The form of the spherical harmonics

Including normalization the spherical harmonics are

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}$$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_1^{\pm 1} = \sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi}$$

$$Y_2^0 = \sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta - 1\right)$$

$$Y_2^{\pm 1} = \sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{\pm i\phi}$$

$$Y_2^2 = \sqrt{\frac{15}{32\pi}}\sin^2\theta e^{\pm 2i\phi}$$

The form commonly used to represent p and d orbitals are linear combinations of these functions

Solutions to the 3-D rotational hamiltonian

- There are two quantum numbers

  ℓ is the total angular momentum quantum number

  m is the z-component of the angular momentum

- The spherical harmonics called $Y_{\ell m}$ are functions whose probability $|Y_{\ell m}|^2$ has the well known shape of the s, p and d orbitals etc.

  $\ell = 0$ is s , $m = 0$

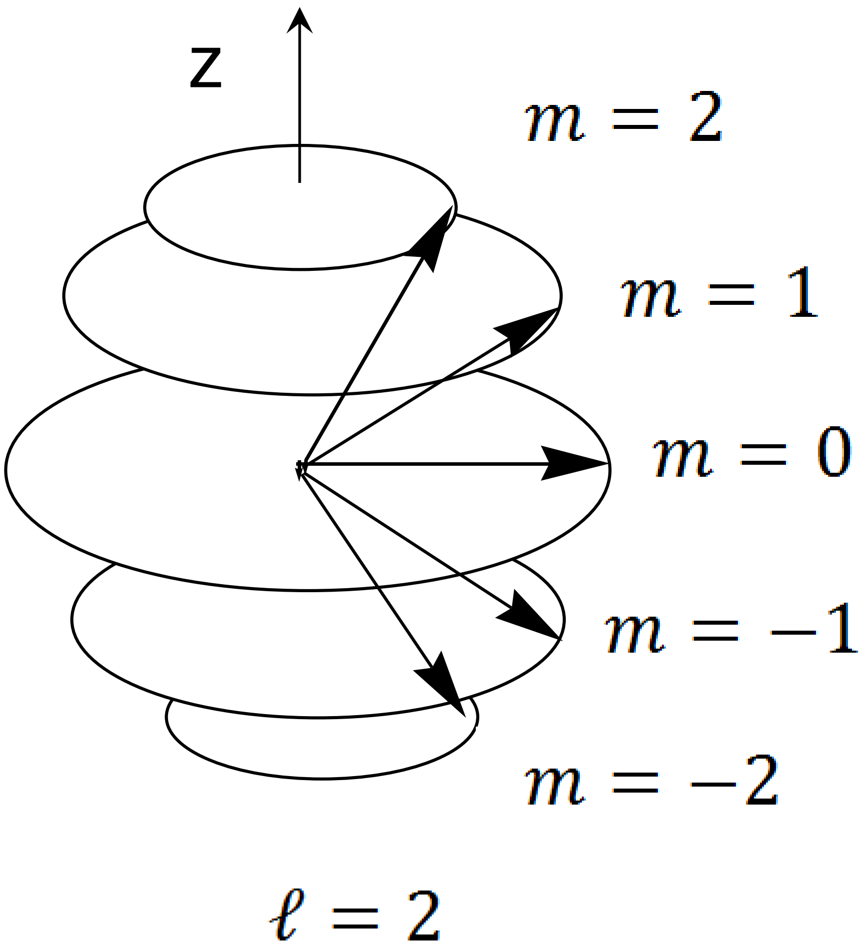
  $\ell = 1$ is p , $m = -1, 0, 1$

  $\ell = 2$ is d , $m = -2, -1, 0, 1, 2$

  $\ell = 3$ is f , $m = -3, -2, -1, 0, 1, 2, 3$

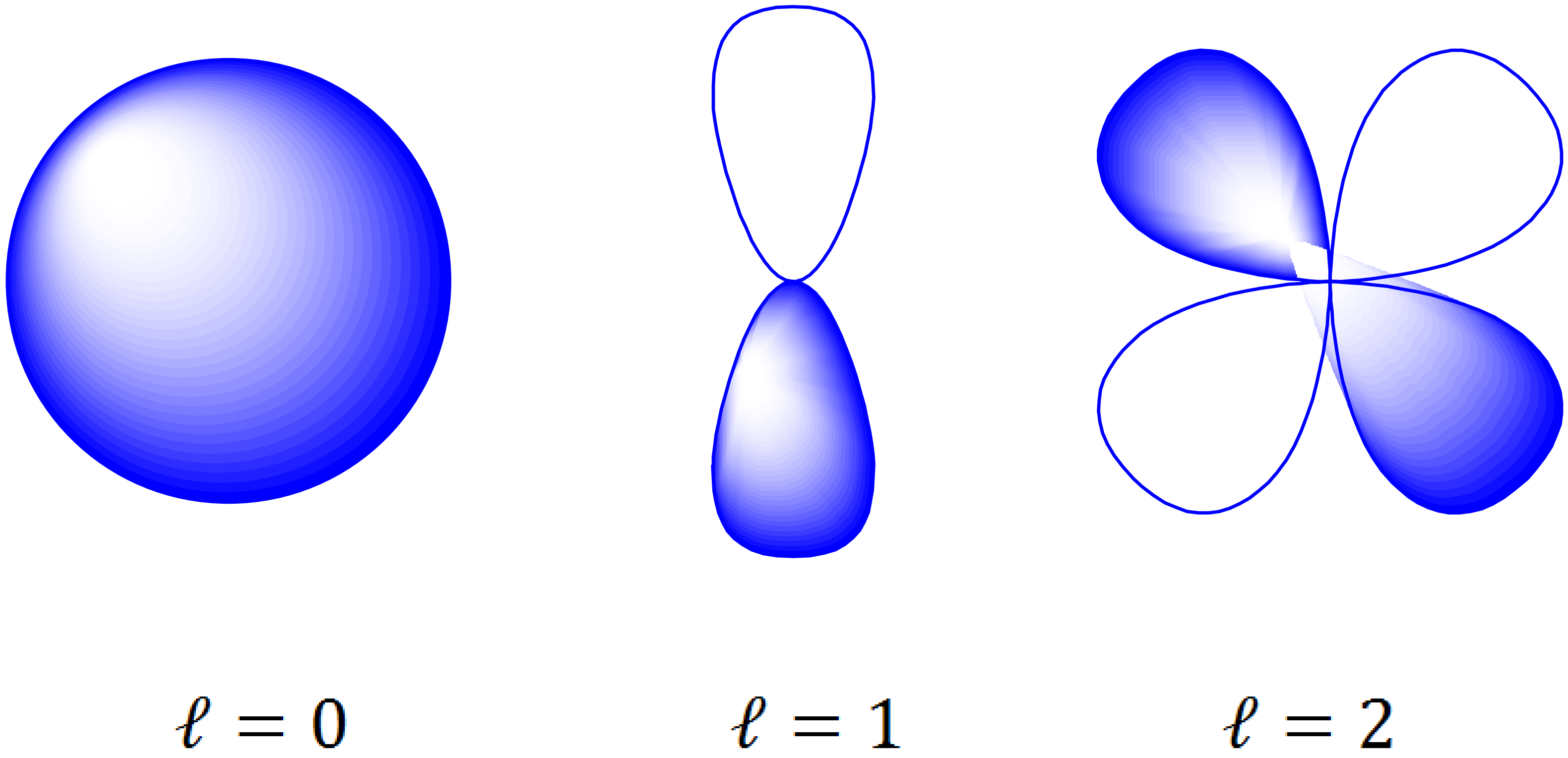
  etc.

Space quantization in 3D



