Physics 221A
Fall 1996
Notes 12
Orbital Angular Momentum and Spherical Harmonics

We now consider the spatial degrees of freedom of a particle moving in 3-dimensional space, which of course is an important case in practice. We will assume either that the particle is spinless, or that we can ignore the spin degrees of freedom. Thus, the position operator $\mathbf{r}$ (i.e., its three components) constitutes a complete set of commuting observables, and the basis kets in the ket space can be taken to be the position eigenkets $|\mathbf{r}\rangle$. The ket space is of course isomorphic to the Hilbert space of wave functions $\psi(\mathbf{r})$. Rotation operators act on this ket space, just as indicated in the general theory laid out in Notes 11, and the study of them leads into the theory of the spherical harmonics and other useful topics.

You have previously learned that the angular momentum operator in wave mechanics in three dimensions, the so-called orbital angular momentum, is $\mathbf{L} = \mathbf{r}\times\mathbf{p}$, which is usually motivated by appeal to classical mechanics. (Here we follow the custom common in the physics literature of using the symbol $\mathbf{L}$ for orbital angular momentum instead of the general notation $\mathbf{J}$, and of using ℓ instead of j for the eigenvalues.) But the philosophy in this course is that the angular momentum of a system should be defined as the generator of rotations. Therefore, before defining the angular momentum, we should first define rotation operators based on the physical and mathematical properties we expect of such operators, and then derive the angular momentum operators from them.

We adopt the following definition of the rotation operators on our ket space:

$$U(\mathsf{R})|\mathbf{r}\rangle = |\mathsf{R}\mathbf{r}\rangle. \tag{12.1}$$

This definition is physically reasonable, because the position eigenket $|\mathbf{r}\rangle$ is the state of the system after a measurement of the position operator has yielded the value $\mathbf{r}$, while $|\mathsf{R}\mathbf{r}\rangle$ is the state after such a measurement has given the value $\mathsf{R}\mathbf{r}$. For example, position can be measured by passing particle through a small hole in a screen, and if we rotate the screen so that the hole moves from $\mathbf{r}$ to $\mathsf{R}\mathbf{r}$, then it is logical to call the state produced by the rotated measuring apparatus the rotated state. The only wrinkle in this argument is that we have to admit the possibility that there should be a phase factor present on the right hand side of Eq. (12.1); but we will ignore this complication as it turns out to be unnecessary. (At least this is true for most 3-dimensional problems in quantum mechanics; it would not be true for the motion of a charged particle in the field of a magnetic monopole.)

Actually, a hole in a screen does not really measure the position of a particle, but rather only restricts the two transverse position components of an electron which passes through the hole. To measure all three components of position at a definite time, we could shine a laser beam of small spatial extent across the exit side of a hole in a screen, and if we detect a scattered photon from the particle coming through, then we know at that instant in time that the particle is localized in a definite (and small) region of space. In any case, if we rotate such a measuring device to a new location, we will produce an eigenstate of the position operator with the rotated eigenvalue, as in Eq. (12.1).

Let us note the following features of the definition (12.1). First, the operator $U(\mathsf{R})$ is well defined by Eq. (12.1), because the action of $U(\mathsf{R})$ on an arbitrary basis vector is indicated. By linear superposition, we can find the action of $U(\mathsf{R})$ on an arbitrary state. Next, the operator $U(\mathsf{R})$ is unitary, in accordance with the calculation,

$$\begin{aligned}\langle \mathbf{r}'|U(\mathsf{R})^\dagger U(\mathsf{R})|\mathbf{r}\rangle &= \langle \mathsf{R}\mathbf{r}'|\mathsf{R}\mathbf{r}\rangle = \delta^3\big(\mathsf{R}(\mathbf{r}-\mathbf{r}')\big) = |\det \mathsf{R}|^{-1}\,\delta^3(\mathbf{r}-\mathbf{r}')\\ &= \delta^3(\mathbf{r}-\mathbf{r}') = \langle \mathbf{r}'|\mathbf{r}\rangle,\end{aligned} \tag{12.2}$$

