The 3D Schrodinger Eqn.
and Spherical Harmonics

$$\frac{-\hbar\nabla^2}{2m}\Psi + V(r)\Psi = E\Psi$$

Schrodinger Eqn

↑	↑	↑
Kinetic energy	Potential energy	Total energy

$$\frac{-\hbar\nabla^2}{2m}\Psi + V(r)\Psi = E\Psi$$

Schrodinger Eqn

$$\Psi = R(r)Y(\theta, \phi)$$

separation ansatz

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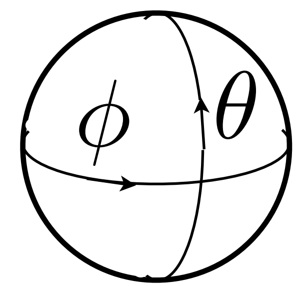
Schrodinger Eqn

$$\Psi = R(r)Y(\theta, \phi)$$

separation ansatz

$$\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{\partial^2 Y}{\partial\phi^2} = -l(l+1)\sin^2\theta\, Y$$

angular equation



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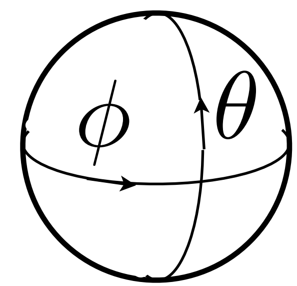

spherical harmonics

$$Y_l^m = \epsilon\sqrt{\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!}}\; e^{im\phi}\; P_l^m(\cos\theta)$$

Condon-Shortley phase

$$\epsilon = (-1)^m \qquad m \geq 0$$
$$\epsilon = 1 \quad m < 0$$

orthonormal

$$\left\langle Y_l^m | Y_{l'}^{m'} \right\rangle = \delta_{ll'}\delta_{mm'}$$

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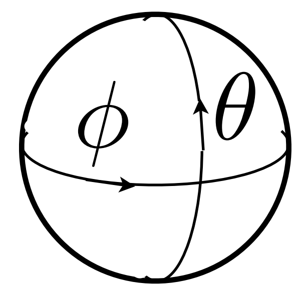
The spherical harmonics are easily visualized by counting the number of zero crossings Re[Y] possess in both the latitudinal (theta) and longitudinal directions (phi).



$\phi -$ longitudinal

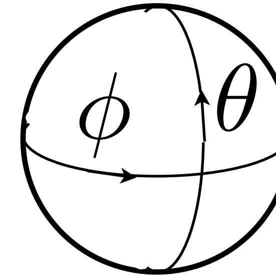
$\theta -$ latitudinal

$$Y_0^0(\theta,\phi) = \frac{1}{2}\sqrt{\frac{1}{\pi}}$$

$l = 0, m = 0$

spherically symmetric

$$Y_l^m(\theta,\phi)$$

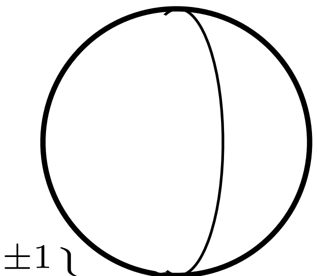


$$Y_1^{-1}(\theta,\phi) = \frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta\; e^{-i\phi}$$

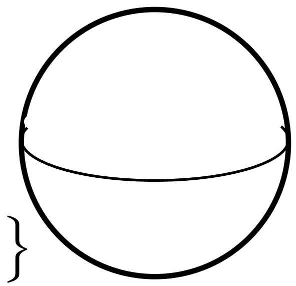
$$Y_1^{0}(\theta,\phi) = \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta$$

$$Y_1^{1}(\theta,\phi) = \frac{-1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta\; e^{i\phi}$$

$l = 1, m = 0, \pm 1$



$\mathbf{Re}\left\{Y_1^{\pm 1}\right\}$



$\mathbf{Re}\left\{Y_1^{0}\right\}$

$$Y_2^{-2}(\theta,\phi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\; e^{-2i\phi}$$

$$Y_2^{-1}(\theta,\phi) = \frac{1}{2}\sqrt{\frac{15}{2\pi}}\sin\theta\cos\theta\; e^{-i\phi}$$

$$Y_2^{0}(\theta,\phi) = \frac{1}{4}\sqrt{\frac{5}{\pi}}(3\cos^2\theta - 1)$$

$$Y_2^{1}(\theta,\phi) = \frac{-1}{2}\sqrt{\frac{15}{2\pi}}\sin\theta\cos\theta\; e^{i\phi}$$

$$Y_2^{2}(\theta,\phi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\; e^{2i\phi}$$

