Associated Legendre Functions and Dipole Transition Matrix Elements

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Summary

Notes on Legendre polynomials, associated Legendre functions, spherical harmonics, and the properties needed from them to get electric dipole transition matrix elements.

1 What is interesting

For an electric dipole transition between two states of known orbital angular momentum, specified by angular quantum numbers l, m for the initial state and l', m' for the final state, one wants to know certain matrix elements between the states, like

$$\langle n'l'm'|\mathbf{r}|nlm\rangle = \int dr\ r^2 R_{n'l'}(r) r R_{nl}(r) \int d\Omega\ Y_{l'}^{m'}(\Omega)\,\hat{r}(\Omega)\,Y_l^m(\Omega) \tag{1.1}$$

The states also are labeled by some other principal quantum number n' and n, that is needed to determine the radial wave functions $R_{nl}(r)$. The volume element for these integrals is $d^3r = r^2 dr d\Omega$, where $d\Omega = -d\phi\, d(\cos\theta) = d\phi \sin\theta\, d\theta$, and the angular integrals are over the surface of a unit sphere. In these notes I am only interested in the angular integrals. The radial unit vector in Cartesian coordinates is

$$\hat{r}(\Omega) = \hat{x}\sin\theta\cos\phi + \hat{y}\sin\theta\sin\phi + \hat{z}\cos\theta = \hat{r}_x\hat{x} + \hat{r}_y\hat{y} + \hat{r}_z\hat{z}. \tag{1.2}$$

Thus I want to discuss how to get these three angular integrals,

$$I_i = \int d\Omega\ Y_{l'}^{m'}(\Omega)\,\hat{r}_i\,Y_l^m(\Omega), \quad i = x, y, z. \tag{1.3}$$

The arguments $\hat{r}_i$ are not unit vectors, however, they can be expressed in terms of spherical harmonics with index $l = 1$. Those spherical harmonics are

$$Y_1^0(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta, \qquad Y_1^{\pm 1}(\theta,\phi) = \mp\sqrt{\frac{3}{8\pi}}e^{\pm i\phi}\sin\theta \tag{1.4}$$

Then one can see that the components of the radial unit vector are written in terms of these, if one so desires, as

$$\hat{r}_x = \sin\theta\cos\phi = -\sqrt{\frac{2\pi}{3}}\left(Y_1^1 - Y_1^{-1}\right) \tag{1.5}$$

$$\hat{r}_y = \sin\theta\sin\phi = i\sqrt{\frac{2\pi}{3}}\left(Y_1^1 + Y_1^{-1}\right) \tag{1.6}$$

$$\hat{r}_z = \cos\theta = \sqrt{\frac{4\pi}{3}}Y_1^0. \tag{1.7}$$

Then one sees that the desired angular integrals involve products of three spherical harmonics. Although I know that there is a lot of theory about how to evaluate these types of integrals for any choices of the quantum indeces, by advanced techniques, here I am considering only the case where one of them has $1\hbar$ unit of orbital angular momentum. Also, I want to see how this can be found more by arithmetic and algebraic approach, using the properties of the differential equation that leads to the spherical harmonics, and especially, the generating functions.

To this end, actually, I will approach this as follows. The spherical harmonics can be expressed as products of two normalized functions, one for the θ dependence, and one for the ϕ dependence:

$$Y_l^m(\theta,\phi) = \Theta_l^m(\theta)\Phi_m(\phi), \qquad \Phi_m(\phi) = \frac{1}{\sqrt{2\pi}}e^{im\phi} \tag{1.8}$$

The ϕ dependence is trivial. The θ dependence is the more interesting part. To be able to get the desired angular integrals, it will suffice to find expressions for products of the spherical harmonic Y_l^m with either $\sin\theta$ or $\cos\theta$, and in fact, try to express those products in terms of other spherical harmonics. This is equivalent to finding what are known as recurrence relations for the angular functions $\Theta_l^m(\theta)$. Those show what can happen to $\Theta_l^m(\theta)$ when multiplied by either $\sin\theta$ or $\cos\theta$, which is exactly what is needed to get the transition matrix elements.

$$\sin\theta\,\Theta_l^m(\theta) = ??, \qquad \cos\theta\,\Theta_l^m(\theta) = ?? \tag{1.9}$$

The calculation also reproduces the electric dipole selection rules along the way.

