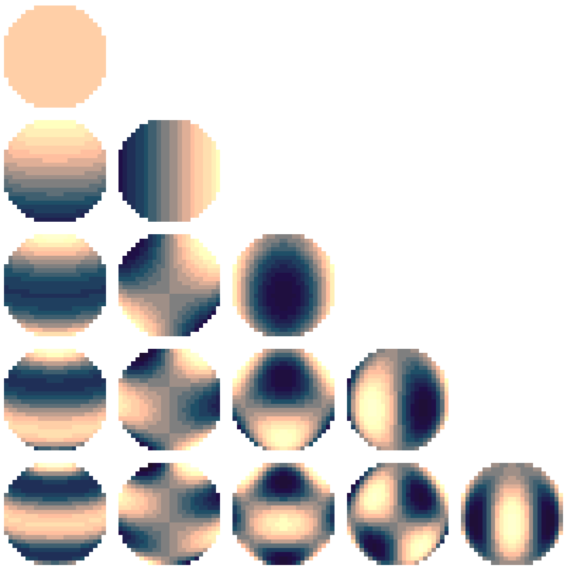
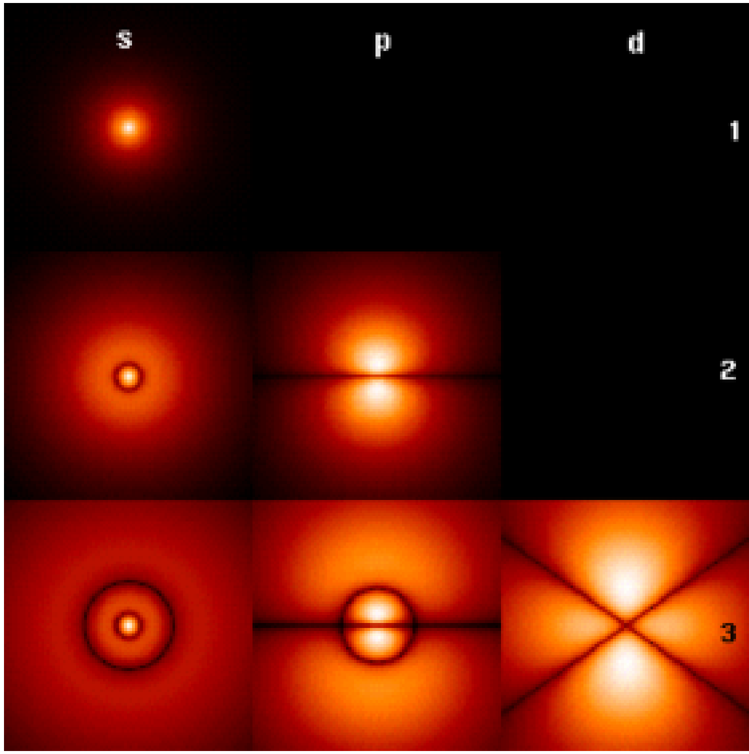
Hydrogen atom

- Next weeks homework should be available by 5pm today and is due next week, 4/22.
- The last homework set will be out on 4/22 and will be due on 4/30 (one day later than normal). It is a normal assignment, **not** an extra credit assignment.





Rest of semester

- **Investigate hydrogen atom (Wednesday 4/15 and Friday 4/17)**
- Learn about intrinsic angular momentum (spin) of particles like electrons (Monday 4/20)
- Take a peak at multielectron atoms including the Pauli Exclusion Principle (Wednesday 4/22)
- Describe some of the fundamentals of quantum mechanics (expectation values, eigenstates, superpositions of states, measurements, wave function collapse, etc.) (Friday 4/24 and Monday 4/27)
- Review of semester (Wednesday 4/29 and Friday 5/1)
- Final exam: Saturday 5/2 from 1:30pm-4:00pm in G125 (this room)

