Welcome back to PHY 3305

Today's Lecture:

Hydrogen Atom Pt 1

Sad, quantum surfer,
Alone, forlorn on the beach,
His wave form collapsed.

ThinkGeek.com
via Ben Wise

ANNOUNCEMENTS

- Reading Assignment for Nov 6th: Krane 7.3 - 7.5.
- Problem set 11 is due Tuesday, Nov 7th at 12:30 pm.
- Regrade for problem set 10 is due Tuesday, Nov 7th at 12:30 pm.
- Second draft slides of presentation are due next week, Tuesday, Nov. 7th at 12:30 pm. Email your slides to Dr. Cooley (cooley@physics.smu.edu).
- Dr. Cooley will be out of town Nov. 5 - 9th. Mr. Thomas will conduct class in her place.
- Dr. Cooley's office hours are cancelled Nov. 6 and 7.
- Thursday, Nov. 16 @ 4pm will be the Nobel Prize discussion Panel. RSVP at http://www.smu.edu/Orgs/FacultyClub/Events

Assigned Presentation Dates

Black Paper Clip - Tuesday, Nov 21st
  Andrew, Gabriel, Connor

Purple Paper Clip - Tuesday, Nov 28th
  Rebecca, Chris, Luke

White Paper Clip - Thursday, Nov 30th
  Ali, Hope , Robert

Particles of energy E are incident from the left, where $U(x) = 0$, and at the origin encounter an abrupt drop in potential energy, whose depth is $-3E$.

a) From a classical perspective, describe the motion of the particles and what happens to their kinetic energy as they propagate?

The particles would continue to the right and the kinetic energy abruptly changes from E to 4E.

Particles of energy E are incident from the left, where U(x) = 0, and at the origin encounter an abrupt drop in potential energy, whose depth is –3E.

b) Now let's consider quantum mechanics. Assume the incident wave is of the form

$$\psi_{inc}(x) = 1e^{ikx}$$

Write the general form of the wave function in all regions.

$$\psi_{x<0}(0) = \psi_{inc}(x) + \psi_{ref}(x)$$
$$= 1e^{ikx} + Ae^{-ikx}$$

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\psi_{x>0}(x) = \psi_{trans}(x)$$
$$= Be^{ik'x}$$

$$k' = \sqrt{\frac{2m(E-U)}{\hbar^2}}$$

Particles of energy E are incident from the left, where U(x) = 0, and at the origin encounter an abrupt drop in potential energy, whose depth is –3E.

c) Solve for the constants A and B and write the wave functions for each region using all numeric values.

Apply Boundary Conditions:

$$\psi_{x<0}(0) = \psi_{x>0}(0)$$

$$1e^{ik0} + Ae^{-ik0} = Be^{ik'0}$$

$$\boxed{1 + A = B} \qquad \text{...(1)}$$

$$\frac{d\psi_{x<0}(0)}{dx} = \frac{d\psi_{x>0}(0)}{dx}$$

$$ike^{ik0} - Aike^{-ik0} = Bik'e^{ik'0}$$

$$\boxed{k(1-A) = k'B} \qquad \text{...(2)}$$

Substitute (1) into (2)

$$k(1-A) = k'(1+A)$$

$$k - kA = k' + k'A$$

$$(k+k')A = (k-k')$$

$$A = \frac{k-k'}{k+k'} \qquad \text{...(3)}$$

$$k' = \sqrt{\frac{2m(E-U)}{\hbar^2}} \qquad k = \sqrt{\frac{2mE}{\hbar^2}}$$

Now examine k'.

$$k' = \sqrt{\frac{2m(E+3E)}{\hbar^2}} = 2\sqrt{\frac{2mE}{\hbar^2}}$$

Substitute into (3).

$$A = \frac{\sqrt{2mE} - 2\sqrt{2mE}}{\sqrt{2mE} + 2\sqrt{2mE}} = \frac{1-2}{1+2} = \frac{1}{3} \qquad \text{...(4)}$$

Substitute into (4) into (1).

$$B = 1 - \frac{1}{3} = \frac{2}{3} \quad \rightarrow$$

$$\psi_{x<0} = 1e^{ikx} - \frac{1}{3}e^{-ikx}$$
$$\psi_{x>0} = \frac{2}{3}e^{ik'x}$$

Particles of energy E are incident from the left, where U(x) = 0, and at the origin encounter an abrupt drop in potential energy, whose depth is -3E.

c) What is the probability the incident particles would be reflected?

$$R = \frac{A^* A}{1 \times 1}$$

$$R = \frac{1}{9}$$

SWE Summary

- Bound States (chapter 5)
  - Particle in a box infinite walls, Particle in a box finite walls, harmonic oscillator
  - Energy was quantized.
- Unbound States (chapter 6)
  - potential steps, barriers and tunneling
  - Energy is NOT quantized.