To proceed, I am going to review some properties of Legendre polynomials $P_l(\cos\theta)$ and the associated Legendre functions $P_l^m(\cos\theta)$, which ultimately give the unit normalized angular functions $\Theta_l^m(\theta)$. Especially, the approach will be to find the desired recurrence relations by manipulating the generating function for the associated Lengendre functions. Note that the only difference between the P_l^m and Θ_l^m is in their normalizations. The Θ_l^m are normalized to unity over $0 \le \theta \le \pi$, while the P_l^m (and the P_l) are normalized in a way so their value at $\theta = 0$ is convenient for matching boundary conditions.

2 Legendre Polynomials

This is not meant to be a reference on all properties of Legendre polynomials. I only want to dicuss their generating function, because it leads to the generating function for the associated Legendre functions. The Legendre polynomials apply to problems with azimuthal symmetry, and hence, no dependence on the quantum index m or on azimuthal angle ϕ. For reference, their differential equation is

$$(1-x^2)P_l''(x) - 2xP_l'(x) + l(l+1)P_l(x) = 0, \qquad x = \cos\theta. \tag{2.1}$$

This is the angular part of Laplace's equation when there is rotational symmetry about the z-axis. It is standard to write the argument as x, but really the argument is the projection onto the z-axis of a position on the unit sphere.

One can solve the equation by series expansion, etc. Eventually, one can show that the solutions are the Legendre polynomials, which can be expressed very compactly using Rodrigues' formula:

$$P_l(x) = \frac{1}{2^l\,l!}\,\frac{d^l}{dx^l}(x^2-1)^l. \tag{2.2}$$

The solutions are defined on the interval $-1 \le x \le +1$. They apply to any kind of problem where Laplace's equation is being solved, where the physical problem has rotational symmetry around the z-axis.

Probably there is a way to get the generating function for the Legendre polynomials directly from the differential equation. Instead, one can realize that the electric potential of a point electric charge on the z-axis, leads to the generating function. The unit electric charge is at position $z' = r'$ (it has $\theta' = 0$). The potential it generates is measured at radius r, with $r > r'$ assumed, at a polar angle θ from the z-axis. That potential is a solution to Laplace's equation and hence a solution to Legendre's equation. It is

$$V(\theta) = \frac{1}{|\mathbf{r}-\mathbf{r}'|} = \frac{1}{\sqrt{r^2+r'^2-2rr'\cos\theta}} = \frac{1}{r}\cdot\frac{1}{\sqrt{1+(r'/r)^2-2(r'/r)\cos\theta}} \tag{2.3}$$

It can be shown that the second factor is a sum over all of the Legendre polynomials. Thus, it is their generating function. With the definitions $t \equiv r'/r < 1$ and $\cos\theta = x$, the generating function is

$$\boxed{g(x,t) = \frac{1}{\sqrt{1-2xt+t^2}} = \sum_{l=0}^{\infty} t^l\, P_l(x)} \tag{2.4}$$

The generating function can be used to produce many relations between the Legendre polynomials. Or it could be used simply to reproduce them, by expanding it in a power series in t. The coefficient of t^l will give $P_l(x)$. For example do a few terms:

$$\begin{aligned} g(x,t) &= (1+t^2-2xt)^{-1/2} = 1 - \frac{1}{2}(t^2-2xt) + \frac{3}{8}(t^2-2xt)^2 - \frac{5}{16}(t^2-2xt)^3 ... \\ &= t^0(1) + t^1(x) + t^2\left(-\frac{1}{2}+\frac{3}{2}x^2\right) + t^3\left(-\frac{3}{2}x+\frac{5}{2}x^3\right) + ... \end{aligned} \tag{2.5}$$

from which we can see the first four Legendre polynomials inside the parenthesis. They are all normalized to give the value $P_l(1) = 1$.