where we use the properties of the δ-function and the fact that R is an orthogonal matrix. Since this is true for all $\mathbf{r}$, $\mathbf{r}'$, we have $U(\mathsf{R})^\dagger U(\mathsf{R}) = 1$, and $U(\mathsf{R})$ is unitary. Finally, the operators $U(\mathsf{R})$ defined in Eq. (12.1) form a unitary representation of $SO(3)$, for we have

$$U(\mathsf{R}_1)U(\mathsf{R}_2) = U(\mathsf{R}_1\mathsf{R}_2). \tag{12.3}$$

This follows directly from the definition, since

$$U(\mathsf{R}_1)U(\mathsf{R}_2)|\mathbf{r}\rangle = U(\mathsf{R}_1)|\mathsf{R}_2\mathbf{r}\rangle = |\mathsf{R}_1\mathsf{R}_2\mathbf{r}\rangle = U(\mathsf{R}_1\mathsf{R}_2)|\mathbf{r}\rangle. \tag{12.4}$$

Furthermore, we note that the representation is single-valued. This fact alone indicates that orbital angular momentum only takes on integral values of ℓ (not half-integers), i.e., the multiplicity of all half-integral values is zero.

Now if Eq. (12.1) holds for all rotations, it holds in particular for infinitesimal rotations. Therefore we have

$$\begin{aligned}\Big(1-\frac{i}{\hbar}\theta\hat{\mathbf{n}}\cdot\mathbf{L}\Big)|\mathbf{r}_0\rangle &= \big|(\mathsf{I}+\theta\hat{\mathbf{n}}\cdot\mathbf{J})\mathbf{r}_0\big\rangle = |\mathbf{r}_0+\theta\hat{\mathbf{n}}\times\mathbf{r}_0\rangle\\ &= |\mathbf{r}_0\rangle + \theta(\mathbf{n}\times\mathbf{r}_0)\cdot\nabla|\mathbf{r}_0\rangle,\end{aligned} \tag{12.5}$$

where we write $\mathbf{L}$ for the generator of rotations, so that $U(\hat{\mathbf{n}},\theta) = \exp(-i\theta\hat{\mathbf{n}}\cdot\mathbf{L}/\hbar)$. This is taken as the definition of $\mathbf{L}$; as yet we do not know what $\mathbf{L}$ is. In Eq. (12.5), we have written the eigenket of position as $|\mathbf{r}_0\rangle$, using the notation $\mathbf{r}_0$ for the c-number eigenvalue, since in the following derivation we will reserve the symbol $\mathbf{r}$ for the operator. But we also have

$$\mathbf{p}|\mathbf{r}_0\rangle = i\hbar\nabla|\mathbf{r}_0\rangle, \tag{12.6}$$

where $\mathbf{p}$ is the momentum operator (not a c-number), so Eq. (12.5) becomes

$$\begin{aligned} \mathbf{L}|\mathbf{r}_0\rangle &= \mathbf{r}_0\times\mathbf{p}|\mathbf{r}_0\rangle = -\mathbf{p}\times\mathbf{r}_0|\mathbf{r}_0\rangle = -\mathbf{p}\times\mathbf{r}|\mathbf{r}_0\rangle \\ &= \mathbf{r}\times\mathbf{p}|\mathbf{r}_0\rangle. \end{aligned} \tag{12.7}$$

But the position kets $|\mathbf{r}_0\rangle$ form a basis in the Hilbert space of wave functions $\psi(\mathbf{r}_0)$, so we obtain

$$\mathbf{L} = \mathbf{r}\times\mathbf{p}. \tag{12.8}$$

Therefore our definition (12.1) of the rotation operators is equivalent to the usual definition of orbital angular momentum.

