Summary of Angular Momentum

C. David Sherrill School of Chemistry and Biochemistry Georgia Institute of Technology November 1999

We start from the classical expression for angular momentum, $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, to obtain the quantum mechanical version $\hat{\mathbf{L}} = \hat{\mathbf{R}} \times \hat{\mathbf{P}}$, where $\hat{\mathbf{L}}$, $\hat{\mathbf{R}}$, and $\hat{\mathbf{P}}$ are all three-dimensional vectors. This definition leads immediately to expressions for the three components of \mathbf{L} :

$$\hat{L}_x = \hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y \tag{1}$$

$$\hat{L}_y = \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z \tag{2}$$

$$\hat{L} = \hat{Y}\hat{P}_x - \hat{X}\hat{P}_z \tag{2}$$

$$\hat{L}_z = \hat{X}\hat{P}_y - \hat{Y}\hat{P}_x. \tag{3}$$

From these definitions, we may easily derive the following commutators

$$\left[\hat{L}_{i},\hat{R}_{j}\right] = \epsilon_{ijk}i\hbar\hat{R}_{k} \tag{4}$$

$$\left[\hat{L}_{i},\hat{P}_{j}\right] = \epsilon_{ijk}i\hbar\hat{P}_{k} \tag{5}$$

$$\left[\hat{L}_{i},\hat{L}_{j}\right] = \epsilon_{ijk}i\hbar\hat{L}_{k}, \qquad (6)$$

where the indices i, j, k can be x, y, or z, and where the coefficient ϵ_{ijk} is unity if i, j, k form a cyclic permutation of x, y, z [i.e., (x, y, z), (y, z, x), or (z, x, y)] and -1 for a reverse cyclic permutation [(z, y, x), (x, z, y), or (y, x, z)]. The final commutator indicates that we cannot generally know L_x , L_y , and L_z simultaneously except if we have an eigenstate with eigenvalue 0 for each of these.

Classically, any component of the angular momentum must be less than or equal to the magnitude of the overall angular momentum vector. Quantum mechanically, the *average* value of any component of the angular momentum must be less than or equal to the square root of the expectation value of $\hat{\mathbf{L}}$ dotted with itself:

$$\langle \hat{L}_i \rangle \leq \sqrt{\langle \hat{\mathbf{L}}^2 \rangle}.$$
 (7)

 $\hat{\mathbf{L}}^2$ is simply $\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$.

Since $\hat{\mathbf{L}}^2$ commutes with any component \hat{L}_i , we *can* have simultaneous eigenfunctions of $\hat{\mathbf{L}}^2$ and a given component \hat{L}_i . We usually pick the *z* axis, since the expression for \hat{L}_z is the easiest of the three when we work in spherical polar coordinates:

$$\hat{L}_x = \frac{\hbar}{i} \left(-\sin\phi \,\frac{\partial}{\partial\theta} - \cos\phi \,\cot\theta \,\frac{\partial}{\partial\phi} \right) \tag{8}$$

$$\hat{L}_y = \frac{\hbar}{i} \left(\cos\phi \, \frac{\partial}{\partial\theta} - \sin\phi \, \cot\theta \, \frac{\partial}{\partial\phi} \right) \tag{9}$$

$$\hat{L}_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi}.$$
(10)

Of course it is also possible to express $\hat{\mathbf{L}}$ in terms of the unit vectors for spherical polar coordinates,

$$\hat{r} = \sin\theta \cos\phi \,\hat{i} + \sin\theta \sin\phi \,\hat{j} + \cos\theta \,\hat{k}$$
(11)

$$\hat{\phi} = -\sin\phi \,\hat{i} + \cos\phi \,\hat{j} \tag{12}$$

$$\hat{\theta} = \cos\theta \cos\phi \,\hat{i} + \cos\theta \sin\phi \,\hat{j} - \sin\theta \,\hat{k}.$$
(13)

Here,

$$\nabla = \hat{r}\frac{\partial}{\partial r} + \hat{\phi}\frac{1}{rsin\theta}\frac{\partial}{\partial\phi} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta}$$
(14)

and

$$\hat{\mathbf{L}} = \hat{\mathbf{R}} \times \hat{\mathbf{P}}
= r\hat{r} \times \frac{\hbar}{i} \nabla
= \frac{\hbar}{i} \left(\hat{\phi} \frac{\partial}{\partial \theta} - \hat{\theta} \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} \right).$$
(15)

The simultaneous eigenfunctions of $\hat{\mathbf{L}}^2$ and \hat{L}_z are called the *spherical harmonics*, $Y_l^m(\theta, \phi)$, where l is the total angular momentum quantum number, and m is the so-called magnetic quantum number. The spherical harmonics are defined as

$$Y_l^m(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} (-1)^m e^{im\phi} P_l^m(\cos\theta),$$
(16)

where P_l^m are the associated Legendre polynomials. We require that $-l \leq m \leq l$, and spherical harmonics with m < 0 are defined in terms of the spherical harmonics with m > 0 according to $Y_l^m = (-1)^m [Y_l^{-m}]^*$. The spherical harmonics are normalized over integration of angular coordinates such that

$$\int_0^\pi \sin\theta \,d\theta \int_0^{2\pi} d\phi \, [Y_{l'}^{m'}(\theta,\phi)]^* Y_l^m(\theta,\phi) = \delta_{l,l'} \delta_{m,m'},\tag{17}$$

and they have the following special properties:

$$\hat{L}_z Y_l^m = m\hbar Y_l^m \tag{18}$$

$$\hat{\mathbf{L}}^2 Y_l^m = l(l+1)\hbar^2 Y_l^m.$$
(19)

It can be useful to define *ladder operators* for angular momentum. The following ladder operators work not only for straight angular momentum $\hat{\mathbf{L}}$, but also for combined angular momenta such as $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$. If

$$\hat{\mathbf{J}}_{\pm} = \hat{J}_x \pm i \hat{J}_y \tag{20}$$

then

$$\hat{\mathbf{J}}_{\pm}|jm\rangle = \hbar \left[(j \mp m)(j \pm m + 1) \right]^{1/2} |j, m \pm 1\rangle.$$
(21)

We can see that these ladder operators raise or lower the magnetic quantum number m but leave l alone.

One can also show that in spherical polar coordinates

$$\hat{\mathbf{L}}^2 = -\hbar^2 \left[\frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \ \frac{\partial}{\partial\theta} \right) \right].$$
(22)

By comparing this expression with that for ∇^2 in spherical polar coordinates,

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 sin\theta} \frac{\partial}{\partial \theta} \left(sin\theta \ \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 sin^2 \theta} \left(\frac{\partial^2}{\partial \phi^2} \right),\tag{23}$$

we can see that the Hamiltonian can be written as

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + \hat{V}
= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{\hat{\mathbf{L}}^2}{2mr^2} + \hat{V}.$$
(24)

Clearly $\hat{\mathbf{L}}^2$ commutes with the kinetic energy term, $\hat{\mathbf{L}}^2$ has no r dependence. Likewise, if $\hat{V} = V(r)$, then $\hat{\mathbf{L}}^2$ commutes with the whole Hamiltonian. Hence, for problems where the potential depends only on r (central force problems), we can find simultaneous eigenfunctions of \hat{H} , $\hat{\mathbf{L}}^2$, and \hat{L}_z .