Another feature of the generating function is that it can give different recurrence relations, depending on how it is manipulated. One way is to take the derivative w.r.t. t on both sides of (2.4).

$$\frac{\partial g}{\partial t} = \frac{-\frac{1}{2}(2t-2x)}{[1-2xt+t^2]^{3/2}} = \sum_l lt^{l-1}\, P_l(x) \tag{2.6}$$

But that reproduces the gen func on LHS, multiplied by $x-t$ and divived by $1-2xt+t^2$, and so

$$(x-t)g(x,t) = (x-t)\sum_l t^l\, P_l = \left[1-2xt+t^2\right]\sum_l lt^{l-1}\, P_l \tag{2.7}$$

Now rearrange by shifting indeces so that all terms have the same power of t:

$$\sum_l t^l\, \{xP_l - P_{l-1} - (l+1)P_{l+1} + 2xlP_l - (l-1)P_{l-1}\} = 0. \tag{2.8}$$

The coefficient of each power of t must vanish, so there results Bonnet's recursion formula,

$$\boxed{lP_{l-1} - (2l+1)xP_l + (l+1)P_{l+1} = 0} \tag{2.9}$$

It can be written as a recurrence:

$$\boxed{P_{l+1} = \frac{1}{l+1}\left[(2l+1)xP_l - lP_{l-1}\right]} \tag{2.10}$$

For instance, use it with $l = 1$ to get P_2 from $P_1 = x$ and $P_0 = 1$, to check it:

$$P_2(x) = \frac{1}{2}\,(3x\cdot x - 1) \tag{2.11}$$

and it can be seen that the result is correct. From this, all the $P_l(x)$ can be generated. (This iteration could even have started with $l = 0$, try it.) By doing other manipulations of $g(x,t)$, like taking more derivatives, derivatives w.r.t. x, multiplying by powers of t before doing derivatives, etc., many other relations can be developed.

Try another manipulation: derivative w.r.t. x.

$$\frac{\partial g}{\partial x} = \frac{-\frac{1}{2}(-2t)}{[1-2xt+t^2]^{3/2}} = \sum_l t^l\, P_l'(x) \tag{2.12}$$

Again some rearrangements to get all terms with the same power of t:

$$t\sum_l t^l\, P_l = [1-2xt+t^2]\sum_l t^l\, P_l' = 0 \tag{2.13}$$

$$\sum_l t^l\, \left\{P_{l-1} - P_l' + 2xP_{l-1}' - P_{l-2}'\right\} = 0 \tag{2.14}$$

Then shifting l up by one gives

$$P_{l-1}' - 2xP_l' - P_l + P_{l+1}' = 0 \tag{2.15}$$

That's not pretty, but try to combine it with the first recurrence relation, by taking the derivative of (2.9):

$$\begin{aligned} & lP_{l-1}' - (2l+1)(P_l + xP_l') + (l+1)P_{l+1}' = 0 \\ \Rightarrow \quad & xP_l' = -P_l + \frac{1}{2l+1}\left[lP_{l-1}' + (l+1)P_{l+1}'\right]. \end{aligned} \tag{2.16}$$

Then using this in (2.15) gives

$$\begin{aligned} P_{l-1}' - 2\left(-P_l + \frac{1}{2l+1}\left[lP_{l-1}' + (l+1)P_{l+1}'\right]\right) - P_l + P_{l+1}' &= 0 \\ \Rightarrow \quad P_{l-1}' + (2l+1)P_l - P_{l+1}' &= 0 \end{aligned} \tag{2.17}$$

Sometimes this last relation is written as

$$\boxed{P_l = \frac{1}{2l+1}\left(P_{l+1}' - P_{l-1}'\right)} \tag{2.18}$$

which is a useful form to have if the integral of $P_l(x)$ is desired, because it makes the integration trivial!

