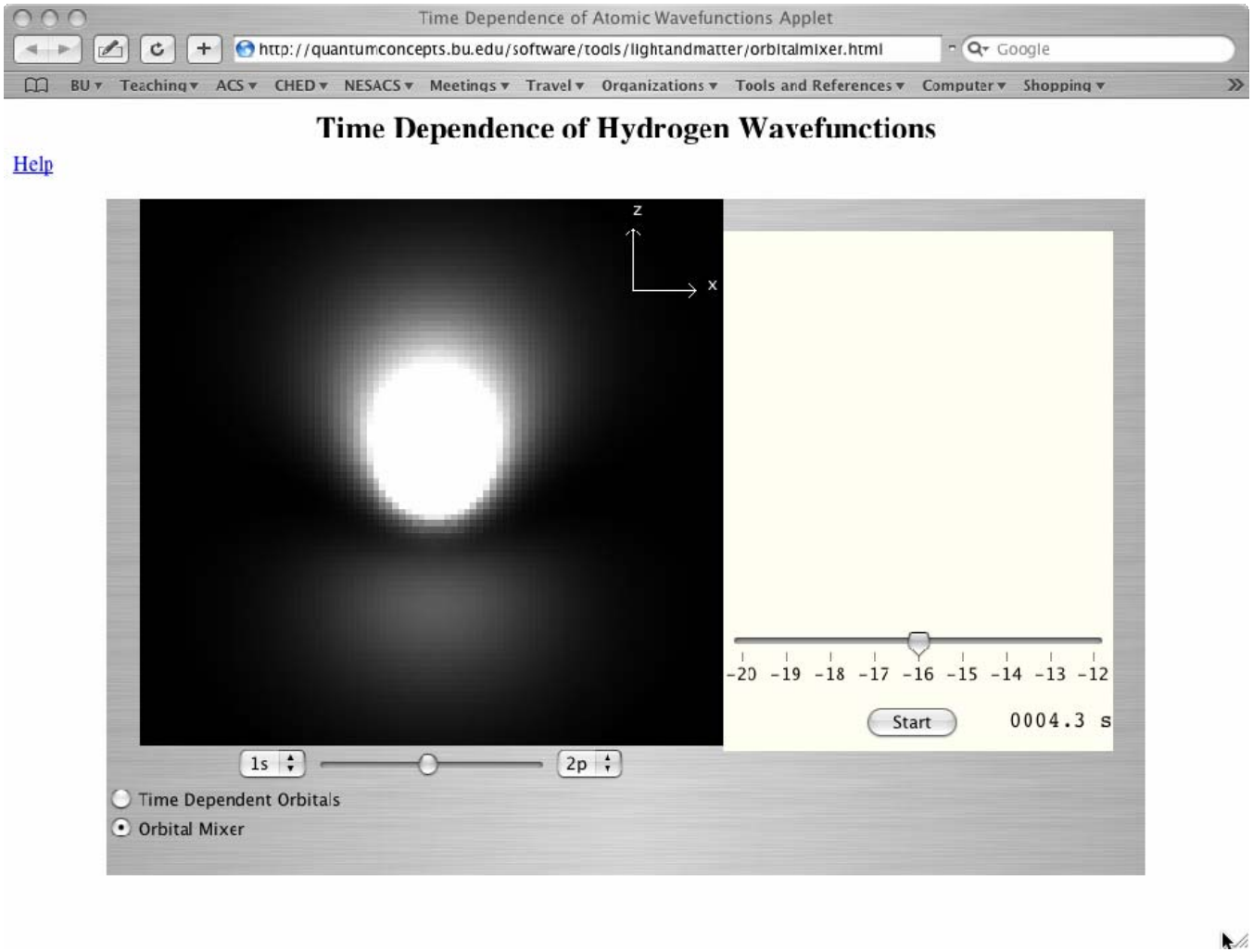

