ANGULAR MOMENTUM

Angular momentum is a far broader concept than the momentum of a rotating single body. In its generalized form, it is the main tool for understanding and classifying energy levels of atomic systems. The spin, which is a major factor in discussing atoms and molecules, is also a form of angular momentum.

Angular momentum of a single body:

Classically, $\vec{L} = \vec{r} \times \vec{p}$. By the rules of quantum mechanics, $\vec{p}$ is replaced by $\frac{\hbar}{i}\vec{\nabla}$, giving the operators

$$\hat{L}_x = \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right),$$

$$\hat{L}_y = \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right),$$

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

The total momentum is

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

The commutation relations are

$$[L_x, L_y] = i\hbar L_z, \quad [L_y, L_z] = i\hbar L_x, \quad [L_z, L_x] = i\hbar L_y.$$

It turns out there are Hermitian operators in many systems which satisfy these commutation relations. Such operators represent generalized angular momenta. We will find properties determined by commutation relations only, which apply to all generalized angular momenta.

Given are three Hermitian operators, L_x, L_y, L_z, which satisfy

$$[L_x, L_y] = i\hbar L_z, \quad [L_y, L_z] = i\hbar L_x, \quad [L_z, L_x] = i\hbar L_y.$$

Nothing else is known about the operators.
Define $L^2 \equiv L_x^2 + L_y^2 + L_z^2$. What is the commutator $[L^2, L_z]$?
Using $[AB, C] = A[B, C] + [A, C]B$, which is easily proved by writing the commutators explicitly, and remembering that the commutator of an operator with itself is always zero, we get

$$[L_x^2, L_z] = L_x[L_x, L_z] + [L_x, L_z]L_x = -i\hbar L_x L_y - i\hbar L_y L_x$$
$$[L_y^2, L_z] = L_y[L_y, L_z] + [L_y, L_z]L_x = +i\hbar L_x L_y + i\hbar L_x L_y$$
$$[L_z^2, L_z] = 0.$$

Adding the three equations gives

$$[L^2, L_z] = 0.$$

L^2 and L_z have therefore a complete set of common eigenfunctions:

$$L^2 Y_{lm} = K_l Y_{lm}$$
$$L_z Y_{lm} = k_m Y_{lm}.$$

From the first equation we get $(L_x^2 + L_y^2 + L_z^2)Y_{lm} = K_l Y_{lm}$, and from the second – $L_z^2 Y_{lm} = k_m^2 Y_{lm}$.
Subtracting the 2nd from the 1st gives

$$(L_x^2 + L_y^2)Y_{lm} = (K_l - k_m^2)Y_{lm}.$$

A scalar product with $\langle Y_{lm}|$ gives

$$\langle Y_{lm}|L_x^2 + L_y^2|Y_{lm}\rangle = K_l - k_m^2.$$

Each of the two integrals in this equation is ≥ 0:

$$\langle Y_{lm}|L_x^2|Y_{lm}\rangle = \langle L_x Y_{lm}|L_x Y_{lm}\rangle \geq 0.$$

The first equality comes from the hermiticity of L_x, and it gives a scalar product of $L_x Y_{lm}$ with itself, which must be ≥ 0. The same holds for L_y^2, and therefore $K_l - k_m^2 \geq 0$, or $\boxed{K_l \geq k_m^2}$.

Define the ladder operators

$$L^+ \equiv L_x + iL_y \quad L^- \equiv L_x - iL_y.$$

These operators are not Hermitian, which is OK since they do not correspond to any observable. $(L^+)^\dagger = L^-$.

$$[L_z, L^+] = [L_z, L_x] + i[L_z, L_y] = i\hbar L_y + \hbar L_x = \hbar L^+.$$

Writing the commutator explicitly, $L_z L^+ - L^+ L_z = \hbar L^+$, gives

$$L_z L^+ = L^+(L_z + \hbar).$$

Applying to Y_{lm},

$$L_z\left(L^+ Y_{lm}\right) = L^+(L_z+\hbar)Y_{lm} = L^+(k_m+\hbar)Y_{lm} = (k_m+\hbar)\left(L^+ Y_{lm}\right),$$

showing that $L^+ Y_{lm}$ is an eigenfunction of L_z with the eigenvalue $k_m + \hbar$. Since L^2 commutes with L^+, $L^+ Y_{lm}$ is also an eigenfunction of L^2 with the eigenvalue K_l. We can also show, in similar manner, that $L^- Y_{lm}$ is an eigenfunction of L^2 with the eigenvalue K_l and an eigenfunction of L_z with the eigenvalue $k_m - \hbar$. These operators can be applied repeatedly, giving an infinite series of eigenfunctions of L^2 and L_z, with the same eigenvalue K_l of L^2 and a series of eigenvalues of L_z, $\cdots k_m - 2\hbar, k_m - \hbar, k_m, k_m + \hbar, \cdots$. This contradicts our finding above that the square of the eigenvalue of L_z must be $\leq$ the eigenvalue of L^2.