3 Associated Legendre Functions

Now onto the main topic. It turns out that the more general version of Laplace's equation, without the assumption of azimuthal symmetry, is the associated Legendre equation,

$$(1-x^2)P''(x) - 2xP'(x) + \left[l(l+1) - \frac{m^2}{1-x^2}\right]P(x) = 0. \tag{3.1}$$

This equation governs the behaviour of the $\Theta(\theta)$ functions. Magically, this equation can be obtained from the regular Legendre equation (2.1) by differentiation m times with respect to x. You could fill in the details, but it helps to know the Leibnitz binomial formula for differentiation of a product m times:

$$\frac{d^m}{dx^m}[A(x)B(x)] = \sum_{s=0}^{m}\left(\begin{array}{c} m \\ s \end{array}\right)\frac{d^s}{dx^s}A(x)\;\frac{d^{m-s}}{dx^{m-s}}B(x). \qquad \left(\begin{array}{c} m \\ s \end{array}\right) = \frac{m!}{s!(m-s)!}. \tag{3.2}$$

For example, the middle term in the Legendre equation requires only $s=0$ and $s=1$ in this sum, and it becomes

$$\frac{d^m}{dx^m}[xP_l'] = xP_l^{(m+1)} + mP_l^{(m)}, \qquad P_l^{(m)} = \frac{d^m}{dx^m}P_l(x). \tag{3.3}$$

Superscripts within parenthesis indicate order of the derivative. Next, one needs terms with $s = 0, 1, 2$ for the first term in Legendre's equation (maximum times $1-x^2$ can be differentiated), and that gives

$$\frac{d^m}{dx^m}[(1-x^2)P_l''] = (1-x^2)P_l^{(m+2)} - 2mxP_l^{(m+1)} - m(m-1)P_l^{(m)} \tag{3.4}$$

Combining all the terms from differentiating m times, Legendre's equation has become

$$(1-x^2)P_l^{(m+2)} - 2mxP_l^{(m+1)} - m(m-1)P_l^{(m)} - 2\left(xP_l^{(m+1)} + mP_l^{(m)}\right) + l(l+1)P_l^{(m)} =$$
$$(1-x^2)P_l^{(m+2)} - 2(m+1)xP_l^{(m+1)} + [l(l+1) - m(m+1)]P_l^{(m)} = 0 \tag{3.5}$$

Due to the $m+1$ on the second term it is not in self-adjoint form. But it *is* a differential equation for the derivative of a Legendre polynomial, $y(x) = P_l^{(m)}(x)$. Further, it is clear that the number of derivatives cannot be more than l. Try to put the equation in self-adjoint form by multiplying by $(1-x^2)^m$:

$$\frac{d}{dx}\left[(1-x^2)^{m+1}\frac{dy}{dx}\right] + (l-m)(l+m+1)(1-x^2)^m y(x) = 0. \tag{3.6}$$

That doesn't quite work, yet, one sees that instead the change to $u(x) = (1-x^2)^{m/2}y(x)$, does lead to a self-adjoint equation, which is the associated Legendre equation (details left as an excercise for you):

$$\frac{d}{dx}\left[(1-x^2)\frac{du}{dx}\right] + \left[l(l+1) - \frac{m^2}{1-x^2}\right]u(x) = 0. \tag{3.7}$$

Due to the way this was constructed from the Legendre equation, its solutions are already known! They are m^{th} derivatives of the Legendre polynomials, multiplied by the adjustment factor $(1-x^2)^{m/2}$. These are the **associated Legendre functions**, where now a superscript m is used to denote them and indicate the number of derivatives that were used,

$$P_l^m(x) \equiv (1-x^2)^{m/2}\,\frac{d^m}{dx^m}P_l(x). \tag{3.8}$$

Since there are formulas for the Legendre polynomials, these functions can be evaluated using this expression for the general case.

Just do a check of the results it gives, for example, for $l=2$. Start from $P_2(x) = \frac{1}{2}(3x^2-1)$. At most, one can do two derivatves w.r.t. x. Scaling by $(1-x^2)^{m/2}$, one gets

$$P_2^0(x) = P_2(x) = \frac{1}{2}(3x^2-1), \tag{3.9}$$
$$P_2^1(x) = (1-x^2)^{1/2}\,P_2'(x) = \sqrt{1-x^2}\,\frac{1}{2}(6x) = 3x\sqrt{1-x^2}, \tag{3.10}$$
$$P_2^2(x) = (1-x^2)^{2/2}\,P_2''(x) = (1-x^2)\,\frac{1}{2}(6) = 3(1-x^2). \tag{3.11}$$