Video Lecture:

Angular Momentum in Quantum Mechanics

The angular momentum properties of a 3-D wave function are described by two quantum numbers.

Angular Momentum Quantum Number: ℓ

determines the length of the angular momentum vector

$$|\vec{L}| = \sqrt{\ell(\ell+1)}\hbar \qquad (\ell = 0, 1, 2, ...)$$

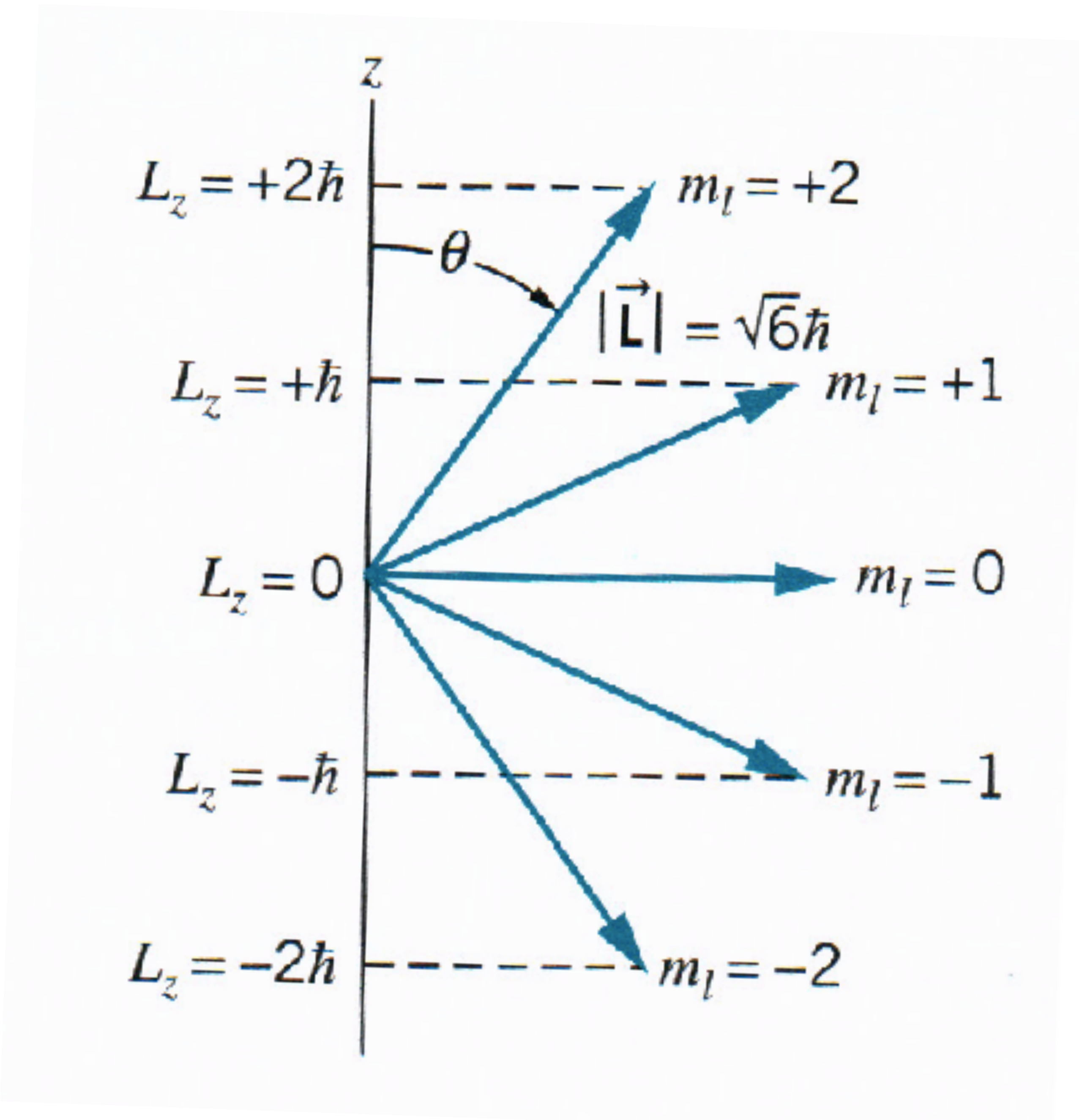
Magnetic Quantum Number: m

$$L_z = m_\ell \hbar \qquad (m_\ell = 0, \pm 1, \pm 2, ... \pm \ell)$$

Note: for each value of ℓ, there are $2\ell + 1$ possible values of m_ℓ

Video Lecture:

Examine angular momentum for case $\ell = 2$



The angle between L and the polar axis is given by

$$\cos\theta = \frac{L_z}{|\vec{L}|} = \frac{m_l}{\sqrt{l(l+1)}}$$

This demonstrates an aspect of quantum mechanics known as **spatial quantization**. Only certain orientations of angular momentum vectors are allowed.

An electron is in an angular momentum state with $\ell = 3$.

a) What is the length of the electron's angular momentum vector?

$$|\vec{L}| = \sqrt{\ell(\ell+1)}\hbar$$

$$= \sqrt{3(3+1)}\hbar$$

$$|\vec{L}| = 2\sqrt{3}\hbar$$

An electron is in an angular momentum state with $\ell = 3$.

b) How many different possible z-components can the angular momentum vector have? List all possible z-components.