To get a feel for the rotation operators defined by Eq. (12.1), let us examine their effect on wave functions. We let $|\psi\rangle$ and $|\psi'\rangle$ be old and new states, respectively, related by some rotation operator,

$$|\psi'\rangle = U(\mathsf{R})|\psi\rangle, \tag{12.9}$$

and we let $\psi(\mathbf{r})$ and $\psi'(\mathbf{r})$ be the associated wave functions,

$$\psi(\mathbf{r}) = \langle\mathbf{r}|\psi\rangle, \qquad \psi'(\mathbf{r}) = \langle\mathbf{r}|\psi'\rangle. \tag{12.10}$$

Then by Eqs. (12.9) and (12.1), we have

$$\psi'(\mathbf{r}) = \langle\mathbf{r}|U(\mathsf{R})|\psi\rangle = \langle\mathsf{R}^{-1}\mathbf{r}|\psi\rangle = \psi\big(\mathsf{R}^{-1}\mathbf{r}\big). \tag{12.11}$$

To summarize this result, let us write $\psi' = \mathcal{R}\psi$, to indicate the relation between the old and new wave functions. Previously (in Notes 9) we used the symbol $\mathcal{R}$ to denote a rotation operator in the sense of a mapping of physical space onto itself which preserves lengths and leaves one point fixed; but now we are generalizing this notation, to allow $\mathcal{R}$ to be the operator which rotates an old function defined on configuration space into a new function. With this notation, we have

$$\boxed{(\mathcal{R}\psi)(\mathbf{r}) = \psi\big(\mathsf{R}^{-1}\mathbf{r}\big).} \tag{12.12}$$

In other words, the value of the rotated wave function at a given point is the value of the unrotated function at the inverse rotated point. This equation is completely equivalent to the definition (12.1).

The use of R^{-1} instead of R in Eq. (12.12) is somewhat counterintuitive (at least if you don't think about it very hard), but is necessary for the active interpretation of the rotation operators. For suppose we have some $\psi(\mathbf{r})$ with a large concentration of probability near some point $\mathbf{r}_0$. Then under an active rotation specified by R, we expect the new wave function to have a large concentration of probability near the (actively rotated) point $\mathsf{R}\mathbf{r}_0$. To say this in words, we expect the value of the new wave function at the new point to be equal to the value of the old wave function at the old point. This is equivalent to

$$\psi'(\mathbf{r}') = \psi(\mathbf{r}) \tag{12.13}$$

whenever $\mathbf{r}' = \mathsf{R}\mathbf{r}$. But this is the same as Eq. (12.12) (with the dummy symbol $\mathbf{r}$ replaced by $\mathsf{R}^{-1}\mathbf{r}$). It is important to see rotations in geometrical terms.

At this point we have identified a Hilbert space [the space of wave functions $\psi(\mathbf{r})$] upon which a vector $\mathbf{L}$ of operators act which are the generators of rotations. Of course, these operators satisfy the angular momentum commutation relations,

$$[L_i, L_j] = i\hbar\,\epsilon_{ijk}\,L_k, \tag{12.14}$$

as is easily verified from the definition (12.8). (A separate calculation is really unnecessary, given that $\mathbf{L}$ constitutes the generators of a representation of the rotation group. But of course if we are insecure we can check it.) Therefore all the hypotheses leading into Notes 11 are satisfied, and we expect to find that the Hilbert space can be broken up into a collection of $(2\ell+1)$-dimensional irreducible subspaces, with some multiplicity for each ℓ value. In fact, as we will see, the multiplicities N_ℓ are zero for all half-integral values of ℓ (half-integral values do not occur), and infinity for all integral values.