The way to solve this apparent contradiction is to require the series of eigenfunctions to be truncated at both ends. This can happen if applying L^+ to the Y_{lm} with the largest k_m and L^- to Y_{lm} with the smallest k_m gives zero:

$$L^+Y_{lm_2} = 0, \quad L^-Y_{lm_1} = 0.$$

L^2 may be expressed as $L^2 = L^-L^+ + L_z^2 + \hbar L_z$, giving $L^-L^+ = L^2 - L_z^2 - \hbar L_z$. Applying L^- to the first equation above and using the last expression gives

$$L^-L^+Y_{lm_2} = 0 = (L^2 - L_z^2 - \hbar L_z)Y_{lm_2} = (K_l - k_{m_2}^2 - \hbar k_{m_2})Y_{lm_2}.$$

From this we get $K_l = k_{m_2}^2 + \hbar k_{m_2}$.

L^2 may also be expressed as $L^2 = L^+L^- + L_z^2 - \hbar L_z$, which gives $L^+L^- = L^2 - L_z^2 + \hbar L_z$. Applying L^+ to the equation with Y_{lm_1} above gives

$$L^+L^-Y_{lm_1} = 0 = (L^2 - L_z^2 + \hbar L_z)Y_{lm_1} = (K_l - k_{m_1}^2 + \hbar k_{m_1})Y_{lm_1},$$

and therefore $K_l = k_{m_1}^2 - \hbar k_{m_1}$.

Equating the two expressions for K_l gives

$$k_{m_2}^2 + \hbar k_{m_2} = k_{m_1}^2 - \hbar k_{m_1}.$$

This is a quadratic equation for k_{m_2}, with the two solutions $k_{m_2} = -k_{m_1}$ or $k_{m_1} - \hbar$. Remember that k_{m_1} is the smallest k_m, whereas k_{m_2} is the largest, and the second solution is therefore not possible, as it implies $k_{m_1} > k_{m_2}$. We get $k_{m_2} = -k_{m_1}$.

The difference $k_{m_2} - k_{m_1}$ is an integer n times $\hbar$, so that $k_{m_1} = -n/2$ and $k_{m_2} = +n/2$. Obviously, n is determined by K_l, because the series of k_m values is truncated so that $k_m^2 \leq K_l$. There is therefore a connection between n and l. This connection may be chosen in many ways, and the choice defines l, which has not been defined so far. We choose $n = 2l$, which gives $k_{m_1} = -l\hbar$ and $k_{m_2} = l\hbar$. Therefore,

$$K_l = k_{m_2}^2 + \hbar k_{m_2} = l(l+1)\hbar^2.$$

$$k_m = -l\hbar, -(l-1)\hbar, \cdots, l\hbar \quad \text{or}$$

$$k_m = m\hbar, \quad m = -l, -l+1, \cdots, l,$$

and the eigenvalue equations look like those of a single particle,

$$\boxed{\begin{array}{l} L^2 Y_{lm} = l(l+1)\hbar^2 Y_{lm} \\ L_z Y_{lm} = m\hbar Y_{lm} \end{array}}$$

Note that l can be integer or half integer, as only n must be an integer. The operators L^2 and L_z, as well as the functions Y_{lm}, are in the coordinates of the system discussed. We know, however, that the eigenvalues will have the form obtained above for any system with generalized angular momentum (obeying the right commutation relations). The various relations we proved for the functions and/or operators will hold in all such cases.

The role of the ladder (or step) operators $L^{\pm}$ in raising or lowering the m value of the eigenfunctions Y_{lm} has been discussed above. Using normalized functions, we obtained (exercise)

$$L^+ Y_{lm} = \hbar\sqrt{(l-m)(l+m+1)}Y_{lm+1}$$

$$L^- Y_{lm} = \hbar\sqrt{(l+m)(l-m+1)}Y_{lm-1}$$

These relations are very useful in obtaining Y_{lm}, as we shall see in many cases.