$l = 2, m = 0, \pm 1, \pm 2$

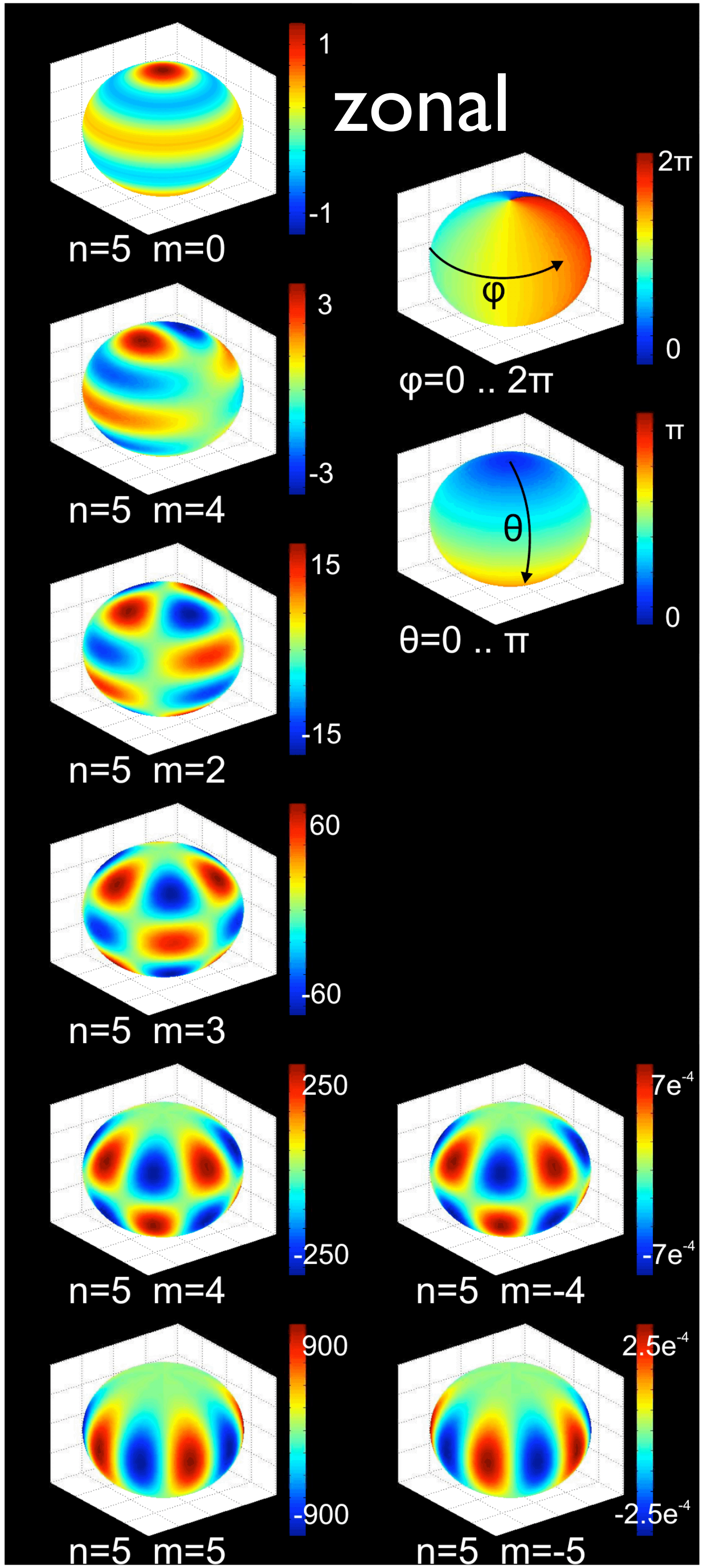
The spherical harmonics are easily visualized by counting the number of zero crossings they possess in both the latitudinal (theta) and longitudinal directions (phi).

They possess (l-|m|) zeros along the theta direction, and 2|m| zeros along the phi direction.

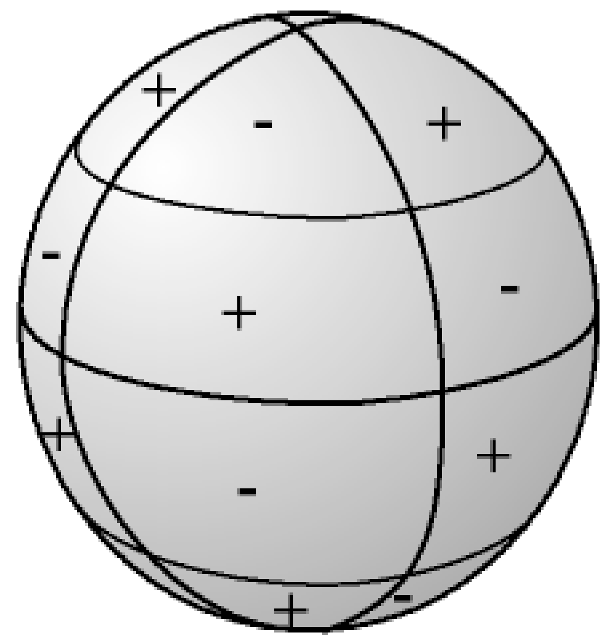
This means Y is equal to 0 along m great circles passing through the poles, and along l-m circles of equal latitude.

Figures from the Wikimedia Commons.