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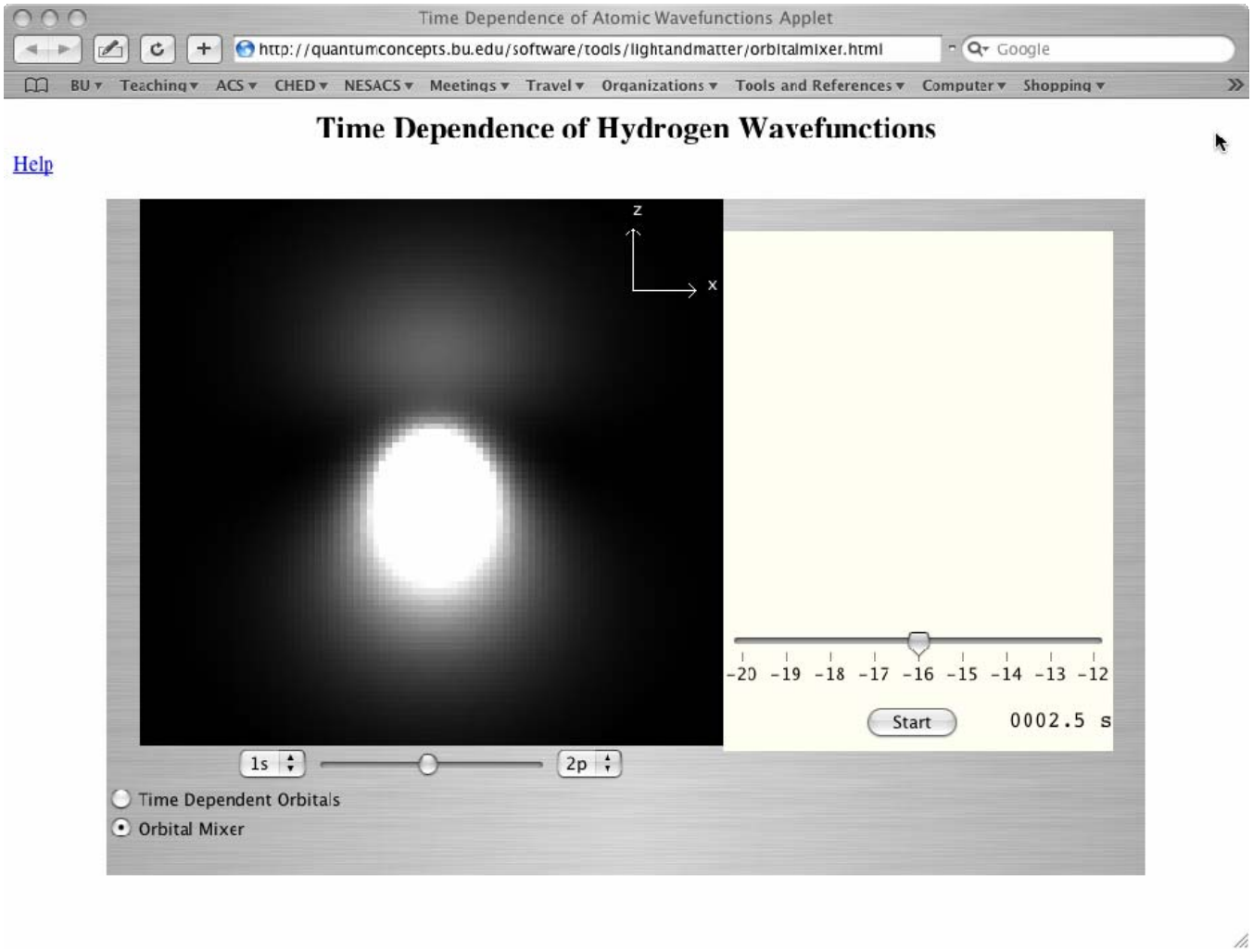

