11) Angular momentum of atomic systems

$$\vec{\nabla}^2\Phi(r,\vartheta,\varphi) = \frac{1}{r}\frac{\partial^2}{\partial r^2}(r\,\Phi) + \frac{1}{r^2\sin\vartheta}\frac{\partial}{\partial\vartheta}(\sin\vartheta\frac{\partial}{\partial\vartheta}\Phi) + \frac{1}{\sin^2\vartheta\, r^2}\frac{\partial^2}{\partial\varphi^2}\Phi$$

$$\vec{L} = \vec{x}\times\vec{p}\,, \quad \vec{L}^2 = (\vec{x}\times\vec{p})\cdot(\vec{x}\times\vec{p}) = \vec{x}^2\vec{p}^2 - (\vec{x}\cdot\vec{p})^2$$

$$E_{kin} = \frac{\vec{p}^2}{2m} = \frac{1}{2m}\left(p_r^2 + \frac{\vec{L}^2}{r^2}\right)$$

$$\frac{\hat{\vec{p}}^2}{2m}\Psi = -\frac{\hbar^2}{2m}\vec{\nabla}^2\Psi = \frac{1}{2m}\left\{-\hbar^2\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\,\Psi) - \hbar^2\frac{\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}(\sin\vartheta\frac{\partial}{\partial\vartheta}\Psi) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\Psi}{r^2}\right\}$$

$$\hat{\vec{L}}^2\Psi = -\hbar^2\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}(\sin\vartheta\frac{\partial}{\partial\vartheta}\Psi) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\Psi\right]$$

$$[\hat{\vec{L}}^2, \hat{L}_z]\Psi = i\hbar^3\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\sin\vartheta\frac{\partial}{\partial\vartheta} + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}, \frac{\partial}{\partial\varphi}\right]\Psi = 0$$

And by rotating the coordinate system, x, y and z can be interchanged leaving also

$$[\hat{\vec{L}}^2, \hat{L}_x] = 0\,, \quad [\hat{\vec{L}}^2, \hat{L}_y] = 0$$

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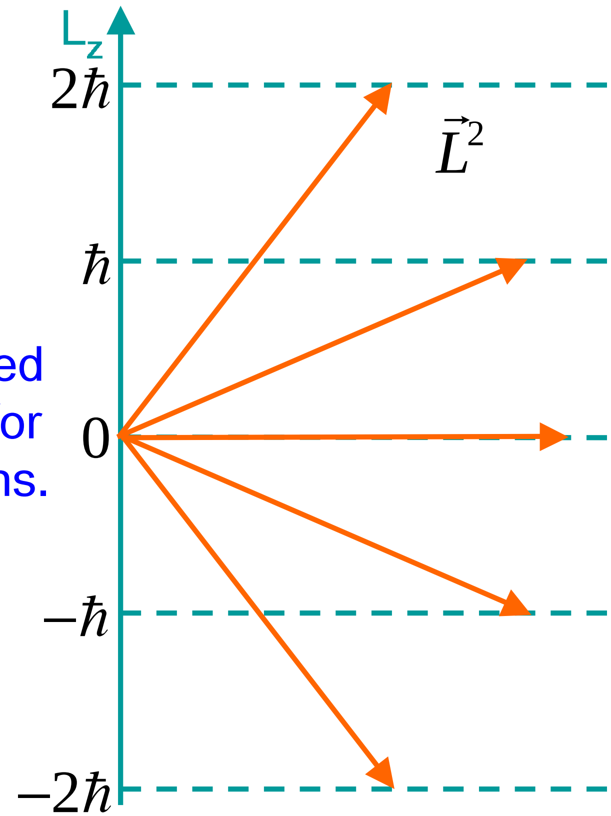
Schematic view of angular momentum

$$[\hat{\vec{L}}^2, \hat{\vec{L}}] = 0$$

There is a complete set of functions in which the square of the angular momentum is simultaneously specified with one of the components of the angular momentum.

If Lz is a quantized value, so is –Lz for symmetry reasons.



While the angular momentum vector and its z component are specified, the orientation in the x-y plane is smeared out.

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Eigenfunctions for L_z and L^2

$$\hat{\vec{L}}^2\Psi = -\hbar^2\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\Psi\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\Psi\right]$$

$$\hat{L}_z\Psi = -i\hbar\frac{\partial}{\partial\varphi}\Psi$$

Simultaneous eigenfunctions must depend on ϑ, φ

Indexing of the eigenfunctions: $Y_{lm}(\vartheta,\varphi)$

So that any function can be written as superposition:

$$\Psi(\vartheta,\varphi) = \sum_{\text{all } l \text{ and } m} A_{lm}Y_{lm}(\vartheta,\varphi)$$

Choice of the indexes:

Eigenfunction of L_z: $\hat{L}_z Y_{lm} = \hbar m Y_{lm}\ , \quad m \in \mathbf{Z}\ , \quad Y_{lm} = f(\vartheta)e^{im\varphi}$

Eigenfunction of L^2: $\hat{\vec{L}}^2 Y_{lm} = \hbar^2\xi(l)Y_{lm}$

What are the eigenvalues $\xi(l)$?