**Please answer this question on your own.
No discussion until after.**

Q. The potential seen by the electron in a hydrogen atom is…

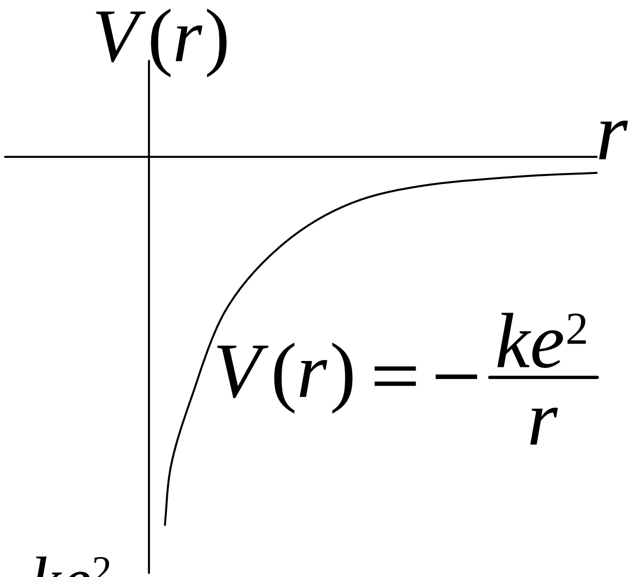
A. Independent of distance

B. Spherically symmetric

C. An example of a central force potential

D. Constant

E. More than one of the above



The potential seen by the electron is $V(r) = -\frac{ke^2}{r}$

Spherically symmetric (doesn't depend on direction). It depends only on distance from proton so it is a central force potential.

3-D central force problems

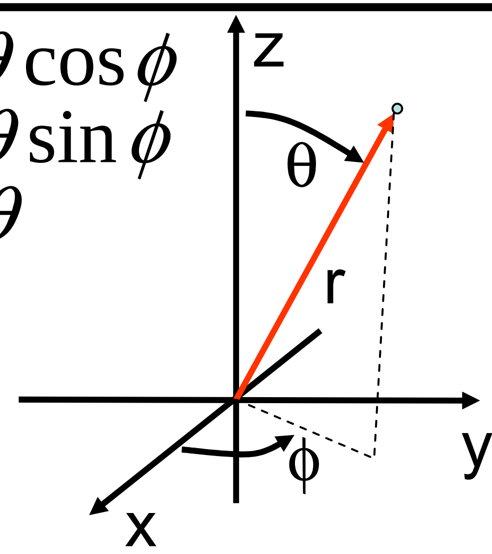
The hydrogen atom is an example of a 3D central force problem.

The potential energy depends only on the distance from a point (spherically symmetric)

Spherical coordinates is the natural coordinate system for this problem.

General potential: $V(r,\theta,\phi)$
Central force potential: $V(r)$

$$x = r\sin\theta\cos\phi$$
$$y = r\sin\theta\sin\phi$$
$$z = r\cos\theta$$



Engineering & math types sometimes swap θ and φ.

The Time Independent Schrödinger Equation (TISE) becomes:

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

We can use separation of variables so $\psi(r,\theta,\phi)=R(r)\Theta(\theta)\Phi(\phi)$

The $\Phi(\phi)$ part

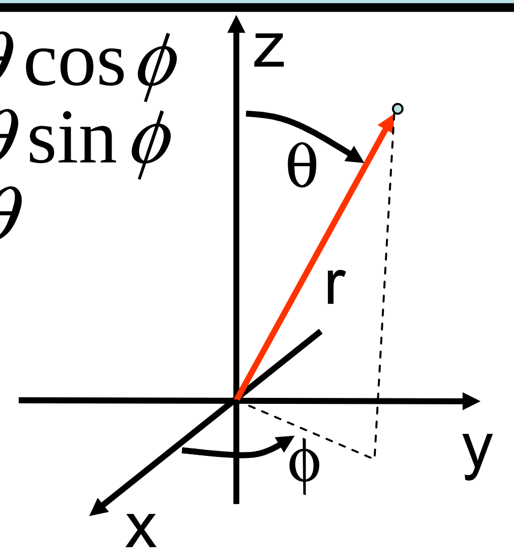
The variable ϕ only appears in the TISE as $\frac{\partial^2 \psi}{\partial \phi^2} \propto -E\psi$

So we should not be surprised that the solution is $\Phi(\phi) = e^{im\phi}$

Note that *m* is a separation variable and not the electron mass.

We use m_e for the electron mass.

$$x = r\sin\theta\cos\phi$$
$$y = r\sin\theta\sin\phi$$
$$z = r\cos\theta$$



Are there any constraints on *m*?

What can we say about $\Phi(\phi)$ and $\Phi(\phi + 2\pi)$?

<u>They have to be the same!</u> $\Phi(\phi) = \Phi(\phi + 2\pi)$

$$\Phi(\phi) = e^{im\phi} = \cos m\phi + i\sin m\phi$$

Since cosine and sine have periods of 2π, as long as *m* is an integer (positive, negative, or 0) the constraint is satisfied.