$Y_l^m(\theta, \phi)$ is equal to 0 along m great circles passing through the poles, and along l-m circles of equal latitude.



$l = 5$
$m = 2$
$l\text{-}m = 3$



sectoral

ϕ — longitudinal

θ — latitudinal

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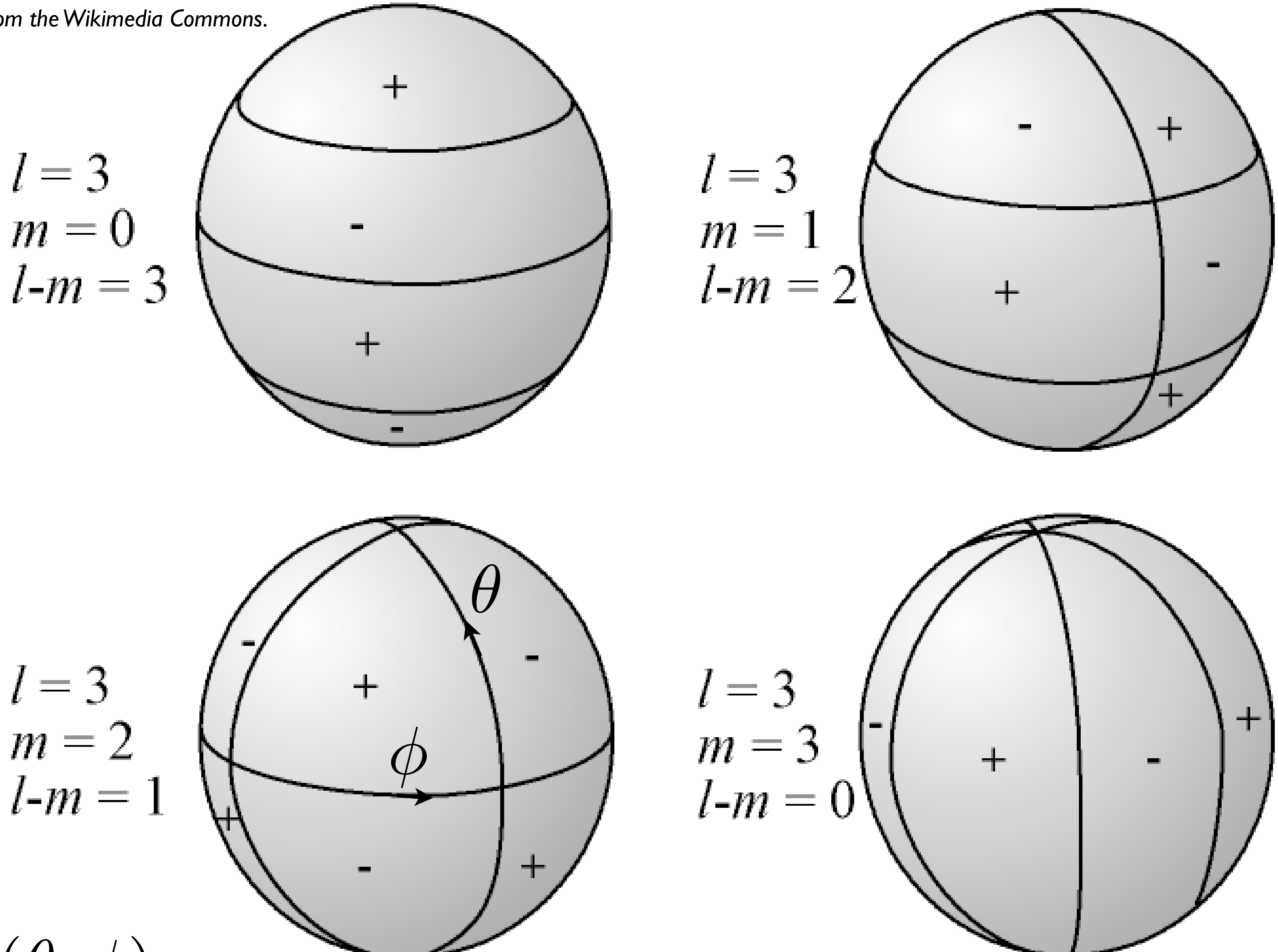

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$$Y_l^m(\theta, \phi)$$

is equal to 0 along m great circles passing through the poles, and along l-m circles of equal latitude. The function changes sign each time it crosses one of these lines