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Properties of Eigenfunctions of L_z and L^2

Simultaneous eigenfunctions of L_z and L^2 are

$$Y_{lm}(\vartheta,\varphi)\,,\quad l\in\{0,1,2,\dots\}\,,\quad m\in\{-l,\dots,l-1,l\}$$

and have the eigenvalues $\hat{\vec{L}}^2 Y_{lm} = \hbar^2 l(l+1) Y_{lm}$

$$\hat{L}_z Y_{lm} = \hbar m Y_{lm}$$

$$\hat{L}^2 Y_{ll} = \frac{\hbar^2}{\sin^2\vartheta}[l^2 f - \sin\vartheta\tfrac{\partial}{\partial\vartheta}(\sin\vartheta\tfrac{\partial}{\partial\vartheta} f)]e^{il\vartheta}$$

$$f(\vartheta)\propto\sin^l\vartheta$$

$$l^2 f - \sin\vartheta\tfrac{\partial}{\partial\vartheta}(\sin\vartheta\tfrac{\partial}{\partial\vartheta} f) = l^2 f - \sin\vartheta\tfrac{\partial}{\partial\vartheta}(\sin\vartheta\cos\vartheta\tfrac{\partial}{\partial\sin\vartheta} f)$$

$$= [l^2\sin^2\vartheta + l\sin^2\vartheta] f = l(l+1) f$$

$$\hat{L}_z Y_{ll} = i l Y_{ll} \quad\to\quad Y_{ll} = f(\vartheta)e^{il\varphi}$$

$$Y_{ll}\propto\sin^l\vartheta\, e^{il\varphi}$$

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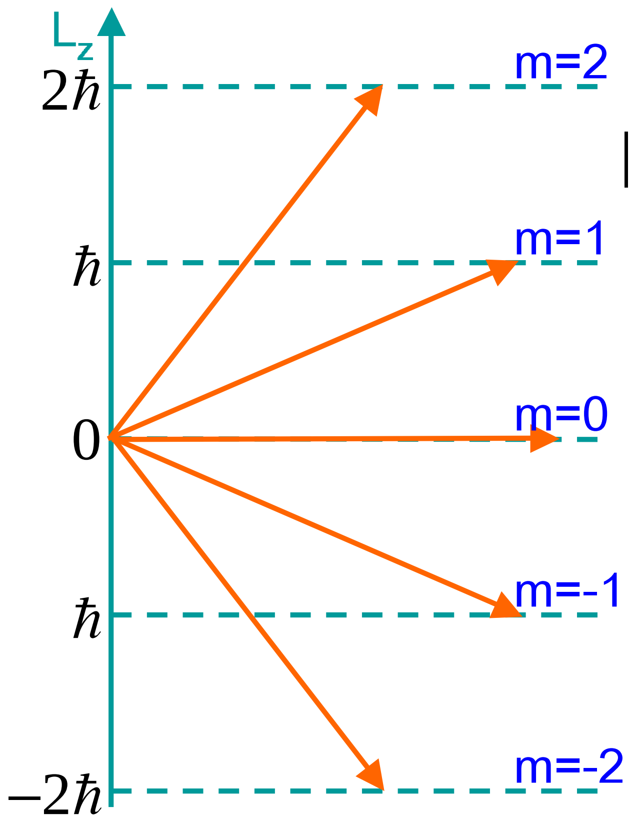
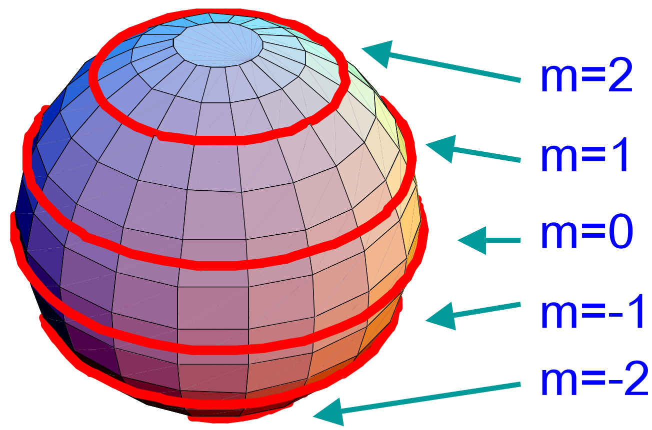
Vector model for angular momentum



$$|\vec{L}| = \hbar\sqrt{l(l+1)} = \hbar\sqrt{6}$$

While the angular momentum vector and its z component are specified, the orientation in the x-y plane is smeared out.