To follow the general theory laid out in Notes 11, we will seek the simultaneous eigenfunctions of L^2 and L_z. We have to admit the possibility (to be confirmed momentarily) that these simultaneous eigenfunctions may be degenerate. To find these eigenfunctions explicitly, we write down the components of angular momentum as differential operators on wave functions, and transform them from rectangular (xyz) to spherical $(r\theta\phi)$ coordinates. The transformation is straightforward but somewhat tedious. The results are

$$\begin{aligned}
L_x &= -i\hbar\Bigl(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\Bigr) = -i\hbar\Bigl(-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}\Bigr),\\
L_y &= -i\hbar\Bigl(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\Bigr) = -i\hbar\Bigl(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\Bigr),\\
L_z &= -i\hbar\Bigl(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\Bigr) = -i\hbar\frac{\partial}{\partial\phi}.
\end{aligned} \tag{12.15}$$

The component L_z is particularly simple in spherical coordinates, and it is not hard to see why: L_z is the generator of rotations about the z-axis, and ϕ is the azimuthal angle.

Another striking feature about these operators is that the radial operator $\partial/\partial r$ does not occur. The geometrical reason for this is that rotations in physical space change the direction of vectors, but not their magnitude; therefore the motion of the tip of a given vector takes place on the surface of a sphere. This is also true of infinitesimal rotations, which connect nearby points of the same r value but different θ and ϕ values. Therefore the components of $\mathbf{L}$, in terms of which infinitesimal rotations are expressed, do not involve any differentiation with respect to r.

Because of this fact, we can think of the angular momentum operators as acting on the Hilbert space of functions $f(\theta,\phi)$ defined on the unit sphere, rather than on functions $\psi(\mathbf{r}) = \psi(r,\theta,\phi)$ defined in the full 3-dimensional space. This is often a useful point of view, and we will now make a small digression for notation for functions defined on the unit sphere.

We denote a point on the unit sphere either by (θ,ϕ) or by $\hat{\mathbf{r}}$, indicating a unit vector. For example, we will write $f(\theta,\phi) = f(\hat{\mathbf{r}})$. We will adopt a Dirac bra-ket notation for functions on the unit sphere, for example making the association,

$$f(\theta,\phi) = f(\hat{\mathbf{r}}) \leftrightarrow |f\rangle. \tag{12.16}$$

We define the scalar product of two such functions by

$$\langle f|g\rangle = \int d\Omega\, f(\theta,\phi)^* g(\theta,\phi), \tag{12.17}$$

where $d\Omega = \sin\theta\, d\theta\, d\phi$. We define a δ-function on the unit sphere by

$$\delta_{\theta_0\phi_0}(\theta,\phi) = \frac{\delta(\theta-\theta_0)\delta(\phi-\phi_0)}{\sin\theta}, \tag{12.18}$$

so that

$$\int d\Omega\, \delta_{\theta_0\phi_0}(\theta,\phi) f(\theta,\phi) = f(\theta_0,\phi_0), \tag{12.19}$$

for any function f, and we associate this δ-function with a ket by

$$\delta_{\theta_0\phi_0}(\theta,\phi) \leftrightarrow |\hat{\mathbf{r}}_0\rangle, \tag{12.20}$$

where $(\theta_0,\phi_0) = \hat{\mathbf{r}}_0$. Then we have

$$f(\theta,\phi) = f(\hat{\mathbf{r}}) = \langle\hat{\mathbf{r}}|f\rangle. \tag{12.21}$$

To return to the construction of the angular momentum basis, we use Eqs. (12.22) to compute the raising and lowering operators,

$$L_\pm = L_x \pm iL_y = -i\hbar\, e^{\pm i\phi}\Big(\pm i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\Big), \tag{12.22}$$

and the Casimir L^2,

$$L^2 = \frac{1}{2}\big(L_+L_- + L_-L_+\big) + L_z^2 = -\hbar^2\Big[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\Big(\sin\theta\frac{\partial}{\partial\theta}\Big) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\Big]. \tag{12.23}$$

At this point we notice the relation of L^2 to the Laplacian operator,

$$|\mathbf{p}|^2\psi = -\hbar^2\nabla^2\psi = -\hbar^2\frac{1}{r^2}\frac{\partial}{\partial r}\Big(r^2\frac{\partial\psi}{\partial r}\Big) + \frac{L^2}{r^2}\psi. \tag{12.24}$$

We will come back to this formula later, but for now we are more interested in angular momentum than kinetic energy.