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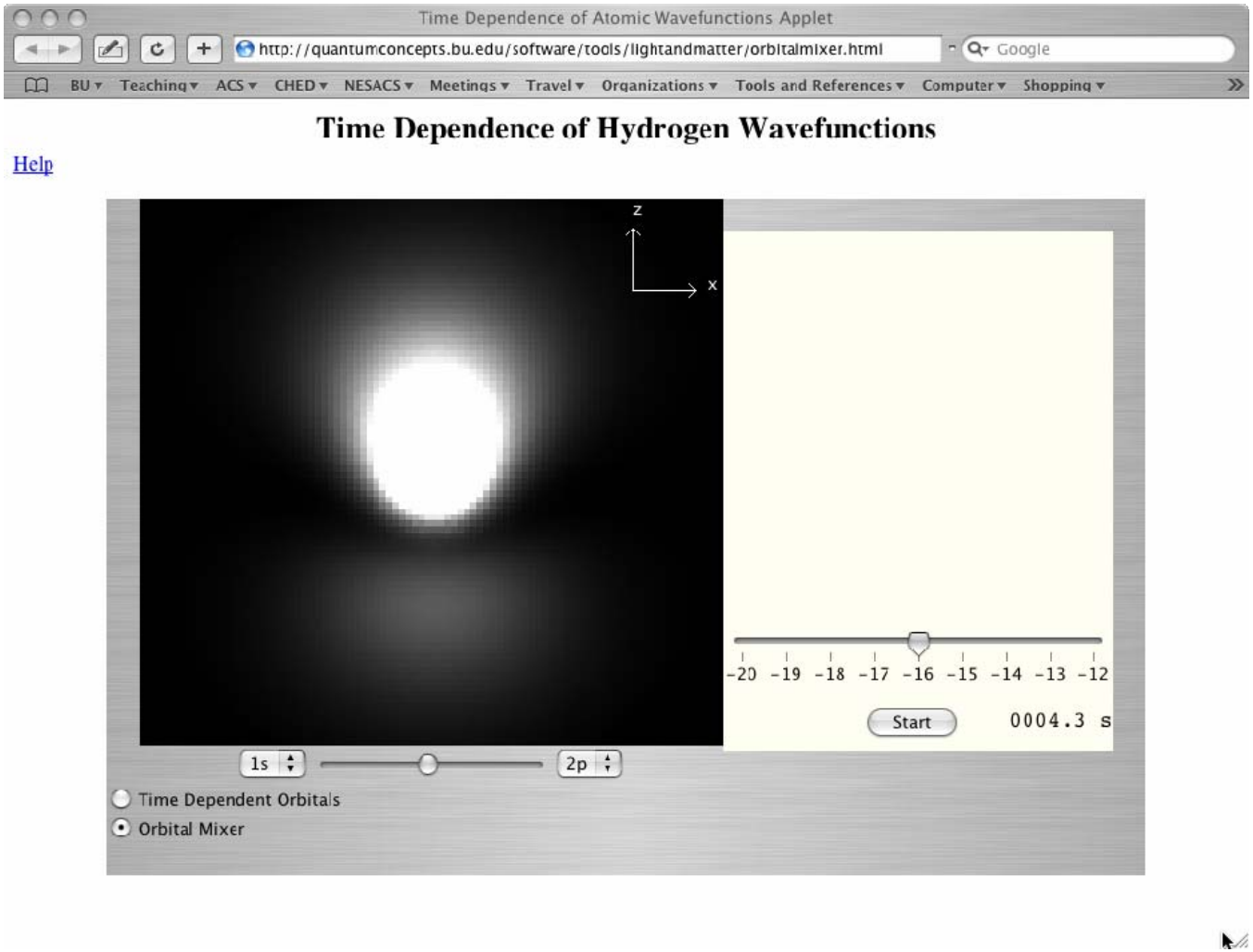