Angular momentum quantization about *z*-axis

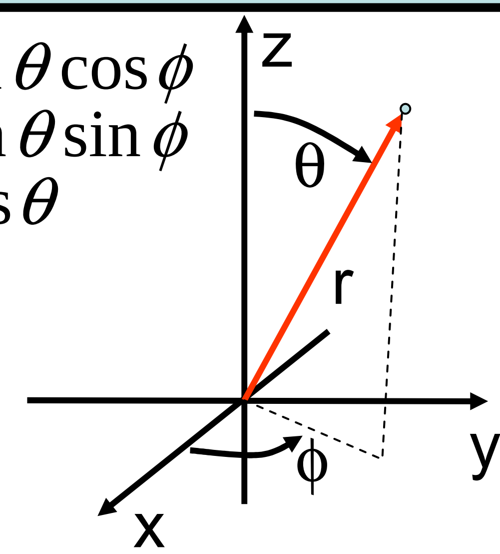
Note $\Phi(\phi) = e^{im\phi}$ is similar to e^{ikx} which is the solution to the free particle with $p = \hbar k$

As *k* gives the momentum in the *x* direction, *m* gives the momentum in the ϕ direction (angular momentum).

$x = r\sin\theta\cos\phi$

$y = r\sin\theta\sin\phi$

$z = r\cos\theta$



Angular momentum about the *z*-axis is quantized: $L_z = m\hbar$

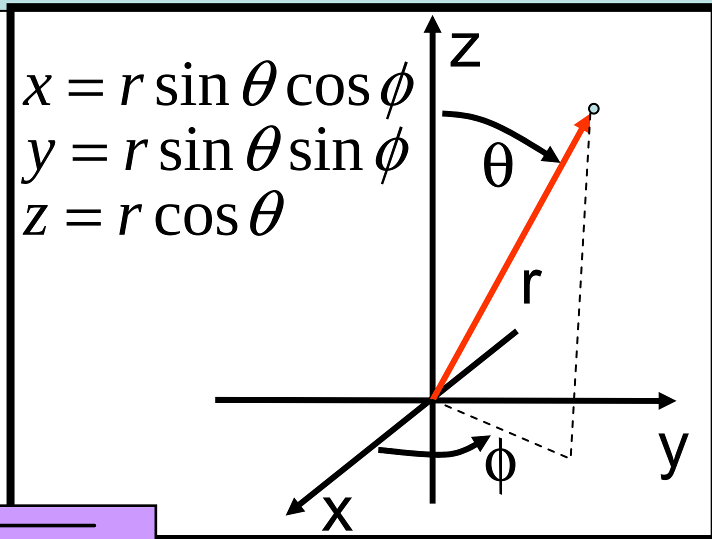
There is nothing truly special about the z-axis.

We can point the z-axis anywhere we want to.

It is just the nature of the coordinate system that treats the z-axis differently than the x and y axes.

The Θ(θ) part

The solution to the Θ(θ) part is more complicated so we skip it.



The end result is that there is another quantum variable ℓ which must be a non-negative integer and ℓ ≥ |m|.

The ℓ variable quantizes the total angular momentum:

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

Note, for large ℓ, $L \approx \ell\hbar$ so ℓ is basically the total angular momentum and *m* is the z-component of the angular momentum.

Since the z-component cannot be larger than the total, |m| ≤ ℓ.

Clicker question 1 — Set frequency to DA

Total angular momentum is $L = \sqrt{\ell(\ell+1)}\hbar$ ℓ can be 0, 1, 2, 3, …

The z-component of the angular momentum is $L_z = m\hbar$

where *m* can be 0, ±1, ±2, … ±ℓ

Just like with any vector, the total angular momentum can be written $L = \sqrt{L_x^2 + L_y^2 + L_z^2}$

Q. Given the rules above, can $L_x = L_y = 0$? That is, can $L = L_z$?

A. Yes, in more than one case
B. Yes, but only in one case
C. Never

It is possible for $L_x = L_y = L_z = 0$ in which case $L = 0$ so $\ell = 0$ and $m = 0$

In general, if $L_x = L_y = 0$ then $L = \sqrt{L_x^2 + L_y^2 + L_z^2}$ simplifies to $L = L_z$

which means $m\hbar = \sqrt{\ell(\ell+1)}\hbar$ or $m^2 = \ell(\ell+1)$. But

$\ell^2 < \ell(\ell+1) < (\ell+1)^2$ and there is no integer between ℓ and ℓ+1

so $m^2 \neq \ell(\ell+1)$ (except for m=ℓ=0)

Spherical harmonics

We have determined the angular part of the wave function so

$\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$ has become $\psi(r,\theta,\phi) = R(r)\Theta_{\ell m}(\theta)e^{im\phi}$

with the quantum numbers ℓ and *m* specifying the total angular momentum and the z-component of angular momentum.

This angular solution works for **any** central force problem.