To find the simultaneous eigenfunctions of L^2 and L_z, we seek first the stretched states $m = \ell$, which we denote by $\psi_{\ell\ell}$. These states must satisfy,

$$L_z\,\psi_{\ell\ell} = \ell\hbar\,\psi_{\ell\ell}, \tag{12.25}$$

and

$$L_+\,\psi_{\ell\ell} = 0. \tag{12.26}$$

Using Eq. (12.15) in Eq. (12.25), we have

$$\frac{\partial\psi_{\ell\ell}}{\partial\phi} = i\ell\,\psi_{\ell\ell}, \tag{12.27}$$

or,

$$\psi_{\ell\ell}(r,\theta,\phi) = F(r,\theta)\,e^{i\ell\phi}, \tag{12.28}$$

where $F(r,\theta)$ is (at this point) an arbitrary function. Equation (12.28) shows once again that only integral values of ℓ are allowed, for the wave functions must be single-valued. Now using Eqs. (12.28) and (12.22) in Eq. (12.26), we find

$$\frac{\partial F}{\partial\theta} = \ell\cot\theta F, \tag{12.29}$$

or,

$$\psi_{\ell\ell}(r,\theta,\phi) = u(r)\sin^\ell\theta\,e^{i\ell\phi}, \tag{12.30}$$

where $u(r)$ is an arbitary radial function. These are the stretched wave functions.

We see that the simultaneous eigenfunctions of L^2 and L_z are indeed degenerate, since any radial function may appear in Eq. (12.30). In order to resolve these degeneracies, we may introduce an arbitrarily chosen basis $\{u_n(r)\}$ of radial wave functions, and write

$$\psi_{n\ell\ell}(r,\theta,\phi) = u_n(r)\sin^\ell\theta e^{i\ell\phi}. \tag{12.31}$$

The index n we use here serves the same purpose as the index α used in Notes 11; it labels an arbitrarily chosen orthonormal basis in the stretched eigenspace. We see that the multiplicity of the integral values of ℓ on the Hilbert space of wave function $\psi(\mathbf{r})$ is infinity.

Another approach is simply to throw away the radial variables, and work on the unit sphere. On the Hilbert space of wave functions $f(\theta,\phi)$ on the unit sphere, the simultaneous stretched eigenfunction of L^2 and L_z is

$$f_{\ell\ell}(\theta,\phi) = \sin^\ell\theta\, e^{i\ell\phi}, \tag{12.32}$$

and it is nondegenerate. Therefore, on this Hilbert space, the multiplicity N_ℓ is zero for half-integral ℓ, and unity for integral ℓ. When we normalize $f_{\ell\ell}$ using the rule

$$\langle f|f\rangle = \int d\Omega\,|f|^2 = 1, \tag{12.33}$$

we find

$$Y_{\ell\ell}(\theta,\phi) = \frac{(-1)^\ell}{2^\ell \ell!}\sqrt{\frac{(2\ell+1)!}{4\pi}}\,\sin^\ell\theta\, e^{i\ell\phi}, \tag{12.34}$$

where we have identified the normalized $f_{\ell\ell}$ with the stretched spherical harmonic $Y_{\ell\ell}$, and where we have introduced the conventional phase factor $(-1)^\ell$. (In the general theory developed in Notes 11, the phase of the stretched state $|jj\rangle$ was left arbitrary.)