The angular momentum vector can have 7 values.

$$m_\ell = 0, \pm 1, \pm 2, \pm 3$$

An electron is in an angular momentum state with $\ell = 3$.

c) What are the values of the angle that the **L** vector makes with the z-axis?

$$\cos\theta = \frac{L_z}{|\vec{\mathbf{L}}|} = \frac{m_l}{\sqrt{l(l+1)}} = \frac{m_\ell}{2\sqrt{3}}$$

$$m_l = +3 \qquad \theta = \cos^{-1} 3/\sqrt{12} = 30°$$

$$m_l = +2 \qquad \theta = \cos^{-1} 2/\sqrt{12} = 55°$$

$$m_l = +1 \qquad \theta = \cos^{-1} 1/\sqrt{12} = 73°$$

$$m_l = 0 \qquad \theta = \cos^{-1} 0 = 90°$$

$$m_l = -1 \qquad \theta = \cos^{-1}(-1/\sqrt{12}) = 107°$$

$$m_l = -2 \qquad \theta = \cos^{-1}(-2/\sqrt{12}) = 125°$$

$$m_l = -3 \qquad \theta = \cos^{-1}(-3/\sqrt{12}) = 150°$$

Video Lecture:

3D Schroedinger equation in spherical coordinates.

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial r^2}+\frac{2}{r}\frac{\partial\psi}{\partial r}+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}\right]$$
$$+U(r)\psi(r,\theta,\phi)=E\psi(r,\theta,\phi)$$

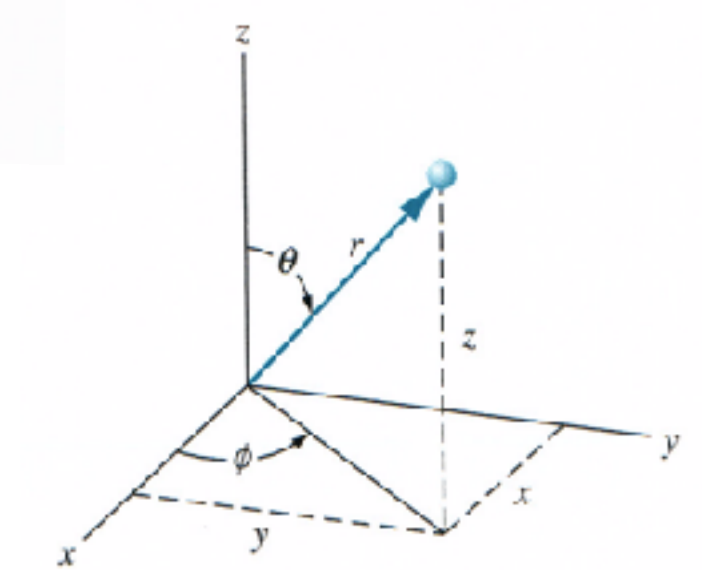
Since we can define the Coulomb potential in terms of only r, the solution is separable.