There is also a definition for negative values of m, which only makes sense as an extension of the above by Rodrigues formula for the derivative (the differential equation only depends on m^2). That definition is

$$P_l^{-m}(x) = (-1)^m\frac{(l-m)!}{(l+m)!}P_l^m(x) \tag{3.12}$$

By this normalization, things work well in various recursion relations. But these really aren't significantly different than the functions at positive m. One has for $l=2$,

$$P_2^{-1}(x) = -1\frac{(2-1)!}{(2+1)!}P_2^1(x) = -\frac{x}{2}\sqrt{1-x^2}, \tag{3.13}$$
$$P_2^{-2}(x) = +1\frac{(2-2)!}{(2+2)!}P_2^2(x) = \frac{1}{8}(1-x^2), \tag{3.14}$$
$$\tag{3.15}$$

When Rodrigues' formula for the Legendre polynomials is combined with the above for the associated functions, one also has an interesting result:

$$P_l^m(x) = \frac{1}{2^l\,l!}(1-x^2)^{m/2}\frac{d^{l+m}}{dx^{l+m}}(x^2-1)^l \tag{3.16}$$

This formula is useful for normalizing these functions. Becausethey come from a Sturn-Liouville problem, the eigenfunctions for different eigenvalues l are orthogonal. After some calculations, one can show the main orthogonality condition,

$$\int_{-1}^{+1} dx P_l^m(x)\, P_{l'}^m(x) = \left(\frac{2}{2l+1}\right) \frac{(l+m)!}{(l-m)!}\, \delta_{ll'}. \tag{3.17}$$

This will be useful for the overall normalization of the spherical harmonics and their polar angle dependent parts, $\Theta_l^m(\theta)$.

Next, I want to develop the generating function for the $P_l^m(x)$ and use it to find the interesting properties.

3.1 Generating function for the $P_l^m(x)$

It is easy to get the generating function because it comes from the generating function for the Legendre polynomials, differentiated m times, then modified by the factor $(1-x^2)^{m/2}$. Start from

$$g_L(x,t) = \frac{1}{\sqrt{1-2xt+t^2}} = \sum_{l=0}^{\infty} t^l\, P_l(x) \tag{3.18}$$

Do a few derivatives to see the pattern,

$$\begin{aligned}
\frac{dg_L}{dx} &= [1-2xt+t^2]^{-3/2}\left(-\frac{1}{2}\right)(-2t) \\
\frac{d^2g_L}{dx^2} &= [1-2xt+t^2]^{-5/2}\left(-\frac{1}{2}\right)\left(-\frac{3}{2}\right)(-2t)^2 \\
\frac{d^3g_L}{dx^3} &= [1-2xt+t^2]^{-7/2}\left(-\frac{1}{2}\right)\left(-\frac{3}{2}\right)\left(-\frac{5}{2}\right)(-2t)^3 \\
\frac{d^mg_L}{dx^m} &= [1-2xt+t^2]^{-m-\frac{1}{2}}\ (2m-1)!!\ t^m.
\end{aligned} \tag{3.19}$$

Then the generating function for the associated Legendre functions at azimuthal quantum number m is

$$\boxed{g(x,t) = (1-x^2)^{m/2}\, \frac{d^mg_L}{dx^m} = (2m-1)!!\ \frac{(1-x^2)^{m/2}\ t^m}{[1-2xt+t^2]^{m+1/2}} = \sum_{l=0}^{\infty} t^l\, P_l^m(x).} \tag{3.20}$$

I still call it $g(x,t)$ so equations that follow are not even further complicated by extra symbols. In principle we could expand the LHS in powers of t, and the coefficient of t^l will be the function $P_l^m(x)$. That would be a hard way to learn about the $P_l^m(x)$. Instead, I'll look at different ways to take derivatives, and avoid any power series expansions.