To obtain the states corresponding to other values of m, we can apply lowering operators. Working from Eqs. (11.37), we readily derive the following formula by induction,

$$|jm\rangle = \sqrt{\frac{(j+m)!}{(2j)!(j-m)!}}\left(\frac{J_-}{\hbar}\right)^{j-m}|jj\rangle, \tag{12.35}$$

where of course in the present context we will change notation and make the replacements, $j\to\ell$, $J_-\to L_-$. Then by induction one can show that

$$\left(\frac{L_-}{\hbar}\right)^{\ell-m}\sin^\ell\theta e^{i\ell\phi} = \frac{e^{im\phi}}{\sin^m\theta}\left[\frac{d}{d(\cos\theta)}\right]^{\ell-m}\sin^{2\ell}\theta, \tag{12.36}$$

so that altogether we have

$$Y_{\ell m}(\theta,\phi) = \frac{(-1)^\ell}{2^\ell \ell!}\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell+m)!}{(\ell-m)!}}\,\frac{e^{im\phi}}{\sin^m\theta}\left[\frac{d}{d(\cos\theta)}\right]^{\ell-m}\sin^{2\ell}\theta. \tag{12.37}$$

This formula is valid for all m in the range, $-\ell \leq m \leq +\ell$.

Equation (12.37) can be expressed in terms of Legendre polynomials and associated Legendre functions. First we consider the case $m = 0$, and invoke the Rodriguez formula for the Legendre polynomial $P_\ell(x)$,

$$P_\ell(x) = \frac{(-1)^\ell}{2^\ell \ell!} \frac{d^\ell}{dx^\ell}(1-x^2)^\ell, \tag{12.38}$$

where we set

$$x = \cos\theta. \tag{12.39}$$

Then Eq. (12.37) becomes

$$Y_{\ell 0}(\theta,\phi) = \sqrt{\frac{2\ell+1}{4\pi}}\, P_\ell(\cos\theta). \tag{12.40}$$

The choice of the phase factor $(-1)^\ell$ in Eq. (12.34) was designed to make $Y_{\ell 0}$ real and positive at the north pole ($\cos\theta = 1$); this follows from

$$P_\ell(1) = 1. \tag{12.41}$$

Now let us consider the case $m \geq 0$. We can construct the $Y_{\ell m}$ for this case by applying raising operators to the state $Y_{\ell 0}$. Again using induction on Eq. (11.37), we obtain

$$|\ell m\rangle = \sqrt{\frac{(\ell-m)!}{(\ell+m)!}} \Big(\frac{L_+}{\hbar}\Big)^m |\ell 0\rangle. \tag{12.42}$$

(This formula only works for integer angular momentum, since the value $m = 0$ is possible only in this case.) Next we use induction to obtain

$$\begin{aligned} \Big(\frac{L_+}{\hbar}\Big)^m P_\ell(\cos\theta) &= (-1)^m \sin^m\theta\, e^{im\phi} \Big[\frac{d}{d(\cos\theta)}\Big]^m P_\ell(\cos\theta) \\ &= (-1)^m e^{im\phi}\, P_{\ell m}(\cos\theta), \end{aligned} \tag{12.43}$$

where we have introduced the associated Legendre function, defined by

$$P_{\ell m}(x) = (1-x^2)^{m/2} \frac{d^m P_\ell(x)}{dx^m}. \tag{12.44}$$

Altogether, for $m \geq 0$ we have

$$Y_{\ell m}(\theta,\phi) = (-1)^m \sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\, e^{im\phi}\, P_{\ell m}(\cos\theta). \tag{12.45}$$

For the case $m < 0$, we go back to Eq. (12.37), we set $m = -|m|$, and we use Eqs. (12.38) and (12.44). The result is

$$Y_{\ell,-|m|}(\theta,\phi) = \sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}}\, e^{-i|m|\phi}\, P_{\ell,|m|}(\cos\theta). \tag{12.46}$$

This is equivalent to

$$Y_{\ell,-m}(\theta,\phi) = (-1)^m Y_{\ell m}(\theta,\phi)^*, \tag{12.47}$$

which is valid for any value of m.

