m_l: is called the magnetic quantum number and can take the values:

$$m_l = 0, \pm 1, \pm 2, \ldots, \pm l$$

m_l number is associated with the space quantization of orbital angular momentum.

Y_{lm_l} can be further factorized to give:

$$Y_{lm_l}(\theta, \phi) = \Theta_{lm_l}(\theta)\, \Phi_{m_l}(\phi)$$

Φ is the angular distribution about the z-axis for the wave function.

$$\Phi_{m_l}(\phi) = \frac{1}{\sqrt{2\pi}}\, e^{im_l\phi}$$

Since Φ_{m_l} must have the same values for

$$\phi = 0, 2\pi, 4\pi, 6\pi, \ldots$$

Then, m_l must be equal to $0, \pm 1, \pm 2, \ldots$

Θ_{lm_l} functions are known as associated Legendre polynomials, and they , and therefore the Y_{lm_l}, are independent of effective nuclear charge Z

Thus the wavefunction ψ can be given by:

$$\psi(r, \theta, \phi) = R_{nl}(r)\, \frac{1}{\sqrt{2\pi}}\, e^{im_l\phi}\, \Theta_{lm_l}$$

The radial wave function R_{nl} depnends on the nuclear charge, unlike the spherical harmonic waeve function.

Also, the quantity a_0, which is Bohr radius, is involved, where

$$a_0 = \frac{\hbar^2 4\pi\varepsilon_0}{m_e e^2} = 0.529\ \text{Å}$$

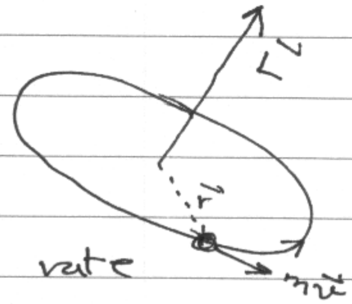
which is the radius of the hydrogen orbital with $n=1$.

The radial wave function R_{nl}, the radial probability distribution function R^2_{nl}, and the radial charge density function $4\pi r^2 R^2_{nl}$ aginst $\rho = \frac{Z}{a_0} r$ can be plotted.

The spherical harmonics wave function, Y_{lm_l}, can be sketched diagrammatically, after conveting them to real functions, to get the orbital shapes.

Quantization of Angular Momentum

Angular momentum $(\vec{L})$ is used to describe the rotational motion of a particle about a fixed center.



$\vec{L}$ is a vector: its magnitud gives the rate at which a particle circulates, and its direction indicates the axis of ratation.

The classical angular momentum is given by:

$$\vec{L} = \vec{r} \times \vec{p}$$

$\vec{r}$: vector representing the particle's position with respect to the fixed center.

$\vec{p}$: linear momentum; $m\vec{v}$

The energy of the particle in terms of classical mechanics is associated to the kinetic energy $E = \frac{1}{2}mv^2$

Thus, for an angular momentum quantity around the Z-axis (L_z) which lies perpendicular to the xy plane,

$$L_z = \pm pr$$

and $$E = L_z^2/2mr^2$$

In QM, not all values of L is permitted and, therefore, both angular momentum and rotational energy are quantized.

QM operators of linear momentum are given by

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x} \quad , \hat{p}_y = -i\hbar \frac{\partial}{\partial y} , \quad \hat{p}_z = -i\hbar \frac{\partial}{\partial z}$$

$$\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)$$

$$\hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) = i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)$$

$$\hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\hbar\frac{\partial}{\partial\phi}$$

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

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

It turned out from the solution of the Schrödinger equation that the rotational energy of a particle is restricted to the values:

$$E_{rot} = L(L+1)\hbar^2/2I \qquad L = 0, 1, 2, \ldots$$

I : moment of inertia for the particle $I = mr^2$

The magnitude of the angular momentum is given by:

$$L = \sqrt{l(l+1)}\,\hbar \quad ; \quad L^2 = l(l+1)\hbar^2$$

l : Azimuthal (or orbital) quantum number

$l = 0, 1, 2, \ldots, n-1$

Thus, the angular momentum quantum number determines the magnitude of the orbital angular momentum.

The z-component of the angular momentum is given by:

$$L_z = m_\ell \hbar$$ (This is called space quantization)

m_ℓ can take $2\ell+1$ possible values which are:

$$m_\ell = \ell, \ell-1, \ell-2, \dots, 0, \dots, -(\ell-2), -(\ell-1), -\ell$$

m_ℓ is known as magnetic quantum number.

From QM results, L_x and L_y values can't be defined, which means that the positions of the ends of the vector can be located anywhere within a circle about the z-axis. This is called "Precession".