3.2 A first recurrence relation for $P_l^m(x)$, at $\Delta m = 0$

We are looking for relations involving the functions at closely spaced l, possible for the same m or nearby m's. Especially, we want relationships where one term in the equation contains either xP_l^m or $\sqrt{1-x^2}P_l^m$, where $x = \cos\theta$, because these will be useful in the dipole matrix elements. One of the simplest things to try is to move the t^m in (3.20) to the opposite side, and differentiate w.r.t. t. To help, denote $(2m-1)!!\ (1-x^2)^{m/2} = c_m$ as this does not change under these operations. One has

$$\begin{aligned}
\frac{d}{dt}\cdot \qquad & \frac{c_m}{[1-2xt+t^2]^{m+1/2}} = \sum_l t^{l-m}\, P_l^m(x), \\
\Rightarrow \qquad & \frac{c_m(m+1/2)(2x-2t)}{[1-2xt+t^2]^{m+3/2}} = \sum_l (l-m)t^{l-m-1}\, P_l^m(x), \\
\Rightarrow \qquad & (2m+1)(x-t)\frac{c_m t^m}{[1-2xt+t^2]^{m+1/2}} = [1-2xt+t^2]\sum_l (l-m)t^{l-1}\, P_l^m(x), \\
\Rightarrow \qquad & (2m+1)(x-t)\sum_l t^l\, P_l^m = \sum_l [1-2xt+t^2](l-m)t^{l-1}\, P_l^m, \qquad (3.21)
\end{aligned}$$

As before for the Legendre polynomial relations, arrange so all terms have the same power of t, by shifting indeces,

$$\begin{aligned}
\sum_l t^l \left\{(2m+1)xP_l^m - (2m+1)P_{l-1}^m\right\} \quad &= \\
& \sum_l t^l \Big\{(l+1-m)P_{l+1}^m \quad - \quad 2x(l-m)P_l^m + (l-1-m)P_{l-1}^m\Big\} \qquad (3.22)
\end{aligned}$$

Collecting some common terms, the coefficient of each power of t gives the first recurrence relation, for functions all at the same azimuthal quantum number,

$$\boxed{(2l+1)x\, P_l^m(x) = (l+m)P_{l-1}^m(x) + (l-m+1)P_{l+1}^m(x).} \qquad (3.23)$$

Since $x = \cos\theta$, this will give the selectrion rule for transitions that involve the operator $\hat{r}_z$. Because the m's are the same on both sides of this equation, those are the type of transitions that conserve azimuthal quantum number. Or, they obey the selection rule $\Delta m = 0$. In addition to this, oe also sees that the original state at l (on the LHS) gets connected only to states at $l \pm 1$ (on the RHS). These selection rules will be clarified more so below.

3.3 A second recurrence relation for $P_l^m(x)$, at $\Delta m = +1$

Now I want to get a relation which relates the functions at different values of m. To do that, the operations on the generating function have to be done in a different order. In this case, first rearrange the expression (3.20), then differentiate w.r.t. t. Again, the factor $(2m-1)!!\,(1-x^2)^{m/2} = c_m$ does not change during these operations.

$$\begin{aligned}
g(x,t) \quad &= \quad \frac{c_m t^m}{[1-2xt+t^2]^{m+1/2}} = \sum_l t^l\, P_l^m(x), \qquad (3.24) \\
c_m t^m \quad &= \quad \sum_l [1-2xt+t^2]^{m+1/2}\, t^l\, P_l^m(x), \quad \Leftarrow \text{do } \frac{d}{dt} \\
c_m m t^{m-1} \quad &= \quad \sum_l \Big\{(m+\frac{1}{2})[1-2xt+t^2]^{m-1/2}\,(2t-2x)t^l + [1-2xt+t^2]^{m+1/2}\, l t^{l-1}\Big\}P_l^m(x) \\
& \frac{m c_m t^{m-1}}{[1-2xt+t^2]^{m-1/2}} = \sum_l \Big\{(2m+1)(t-x)t^l + [1-2xt+t^2] l t^{l-1}\Big\}P_l^m(x)
\end{aligned}$$

At this point, the LHS has the generating function (almost) at m shifted downward by 1. It only needs the c_m part corrected to be c_{m-1}, but that is easy,

$$\begin{aligned}
c_m \quad &= \quad (2m-1)!!\,(1-x^2)^{m/2} \\
&= \quad (2m-1)(1-x^2)^{1/2}\,\Big[(2m-3)!!\,(1-x^2)^{(m-1)/2}\Big] \\
&= \quad (2m-1)(1-x^2)^{1/2}\, c_{m-1}. \qquad (3.25)
\end{aligned}$$