Hydrogen atom: electron wave function

$$\Psi_{n,l,m} = A\left(\frac{2r}{na}\right)e^{-r/na}\left[L_{n-l-1}^{2l+1}(2r/na)\right]Y_l^m(\theta,\phi)$$

degree of polynomial

$n-l-1$ radial zeros

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degree of polynomial

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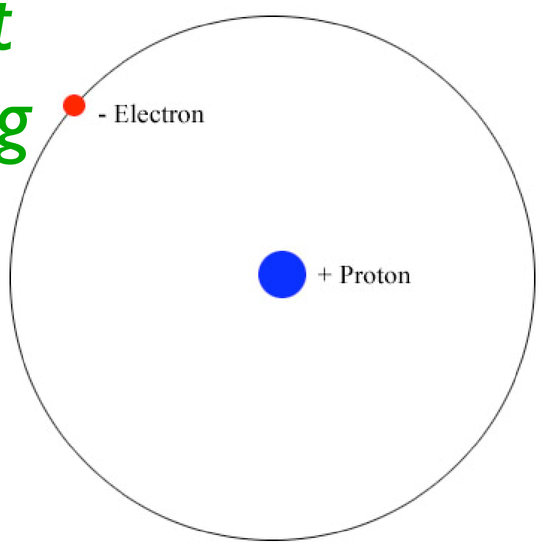
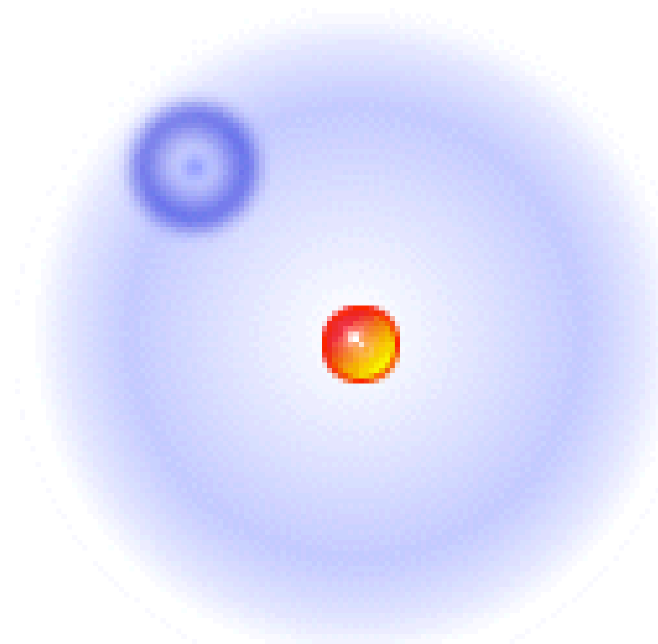
quantum wave function

planet orbiting sun



classical picture



probability distribution

quantum picture

Hydrogen atom: electron wave function

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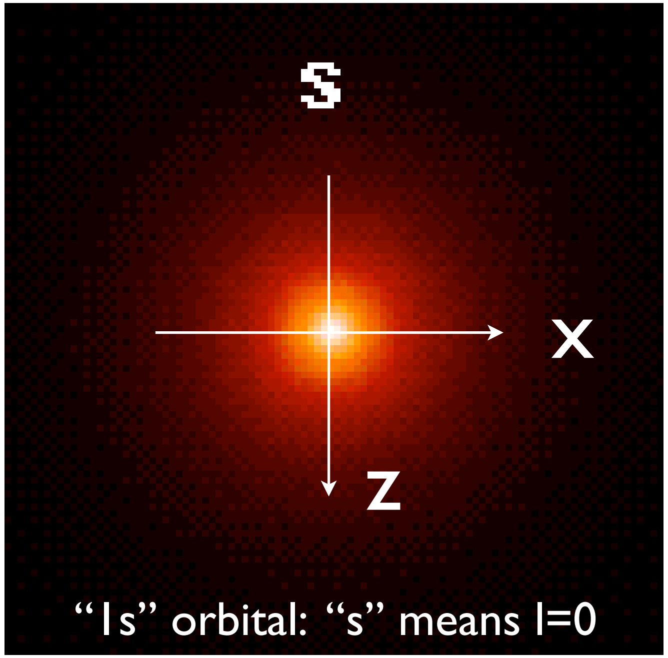
$$\Psi_{n,l,m} = A\left(\frac{2r}{na}\right) e^{-r/na}\left[L^{2l+1}_{n-l-1}(2r/na)\right] Y_l^m(\theta,\phi)$$

degree of polynomial

$n-l-1$ radial zeros

Ground state: $n=1,\ l=0,\ m=0$

$$\Psi_{100} = \frac{1}{\sqrt{\pi a^3}}\, e^{-r/a}$$



cross-section of the probability density
black = zero density, white = highest density