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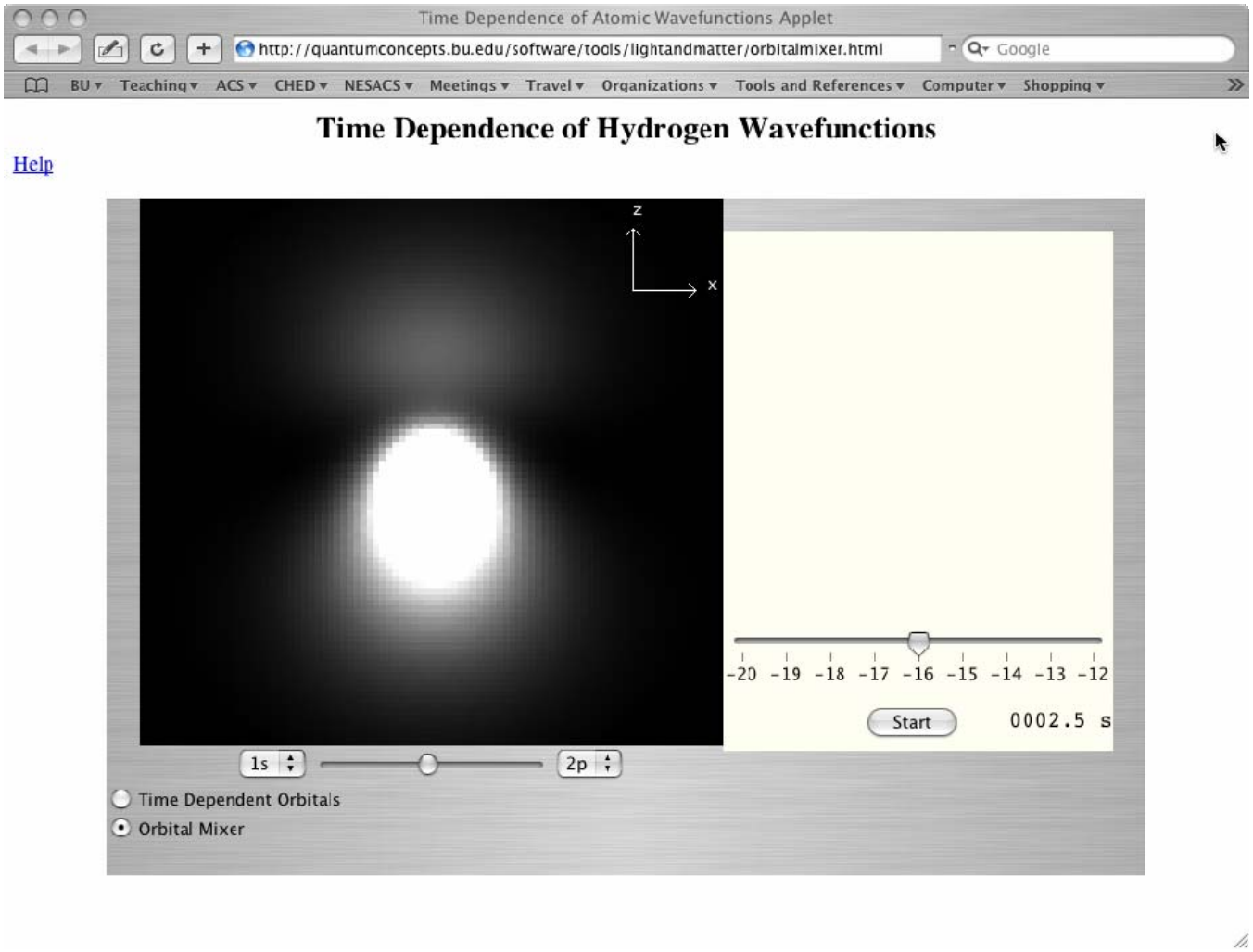

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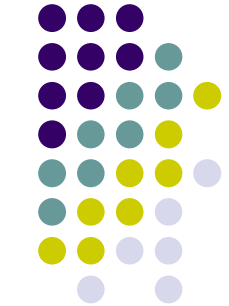
The Resolution: *Include Time!*

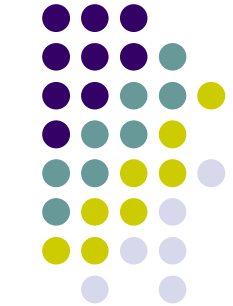
- Proper treatment of “time” in quantum systems is crucial.
- It provides the correct framework on which students can reason about quantum change.
- Without this framework, myths and misconceptions are the inevitable consequence.

Why Should Students in General Chemistry Learn This?



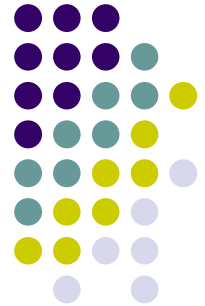
- Nature continually undergoes change.
- Chemistry is the science of the change.
- Time dependence in the quantum world is the analogue for all change in chemistry.
- Quantum time dependence is the basis for students to learn how and why things happen.

The Challenge



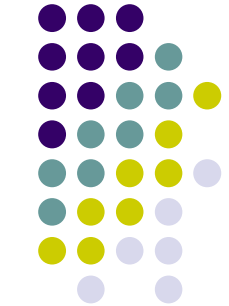
- Incoming students have a good understanding of the spatial description of waves (wavelength and amplitude).
- They have a poor understanding of the temporal description of waves (period and frequency).
- They have difficulty linking the spatial and temporal behavior of waves, and are weak in their understanding of the energetics of waves.

Our Approach



- Interactive guided-inquiry software that examines spectroscopy and the Planck relationship for electron orbital energies.
- Interactive graphics and renderings of time-dependent atomic orbitals.
- Activities that provide a visual means to understand the beats that correspond to dipole excitations of atoms, and a visual introduction to the selection rules for quantum absorption and emission.