With that used in the LHS, there results

$$m(2m-1)(1-x^2)^{1/2}\sum_l t^l\, P_l^{m-1} = \sum_l \left\{(2m+1)(t-x)t^l + [1-2xt+t^2]lt^{l-1}\right\}P_l^m(x) \quad (3.26)$$

The usual procedure of getting all powers of t the same gives

$$m(2m-1)\sqrt{1-x^2}P_l^{m-1} = (2m+1)P_{l-1}^m - (2m+1)xP_l^m + (l+1)P_{l+1}^m - 2lxP_l^m + (l-1)P_{l-1}^m \quad (3.27)$$

$$m(2m-1)\sqrt{1-x^2}P_l^{m-1} = (2m+l)P_{l-1}^m - (2m+2l+1)xP_l^m + (l+1)P_{l+1}^m \quad (3.28)$$

OK, it doesn't look real promising, but the term with xP_l^m on the RHS can be substituted from the first recurrence relation, to give

$$\begin{aligned}
\text{RHS} &= (2m+l)P_{l-1}^m + (l+1)P_{l+1}^m \\
&\quad -(2m+2l+1)\frac{1}{2l+1}\left[(l+m)P_{l-1}^m(x) + (l-m+1)P_{l+1}^m(x)\right], \\
(2l+1)\times\text{RHS} &= [(2l+1)(2m+l) - (2l+1+2m)(l+m)]P_{l-1}^m \\
&\quad +[(2l+1)(l+1) - (2l+1+2m)(l-m+1)]P_{l+1}^m \\
&= -m(2m-1)P_{l-1}^m + m(2m-1)P_{l+1}^m. \qquad (3.29)
\end{aligned}$$

After all of this a remarkably simple relation comes out, due to the cancellation of the factor $m(2m-1)$,

$$\boxed{(2l+1)\sqrt{1-x^2}\,P_l^{m-1}(m) = P_{l+1}^m(x) - P_{l-1}^m(x).} \quad (3.30)$$

Now since $\sqrt{1-x^2} = \sin\theta$, this gives a relation that is useful for the transition matrix elements of $\hat{r}_x$ and $\hat{r}_y$, where the azimuthal quantum number increases by 1. Again, the selection rule in magntiude of angular momentum is that the original state at l is connected only to states at $l \pm 1$. Transitions changing by more than 1 would have a zero matrix element.

3.4 A third recurrence relation for $P_l^m(x)$, at $\Delta m = -1$

One also can find another relation that corresponds to the azimuthal quantum number decreasing. For some reason, this relation seems harder to obtain. Perhaps I do not have the simplest derivation! I want some manipulations of $g(x,t)$ that will cause the power $m+\frac{1}{2}$ in its denominator to change to $m+\frac{3}{2}$, and then rewrite the result in terms of sums of P_l^{m+1}. At the same time, I also want an extra factor of $\sin\theta = \sqrt{1-x^2}$ to appear on that same side of the equation.

Here is the way I found to do this: (1) derivative of g w.r.t. t. (2) rescale by $[1-2xt+t^2]^{m+1}$ on both sides. (3) do another derivative w.r.t. t. Let's see what happens, starting after the first derivative, which is the same as for the first recurrence relation:

$$\frac{(2m+1)(x-t)c_m}{[1-2xt+t^2]^{m+3/2}} = \sum_l (l-m)t^{l-m-1}\,P_l^m(x), \quad \leftarrow \text{after } \frac{d}{dt} \quad (3.31)$$

$$\frac{(2m+1)(x-t)c_m}{[1-2xt+t^2]^{1/2}} = [1-2xt+t^2]^{m+1}\sum_l (l-m)t^{l-m-1}\,P_l^m(x), \quad \leftarrow \text{do another } \frac{d}{dt}$$

Note what happens on the LHS, which is why I did it this way,

$$\begin{aligned}
\frac{d}{dt}\frac{x-t}{[1-2xt+t^2]^{1/2}} &= -\frac{1}{[1-2xt+t^2]^{1/2}} - \frac{\frac{1}{2}(x-t)(2t-2x)}{[1-2xt+t^2]^{3/2}} \\
&= -\frac{1-2xt+t^2-t^2-x^x+2xt}{[1-2xt+t^2]^{3/2}} = -\frac{1-x^2}{[1-2xt+t^2]^{3/2}} \qquad (3.32)
\end{aligned}$$