Hydrogen atom: electron wave function

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degree of polynomial

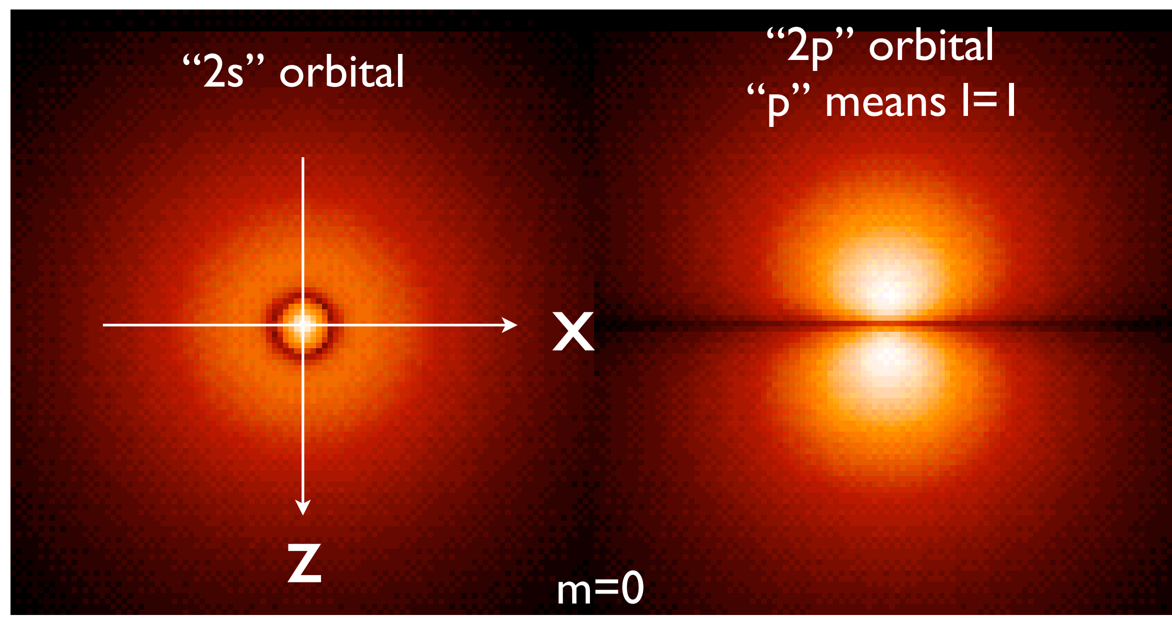
$n-l-1$ radial zeros

First excited state:

$n=2,\ l=0,\ m=0$

$n=2,\ l=1,\ m=\{-1,0,+1\}$

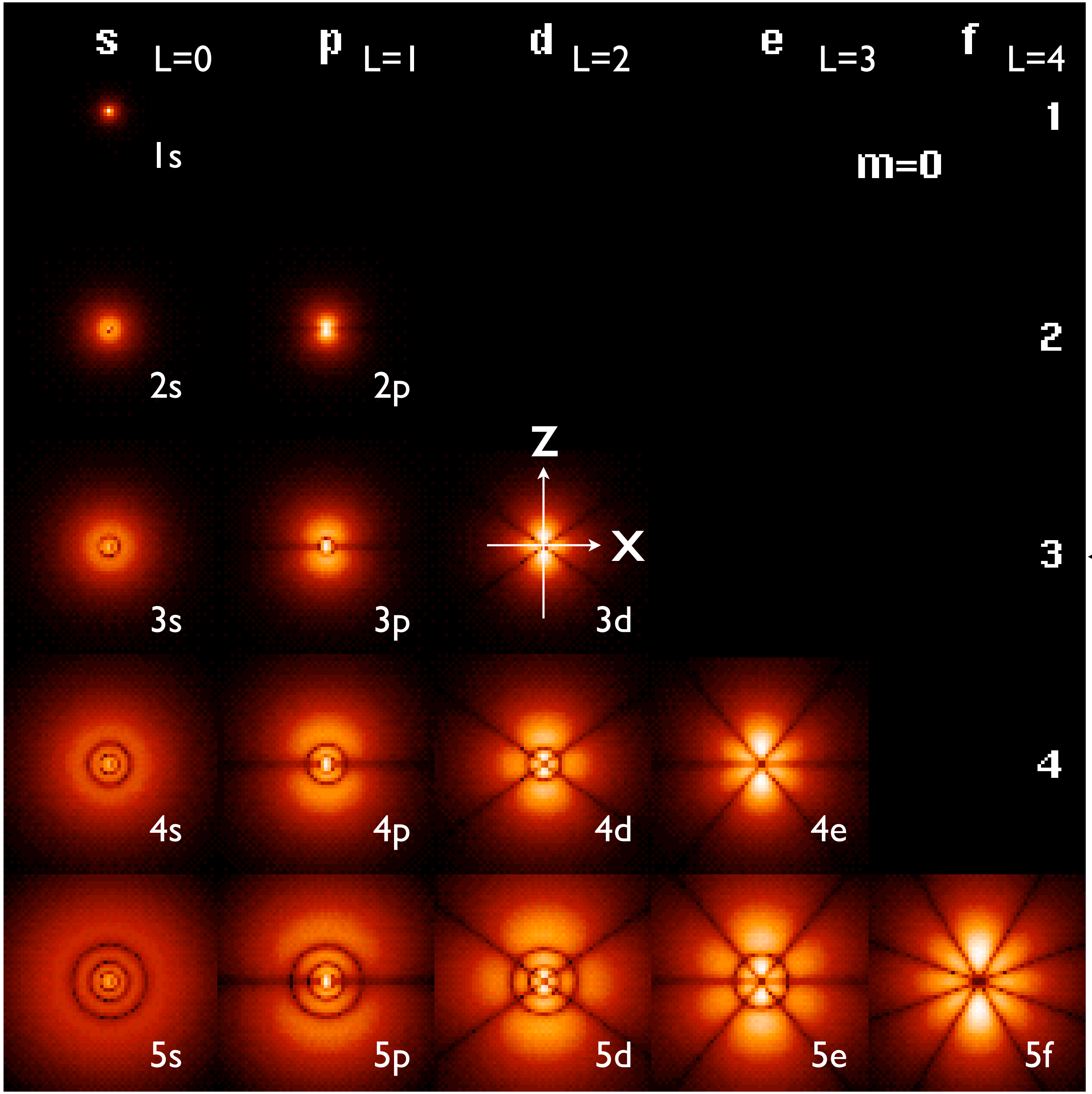
4 states



one radial node *no radial nodes*

The probability density in three-dimensional space is obtained by rotating the one shown here around the z-axis