The combination $\Theta_{\ell m}(\theta)e^{im\phi}$ are the spherical harmonics $Y_\ell^m(\theta,\phi)$

Spherical harmonics are 3-D and complex (real and imaginary terms), making it very difficult to display.

A few of the spherical harmonics

Real part only

Red = +1

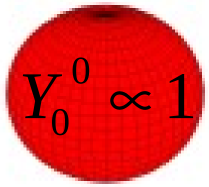
Cyan = -1

Colors give phase

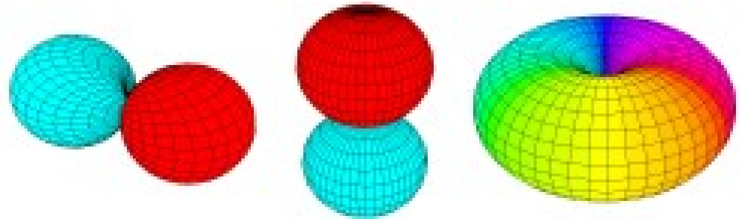
Purple = +*i*

Green = -*i*

$\ell = 0$



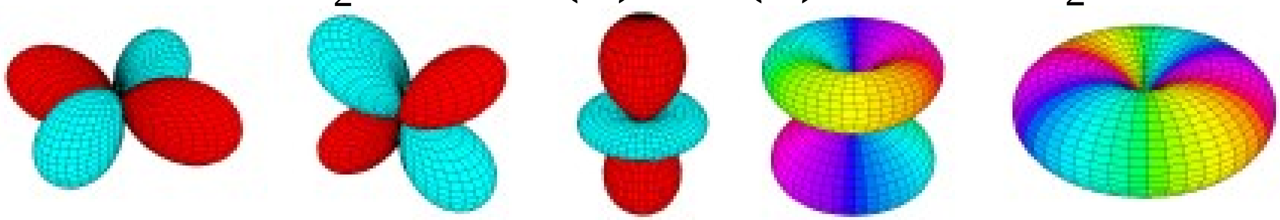
$\ell = 1$ $\quad Y_1^0 \propto \cos(\theta)$



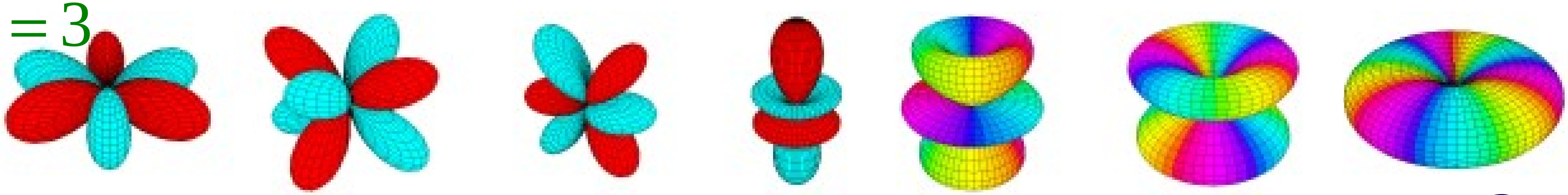
$Y_1^{\pm 1} \propto \sin(\theta) e^{\pm i\phi}$

$Y_2^0 \propto 3\cos^2(\theta) - 1$ $\quad Y_2^{\pm 1} \propto \sin(\theta)\cos(\theta) e^{\pm i\phi}$ $\quad Y_2^{\pm 2} \propto \sin^2(\theta) e^{\pm 2i\phi}$

$\ell = 2$



$\ell = 3$



$m = 3$ $\quad m = 2$ $\quad m = 1$ $\quad m = 0$ $\quad m = 1$ $\quad m = 2$ $\quad m = 3$

http://www.colorado.edu/physics/

http://oak.ucc.nau.edu/jws8/dpgraph/Yellm.html

Clicker question 2

Set frequency to DA

For any central force potential we can write the wave function as

$$\psi(r,\theta,\phi) = R(r)\Theta_{\ell m}(\theta)e^{im\phi}$$
$$\psi(r,\theta,\phi) = R(r)Y_{\ell m}(\theta,\phi)$$

Q. What are the boundary conditions on the radial part R(r)?

A. R(r) must go to zero as r goes to 0

B. R(r) must go to zero as r goes to infinity

C. R(∞) must equal R(0)

D. R(r) must equal R(r+2π).

E. More than one of the above.

In order for ψ(r,θ,φ) to be normalizable, it must go to zero as r goes to infinity. Therefore, $R(r) \rightarrow 0$ as $r \rightarrow \infty$.

Physically makes sense as well. Probability of finding the electron very far away from the proton is very small.