Self-Study Computer Labs



Used in conjunction with lecture demonstrations and lecture/discussion periods.

- Lab 1: spectroscopy of atomic hydrogen and hydrogen-like ions.
- Lab 2: introduction to the normal modes of one- (cable) and two-dimensional (square and circular membranes) waves with analogy to the modes of a bound electron.
- Lab 3: time-dependent behavior of electron orbitals and their interaction with light.

Assessing the Efficacy of the Approach

- Post-test and student evaluations were used.
- The sophistication of the questions demonstrated our level of expectation to the students.
- The response from almost 600 students suggests that students can master the concepts that underlie the modern quantum model of chemistry.
- The students appreciated the interactive computer tools and graphics and felt the exercises help them understand quantum concepts.

Post-Test Comparisons With Chemistry Majors

- Subject matter in physical chemistry: Schrödinger equation, spherical harmonics, quantization of angular momentum, etc.
- Taught at the same time by the same instructor in CH101.
- No use of the interactive computer tools and graphics.

The general chemistry students did as well or somewhat better on many questions than did the physical chemistry students.

Conclusions-I

Our experience is that general chemistry students can understand quantum concepts through the use of guided-inquiry interactive graphics and visualizations, and can go on to other chemistry courses without persistent myths and misconceptions that block learning.

Conclusions-II

The vocabulary of time-dependent electron orbitals will provide new insights to the students about the absorption and emission of electromagnetic radiation across the spectrum, van der Waals interactions, and London dispersion forces.

Quantum change accounts for the stickiness of atoms and molecules.

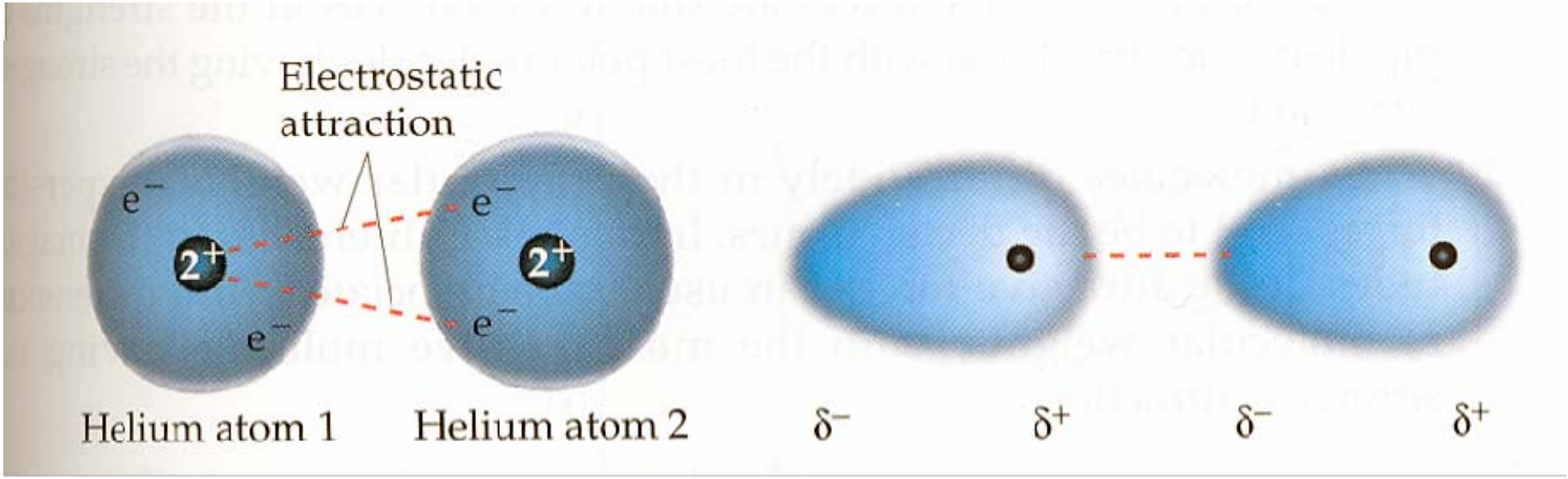


Figure 11.5, p. 397 in "Chemistry, The Central Science," Eighth Edition, by Theodore L. Brown, H. Eugene LeMay, Jr., and Bruce E. Burstein, Upper Saddle River, New Jersey: Prentice Hall, 2000. ISBN 0-13-010310-1

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