Hydrogen atom: electron wave function



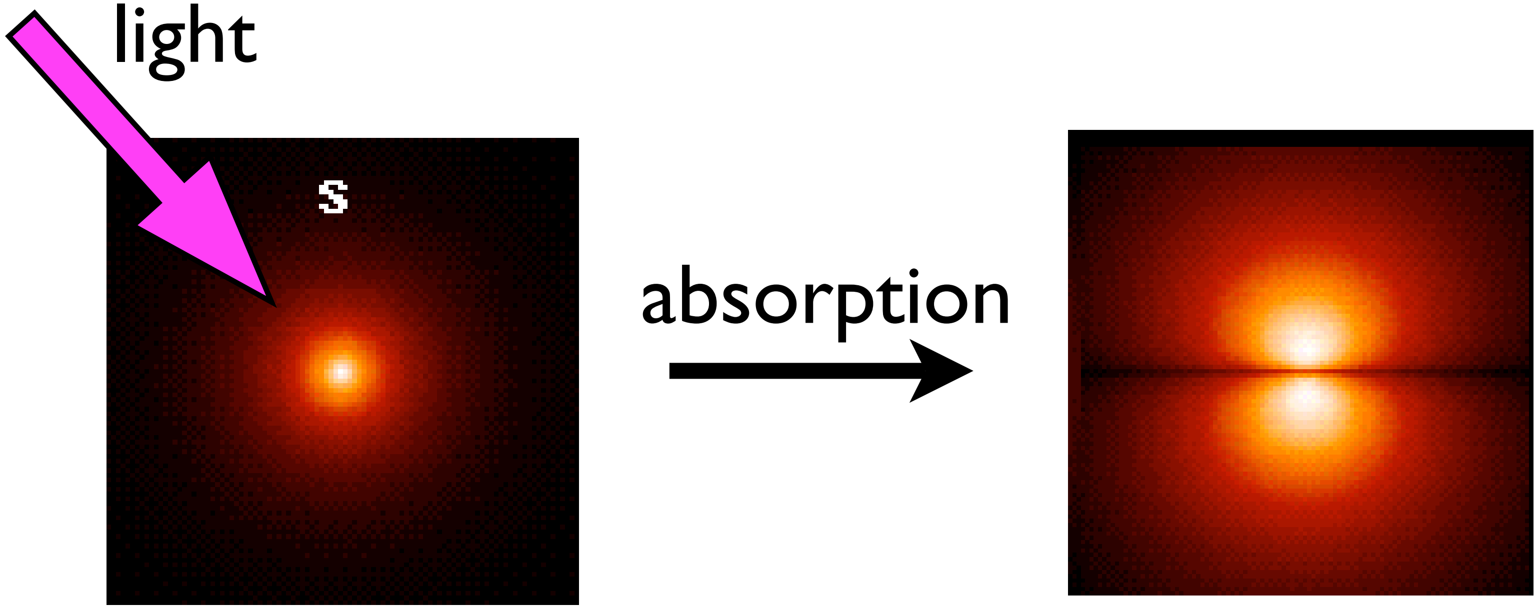
principal quantum number

n

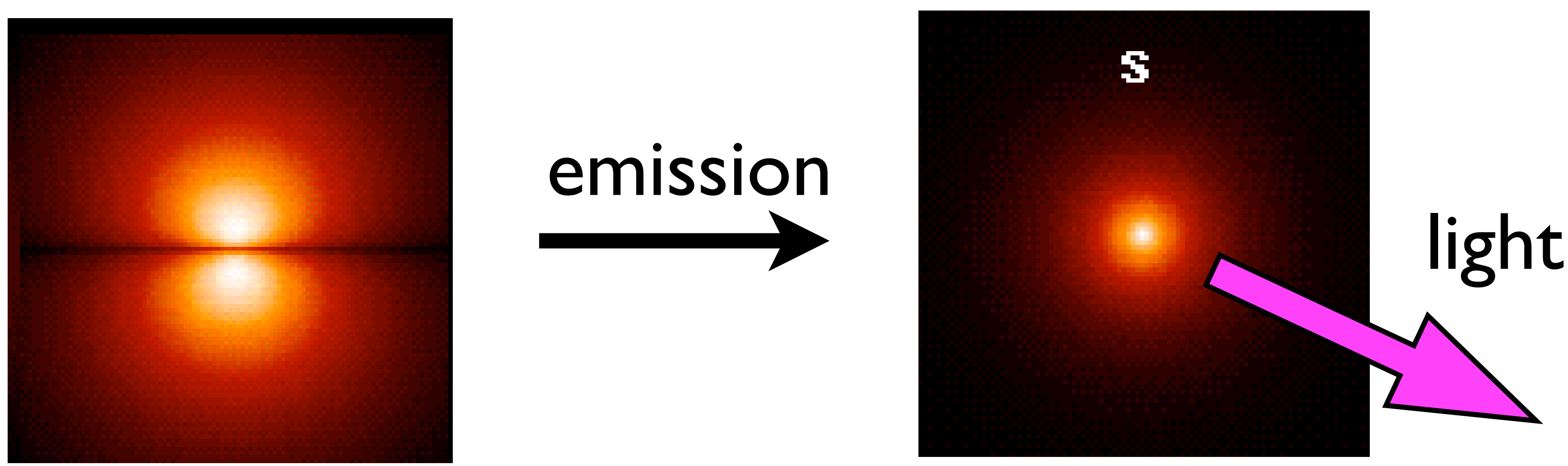
The probability density in three-dimensional space is obtained by rotating the one shown here around the z-axis

Quantum jumps: quantum state change

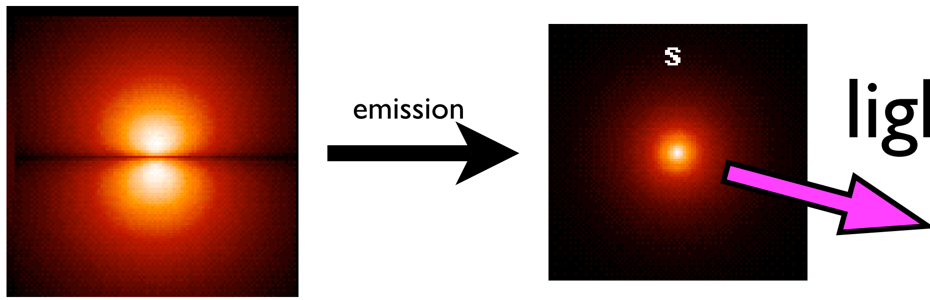
Quantum jumps: excitation by absorption of light