$$\psi(r,\theta,\phi)=R(r)\Theta(\theta)\Phi(\phi)$$

R(r) = radial function

$\Theta(\theta)$ = polar function

$\Phi(\varphi)$ = azimuthal function



Video Lecture:

If you were to solve this equation, three quantum numbers emerge from the solution.

n	principle quantum number	1, 2, 3 ...
ℓ	angular momentum quantum number	0, 1, 2, ... (n-1)
m_ℓ	magnetic quantum number	0, ±1, ±2,...±(n-1)

The principle quantum number determines the quantized energy levels.

$$E = -\frac{me^4}{2(4\pi\epsilon_0)^2\hbar^2}\frac{1}{n^2}$$

Video Lecture:

The solutions of the 3D SWE, complete quantum numbers, can be written as

$$\psi_{n,\ell,m_\ell}(r,\theta,\phi) = R_{n,m_\ell}(r)\Theta_{\ell,m_\ell}(\theta)\Phi_{m_\ell}(\phi)$$

n	l	m_l	$R(r)$	$\Theta(\theta)$	$\Phi(\phi)$
1	0	0	$\frac{2}{a_0^{3/2}}e^{-r/a_0}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2\pi}}$
2	0	0	$\frac{1}{(2a_0)^{3/2}}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2\pi}}$
2	1	0	$\frac{1}{\sqrt{3}(2a_0)^{3/2}}\frac{r}{a_0}e^{-r/2a_0}$	$\sqrt{\frac{3}{2}}\cos\theta$	$\frac{1}{\sqrt{2\pi}}$
2	1	±1	$\frac{1}{\sqrt{3}(2a_0)^{3/2}}\frac{r}{a_0}e^{-r/2a_0}$	$\mp\frac{\sqrt{3}}{2}\sin\theta$	$\frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$
3	0	0	$\frac{2}{(3a_0)^{3/2}}\left(1-\frac{2r}{3a_0}+\frac{2r^2}{27a_0^2}\right)e^{-r/3a_0}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2\pi}}$
3	1	0	$\frac{8}{9\sqrt{2}(3a_0)^{3/2}}\left(\frac{r}{a_0}-\frac{r^2}{6a_0^2}\right)e^{-r/3a_0}$	$\sqrt{\frac{3}{2}}\cos\theta$	$\frac{1}{\sqrt{2\pi}}$
3	1	±1	$\frac{8}{9\sqrt{2}(3a_0)^{3/2}}\left(\frac{r}{a_0}-\frac{r^2}{6a_0^2}\right)e^{-r/3a_0}$	$\mp\frac{\sqrt{3}}{2}\sin\theta$	$\frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$
3	2	0	$\frac{4}{27\sqrt{10}(3a_0)^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}$	$\sqrt{\frac{5}{8}}(3\cos^2\theta-1)$	$\frac{1}{\sqrt{2\pi}}$
3	2	±1	$\frac{4}{27\sqrt{10}(3a_0)^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}$	$\mp\sqrt{\frac{15}{4}}\sin\theta\cos\theta$	$\frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$
3	2	±2	$\frac{4}{27\sqrt{10}(3a_0)^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}$	$\frac{\sqrt{15}}{4}\sin^2\theta$	$\frac{1}{\sqrt{2\pi}}e^{\pm 2i\phi}$

Ground state ($n=1$; $\ell = 0$; $m_\ell = 0$)

($n=2$; $\ell = 0, 1$; $m_\ell = 0, \pm1$)

($n=3$; $\ell = 0, 1, 2$; $m_\ell = 0, \pm1, \pm2$)

Group 1:

Show by direct substitution that the n = 2, ℓ = 0, m_ℓ = 0 wave functions are solutions to the 3D Schrodinger equation corresponding to the energy of the first excited state.