Notice that the theory of the $Y_{\ell m}$'s is completely founded on the general theory of raising and lowering operators as laid out in Notes 11, and that even the phase conventions are the standard ones presented in those Notes. Only the phase $(-1)^\ell$ in Eq. (12.34) goes beyond the conventions established in those Notes.

There are several interesting and useful results which follow from applying rotation operators to the $Y_{\ell m}$'s. It is often important to rotate the $Y_{\ell m}$'s, because by the very definition of the spherical coordinates (θ,ϕ), a privileged role has been assigned to the z-axis. In addition, the z-axis has been selected out again for a privileged role by the standard convention of working with eigenfunctions of L^2 and L_z. In many problems it is necessary to refer calculations to another axis, which can be done with rotation operators.

First let us write the ket $|\ell m\rangle$ to stand for the function $Y_{\ell m}(\theta,\phi)$, regarded as a function defined on the unit sphere, so that

$$Y_{\ell m}(\hat{\mathbf{r}}) = \langle\hat{\mathbf{r}}|\ell m\rangle. \tag{12.48}$$

Since we have determined that $Y_{\ell m}$ is the nondegenerate eigenfunction of L^2 and L_z on the unit sphere, we do not need any extra quantum numbers in $|\ell m\rangle$. We now apply a rotation operator specified by $\mathcal{R}$ or R to a $Y_{\ell m}$. We have

$$\big(\mathcal{R}Y_{\ell m}\big)(\hat{\mathbf{r}}) = Y_{\ell m}\big(\mathsf{R}^{-1}\hat{\mathbf{r}}\big) = \langle\hat{\mathbf{r}}|U(\mathsf{R})|\ell m\rangle = \sum_{m'}\langle\hat{\mathbf{r}}|\ell m'\rangle\langle\ell m'|U(\mathsf{R})|\ell m\rangle, \tag{12.49}$$

where in effect we rotate the $Y_{\ell m}$ in two ways, once by rotating the argument in 3-dimensional space, and the other time by rotating it as a basis function in its irreducible subspace of Hilbert space. The matrix element in the final expression is a D matrix, so we obtain

$$\boxed{\big(\mathcal{R}Y_{\ell m}\big)(\hat{\mathbf{r}}) = Y_{\ell m}(\mathsf{R}^{-1}\hat{\mathbf{r}}) = \sum_{m'} Y_{\ell m'}(\hat{\mathbf{r}})\, D^{\ell}_{m'm}(\mathsf{R}),} \tag{12.50}$$

which may be recognized as a special case of Eq. (11.56).

Equation (12.50) gives $Y_{\ell m}$ at one point on the sphere as a linear combination of other $Y_{\ell m}$'s, for the same value of ℓ but all values of m, at another point on the sphere. The fact that the linear combination does not involve other values of ℓ is due to the irreducibility of the subspace spanned by the $Y_{\ell m}$'s for fixed ℓ but variable m.

Equation (12.50) can be used to express the values of the $Y_{\ell m}$'s at a point of interest in terms of the their values at the north pole (a convenient reference point). To put this in convenient form, we change notation in Eq. (12.50), and replace $\hat{\mathbf{r}}$ by $\hat{\mathbf{z}}$, and replace R by R^{-1}. Then we write $\hat{\mathbf{r}} = \mathsf{R}\hat{\mathbf{z}}$, so that R is interpreted as a rotation which maps the $\hat{\mathbf{z}}$-axis into some direction $\hat{\mathbf{r}}$ of interest. Then we obtain,

$$Y_{\ell m}(\hat{\mathbf{r}}) = \sum_{m'} Y_{\ell m'}(\hat{\mathbf{z}})\, D^{\ell}_{m'm}(\mathsf{R}^{-1}). \tag{12.51}$$