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Some spherical harmonics Y_{lm}

$$Y_{lm}(\vartheta,\varphi) = P_{lm}(\vartheta)e^{im\varphi}$$

The

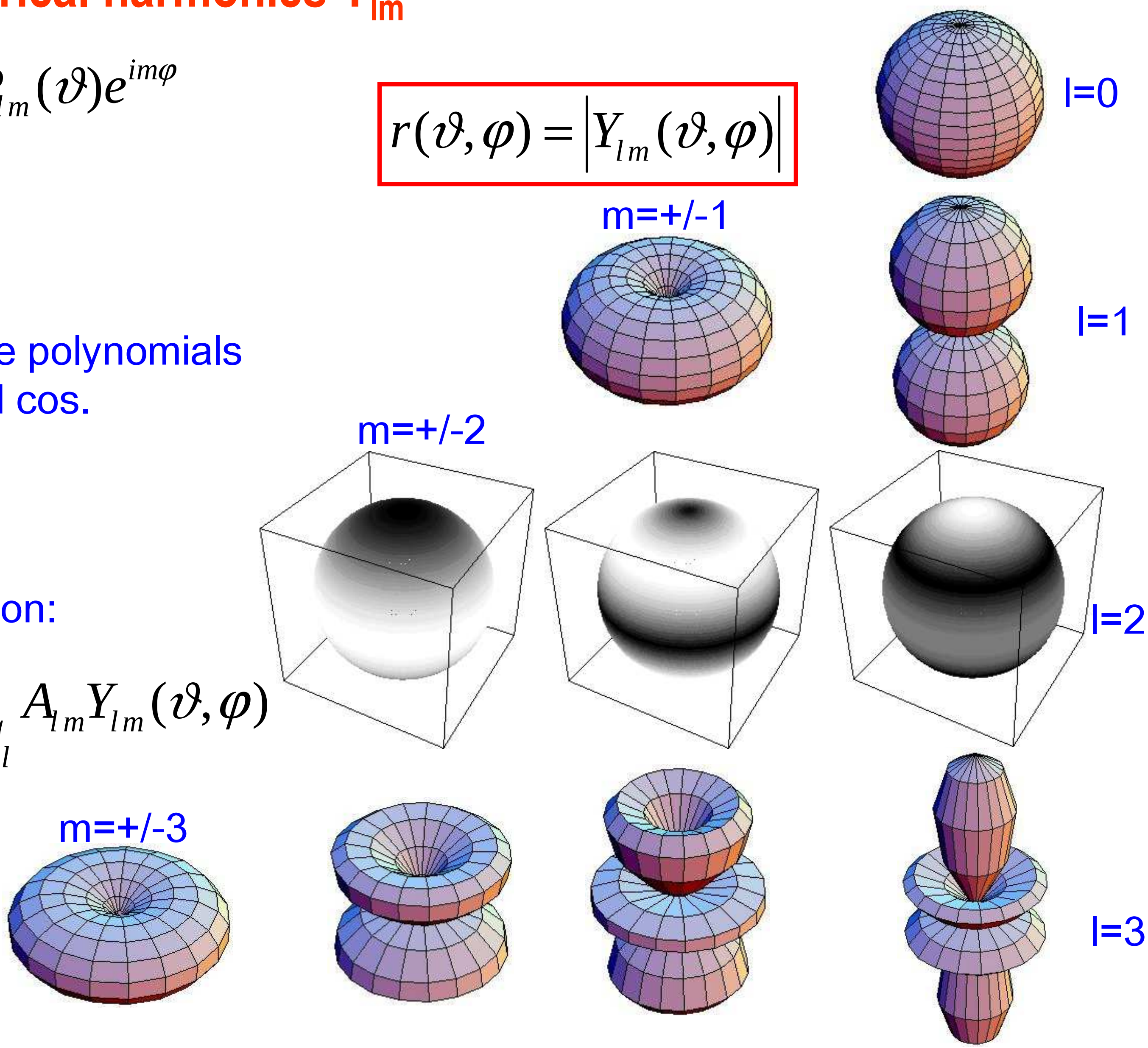
$$P_{lm}(\vartheta)$$

are simple polynomials of sin and cos.

Function expansion:

$$f(\vartheta,\varphi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} A_{lm}Y_{lm}(\vartheta,\varphi)$$

$$r(\vartheta,\varphi) = \left|Y_{lm}(\vartheta,\varphi)\right|$$



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