Group 2:

Show by direct substitution that the n = 2, ℓ = 1, m_ℓ = 0 wave functions are solutions to the 3D Schrodinger equation corresponding to the energy of the first excited state.

n	ℓ	m_ℓ	$R(r)$	$\Theta(\theta)$	$\Phi(\phi)$
1	0	0	$\frac{2}{a_0^{3/2}} e^{-r/a_0}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2\pi}}$
2	0	0	$\frac{1}{(2a_0)^{3/2}}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2\pi}}$
2	1	0	$\frac{1}{\sqrt{3}(2a_0)^{3/2}}\frac{r}{a_0}e^{-r/2a_0}$	$\sqrt{\frac{3}{2}}\cos\theta$	$\frac{1}{\sqrt{2\pi}}$
2	1	±1	$\frac{1}{\sqrt{3}(2a_0)^{3/2}}\frac{r}{a_0}e^{-r/2a_0}$	$\mp\frac{\sqrt{3}}{2}\sin\theta$	$\frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$
3	0	0	$\frac{2}{(3a_0)^{3/2}}\left(1-\frac{2r}{3a_0}+\frac{2r^2}{27a_0^2}\right)e^{-r/3a_0}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2\pi}}$
3	1	0	$\frac{8}{9\sqrt{2}(3a_0)^{3/2}}\left(\frac{r}{a_0}-\frac{r^2}{6a_0^2}\right)e^{-r/3a_0}$	$\sqrt{\frac{3}{2}}\cos\theta$	$\frac{1}{\sqrt{2\pi}}$
3	1	±1	$\frac{8}{9\sqrt{2}(3a_0)^{3/2}}\left(\frac{r}{a_0}-\frac{r^2}{6a_0^2}\right)e^{-r/3a_0}$	$\mp\frac{\sqrt{3}}{2}\sin\theta$	$\frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$
3	2	0	$\frac{4}{27\sqrt{10}(3a_0)^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}$	$\sqrt{\frac{5}{8}}(3\cos^2\theta-1)$	$\frac{1}{\sqrt{2\pi}}$
3	2	±1	$\frac{4}{27\sqrt{10}(3a_0)^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}$	$\mp\sqrt{\frac{15}{4}}\sin\theta\cos\theta$	$\frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$
3	2	±2	$\frac{4}{27\sqrt{10}(3a_0)^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}$	$\frac{\sqrt{15}}{4}\sin^2\theta$	$\frac{1}{\sqrt{2\pi}}e^{\pm 2i\phi}$

Group 1:

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial r^2}+\frac{2}{r}\frac{\partial\psi}{\partial r}+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}\right]$$
$$+U(r)\psi(r,\theta,\phi)=E\psi(r,\theta,\phi)$$

$$\psi_{2,0,0}(r,\theta,\phi)=\frac{1}{\sqrt{4\pi}}\frac{1}{\sqrt{8a_0^3}}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0}$$

Step 1: Calculate derivatives.

$$\frac{\partial\psi}{\partial\theta}=0 \text{ and } \frac{\partial\psi}{\partial\phi}=0$$

$$\frac{\partial\psi}{\partial r}=\frac{1}{\sqrt{32\pi a_0^3}}\left[-\frac{1}{a_0}e^{-r/2a_0}-\frac{1}{2a_0}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0}\right]=\frac{1}{\sqrt{32\pi a_0^3}}\left(-\frac{2}{a_0}+\frac{r}{2a_0^2}\right)e^{-r/2a_0}$$

$$\frac{\partial^2\psi}{\partial r^2}=\frac{1}{\sqrt{32\pi a_0^3}}\left[\frac{1}{2a_0^2}e^{-r/2a_0}+\frac{1}{2a_0^2}e^{-r/2a_0}+\frac{1}{4a_0^2}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0}\right]$$

$$=\frac{1}{\sqrt{32\pi a_0^3}}\left(\frac{3}{2a_0^2}-\frac{r}{4a_0^3}\right)e^{-r/2a_0}$$

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial r^2}+\frac{2}{r}\frac{\partial\psi}{\partial r}+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}\right]$$
$$+U(r)\psi(r,\theta,\phi)=E\psi(r,\theta,\phi)$$

Step 2: Substitute LHS

U(r)

$$-\frac{\hbar^2}{2m}\left[\frac{1}{\sqrt{32\pi a_0^3}}\left(\frac{3}{2a_0^2}-\frac{r}{4a_0^3}\right)e^{-r/2a_0}+\frac{2}{r}\frac{1}{\sqrt{32\pi a_0^3}}\left(-\frac{2}{a_0}+\frac{r}{2a_0^2}\right)e^{-r/2a_0}\right]-\frac{e^2}{4\pi\varepsilon_0 r}\frac{1}{\sqrt{32\pi a_0^3}}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0}$$