If we write $\hat{\mathbf{r}} = (\theta, \phi)$ for the direction of interest, then a rotation which maps the $\hat{\mathbf{z}}$-axis into this direction is easily given in Euler angle form,

$$\mathsf{R}(\phi, \theta, 0)\hat{\mathbf{z}} = \hat{\mathbf{r}}, \tag{12.52}$$

i.e., with $\alpha = \phi$ and $\beta = \theta$, because the first two Euler angles were designed to specify the direction of the rotated $\hat{\mathbf{z}}$-axis. Also, the value of $Y_{\ell m}$ at the north pole is especially simple, because all the associated Legendre functions $P_{\ell m}(\cos\theta)$ vanish at $\theta = 0$ unless $m = 0$, and in that case we have $P_\ell(1) = 1$. Therefore

$$Y_{\ell m}(\hat{\mathbf{z}}) = \sqrt{\frac{2\ell+1}{4\pi}}\, \delta_{m0}. \tag{12.53}$$

Finally, we can use Eq. (11.54) to rewrite the matrix $D(\mathsf{R}^{-1})$, and Eq. (12.51) becomes,

$$\boxed{Y_{\ell m}(\theta, \phi) = \sqrt{\frac{2\ell+1}{4\pi}}\, D^{\ell *}_{m0}(\phi, \theta, 0).} \tag{12.54}$$

In this way we have found a useful connection between the $Y_{\ell m}$'s and the D-matrices.

We can use this to derive another nice result. Consider the following function defined on the unit sphere:

$$f(\theta, \phi) = f(\hat{\mathbf{r}}) = P_\ell(\cos\theta) = P_\ell(\hat{\mathbf{r}} \cdot \hat{\mathbf{z}}) = \sqrt{\frac{4\pi}{2\ell+1}}\, Y_{\ell 0}(\hat{\mathbf{r}}), \tag{12.55}$$

where P_ℓ is the usual Legendre polynomial and $\hat{\mathbf{r}} = (\theta, \phi)$ is some direction of interest. Now let us rotate this function by some rotation specified by $\mathcal{R}$ or R. We have

$$(\mathcal{R}f)(\hat{\mathbf{r}}) = f(\mathsf{R}^{-1}\hat{\mathbf{r}}) = P_\ell(\mathsf{R}^{-1}\hat{\mathbf{r}} \cdot \hat{\mathbf{z}}) = P_\ell(\hat{\mathbf{r}} \cdot \mathsf{R}\hat{\mathbf{z}}), \tag{12.56}$$

where in the final step we use the fact that $\mathsf{R}^{-1} = \mathsf{R}^t$ to transfer the rotation matrix from $\hat{\mathbf{r}}$ to $\hat{\mathbf{z}}$ in the scalar product. Now we choose the matrix R to have the Euler angle form $\mathsf{R}(\phi', \theta', 0)$, so that $\hat{\mathbf{r}}' = (\theta', \phi') = \mathsf{R}\hat{\mathbf{z}}$, where $\hat{\mathbf{r}}'$ is another direction of interest (in addition to $\hat{\mathbf{r}}$). Then Eqs. (12.55) and (12.56) become

$$P_\ell(\hat{\mathbf{r}} \cdot \hat{\mathbf{r}}') = \sqrt{\frac{4\pi}{2\ell+1}}\, Y_{\ell 0}(\mathsf{R}^{-1}\hat{\mathbf{r}}) = \sqrt{\frac{4\pi}{2\ell+1}} \sum_m Y_{\ell m}(\hat{\mathbf{r}})\, D^\ell_{m0}(\theta', \phi', 0), \tag{12.57}$$

where we use Eq. (12.50) to expand the rotated $Y_{\ell m}$. Finally, we use Eq. (12.54) to write the result purely in terms of $Y_{\ell m}$'s, and we have

$$\boxed{P_\ell(\hat{\mathbf{r}} \cdot \hat{\mathbf{r}}') = \frac{4\pi}{2\ell+1} \sum_m Y_{\ell m}(\theta, \phi)\, Y^*_{\ell m}(\theta', \phi'),} \tag{12.58}$$

which is the (very useful) *addition theorem* for the spherical harmonics.