- Specification of the azimuthal quantum number m_z implies that the angular momentum about the z-axis is $J_z = \hbar m$.
- This implies a fixed orientation between the total angular momentum and the z component.
- The x and y components cannot be known due to the Uncertainty principle.

Standing waves on a sphere



These are the spherical harmonics Y_{lm}, which are solutions of the angular Schrodinger equation.

Orthogonality of wavefunctions

- Ignoring normalization we have:
- s 1
- p $\cos\theta$, $\sin\theta\cos\phi$, $\sin\theta\sin\phi$
- d $1/2(3\cos^2\theta - 1)$, $\cos^2\theta\cos 2\phi$, $\cos^2\theta\sin 2\phi$, $\cos\theta\sin\theta\cos\phi$, $\cos\theta\sin\theta\sin\phi$

- The differential angular element is $\sin\theta d\theta d\phi/4\pi$
- The limits $\theta = 0$ to π and $\phi = 0$ to 2π.
- The angular wavefunctions are orthogonal.

Orthogonality of wavefunctions

- For the theta integrals we can use the substitution
- x = cosθ and dx = -sinθdθ
- For example, for s and p-type rotational wave functions we have

$$< s \mid p > \propto \int_0^{\pi} \cos\theta \sin\theta \, d\theta = \int_1^{-1} x \, dx = \left. \frac{x^2}{2} \right|_{-1}^{-1} = \frac{1}{2} - \frac{1}{2} = 0$$