$$=\frac{1}{\sqrt{32\pi a_0^3}}e^{-r/2a_0}\left[-\frac{\hbar^2}{2m}\left(\frac{3}{2a_0^2}-\frac{r}{4a_0^3}-\frac{4}{ra_0}+\frac{1}{a_0^2}\right)-\frac{e^2}{2\pi\varepsilon_0 r}+\frac{e^2}{4\pi\varepsilon_0 a_0}\right]$$

$$=\frac{1}{\sqrt{32\pi a_0^3}}e^{-r/2a_0}\frac{e^2}{4\pi\varepsilon_0}\left(-\frac{5}{4a_0}+\frac{r}{8a_0^2}+\frac{2}{r}-\frac{2}{r}+\frac{1}{a_0}\right)$$

$$=\frac{1}{\sqrt{32\pi a_0^3}}e^{-r/2a_0}\frac{e^2}{4\pi\varepsilon_0}\left(-\frac{1}{4a_0}+\frac{r}{8a_0^2}\right)=\frac{e^2}{4\pi\varepsilon_0}\left(-\frac{1}{8a_0}\right)\psi_{2,0,0}(r,\theta,\phi)$$

$$=E\psi_{2,0,0}(r,\theta,\phi)$$

Step 3: Calculate E

$$E = \frac{e^2}{4\pi\varepsilon_0}\left(-\frac{1}{8a_0}\right)$$

$$= \frac{e^2}{4\pi\varepsilon_0}\left(-\frac{me^2}{32\pi\varepsilon_0\hbar^2}\right)$$

$$E = \frac{1}{4}\left(-\frac{me^4}{32\pi^2\varepsilon_0^2\hbar^2}\right)$$

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial r^2}+\frac{2}{r}\frac{\partial\psi}{\partial r}+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}\right]$$
$$+U(r)\psi(r,\theta,\phi)=E\psi(r,\theta,\phi)$$

Group 2:

$$\psi_{2,1,0}(r,\theta,\phi)=\frac{1}{\sqrt{32\pi a_0^5}}re^{-r/2a_0}\cos\theta$$

Step 1: Calculate derivatives.

$$\frac{\partial\psi}{\partial\phi}=0$$

$$\frac{\partial\psi}{\partial r}=\frac{1}{\sqrt{32\pi a_0^5}}\left(e^{-r/2a_0}-\frac{r}{2a_0}e^{-r/2a_0}\right)\cos\theta$$

$$\frac{\partial^2\psi}{\partial r^2}=\frac{1}{\sqrt{32\pi a_0^5}}\left(-\frac{1}{2a_0}e^{-r/2a_0}-\frac{1}{2a_0}e^{-r/2a_0}+\frac{r}{4a_0^2}e^{-r/2a_0}\right)\cos\theta$$

$$\frac{\partial\psi}{\partial\theta}=\frac{1}{\sqrt{32\pi a_0^5}}re^{-r/2a_0}(-\sin\theta)$$

$$\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)=-\frac{1}{\sqrt{32\pi a_0^5}}re^{-r/2a_0}(2\sin\theta\cos\theta)$$

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial r^2}+\frac{2}{r}\frac{\partial\psi}{\partial r}+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}\right]$$
$$+U(r)\psi(r,\theta,\phi)=E\psi(r,\theta,\phi)$$

Step 2: Substitute LHS

$$\frac{\cos\theta}{\sqrt{32\pi a_0^5}}e^{-r/2a_0}\left(-\frac{\hbar^2}{2m}\left[-\frac{1}{a_0}+\frac{r}{4a_0^2}+\frac{2}{r}\left(1-\frac{r}{2a_0}\right)-\frac{2}{r}\right]-\frac{e^2}{4\pi\varepsilon_0}\right)$$

$$=\frac{e^2}{4\pi\varepsilon_0}\psi_{2,1,0}(r,\theta,\phi)\left(\frac{1}{2r}-\frac{1}{8a_0}+\frac{1}{2r}-\frac{1}{r}\right)$$

$$=\frac{e^2}{4\pi\varepsilon_0}\left(-\frac{1}{8a_0}\right)\psi_{2,1,0}(r,\theta,\phi)=E_2\psi_{2,1,0}(r,\theta,\phi)$$

Recall we calculated: $E=\frac{e^2}{4\pi\varepsilon_0}\left(-\frac{1}{8a_0}\right)$

Thus, both solutions correspond to the first excited state!

The end (for today)