Quantum jumps: dexcitation by emission of light



Quantum jumps: dexcitation by emission



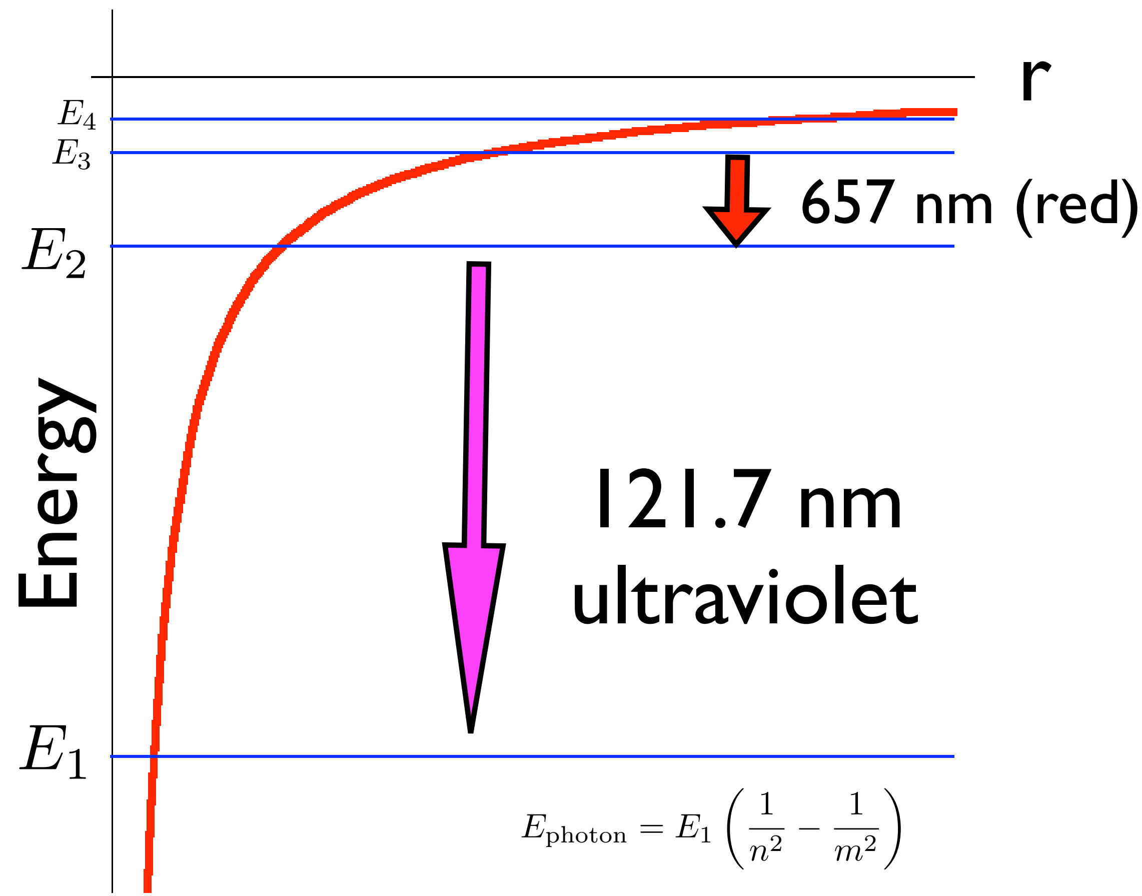
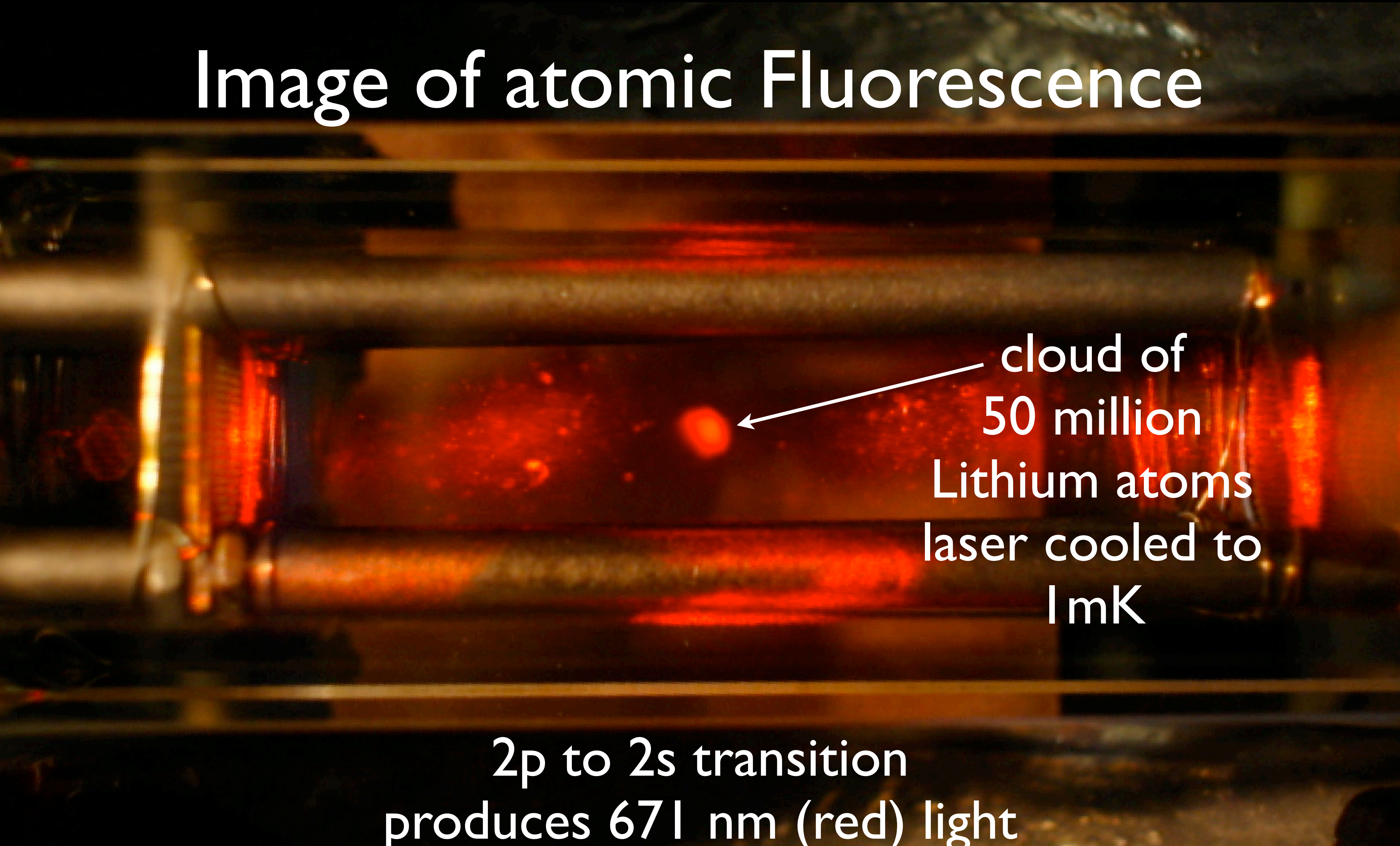


Image of atomic Fluorescence



2p to 2s transition
produces 671 nm (red) light