The operation produced a factor of $(1-x^2)$ and raised the power in the denominator, which is exactly what I wanted. With this, the LHS will be found proportional to a sum of P_l^{m+1}. Again, one needs to see how c_m gets changed into c_{m+1}:

$$\begin{aligned}
c_m &= (2m-1)!!\,(1-x^2)^{m/2} \\
(2m+1)(1-x^2)c_m &= (2m+1)(2m-1)!!\,(1-x^2)^{(m+1)/2+1/2} \\
&= (2m+1)!!\,(1-x^2)^{(m+1)/2}\sqrt{1-x^2} = c_{m+1}\sqrt{1-x^2}. && (3.33) \\
\frac{d}{dt}\cdot \text{LHS} &= -\frac{c_{m+1}\sqrt{1-x^2}}{[1-2xt+t^2]^{3/2}}. && (3.34)
\end{aligned}$$

Now for the RHS of (3.31),

$$\begin{aligned}
\frac{d}{dt}\cdot \text{RHS} &= \sum_l (l-m)\Big\{(l-m-1)t^{l-m-2}[1-2xt+t^2]^{m+1} \\
&\quad + t^{l-m-1}(m+1)(2t-2x)[1-2xt+t^2]^m\Big\}P_l^m
\end{aligned}$$

$$\frac{d}{dt}\cdot \text{RHS} = t^{-m-1}[1-2xt+t^2]^m\sum_l (l-m)\Big\{(l-m-1)[1-2xt+t^2]t^{l-1}+2(m+1)(t-x)t^l\Big\}P_l^m \quad (3.35)$$

Now moving those factors in front of the sum to the LHS term, it becomes the generating function at $m+1$. There results from these manipulations,

$$-\sqrt{1-x^2}\frac{c_{m+1}\sqrt{1-x^2}}{[1-2xt+t^2]^{m+3/2}} = -\sqrt{1-x^2}\sum_l t^l\, P_l^{m+1} =$$

$$= \sum_l (l-m)\Big\{(l-m-1)[1-2xt+t^2]t^{l-1}+2(m+1)(t-x)t^l\Big\}P_l^m \quad (3.36)$$

Then looking at the coefficient of t^l gives a desired relation,

$$\begin{aligned}
-\sqrt{1-x^2}P_l^{m+1} &= (l+1-m)(l-m)P_{l+1}^m - 2x(l-m)[(l-m-1)+(m+1)]P_l^m \\
&+ (l-1-m)[(l-2-m)+2(m+1)]P_{l-1}^m
\end{aligned}$$

$$-\sqrt{1-x^2}P_l^{m+1} = (l+1-m)(l-m)P_{l+1}^m - 2xl(l-m)P_l^m + (l-1-m)(l+m)P_{l-1}^m. \quad (3.37)$$

That's a good result, because it gives a higher m in terms of three lower m's. But this raw result can be improved, by combining it with the first recurrence formula (3.23) to get rid of the term with xP_l^m on the RHS:

$$\begin{aligned}
-\sqrt{1-x^2}P_l^{m+1} &= (l+1-m)(l-m)P_{l+1}^m \\
&- 2l(l-m)\frac{1}{2l+1}\left[(l+m)P_{l-1}^m+(l-m+1)P_{l+1}^m\right] \\
&+ (l-1-m)(l+m)P_{l-1}^m \\
&= \frac{l+m}{2l+1}[(2l+1)(l-1-m)-2l(l-m)]P_{l-1}^m \\
&+ \frac{l-m}{2l+1}[(2l+1)(l+1-m)-2l(l-m+1)]P_{l+1}^m \\
&= \frac{1}{2l+1}\left\{(l+m)(-l-1-m)P_{l-1}^m+(l-m)(l-m+1)P_{l+1}^m\right\} && (3.38)
\end{aligned}$$

So finally this gives a good recurrence relation,

$$\boxed{(2l+1)\sqrt{1-x^2}\,P_l^{m+1}(x) = (l+m)(l+m+1)P_{l-1}^m(x)-(l-m)(l-m+1)P_{l+1}^m(x).} \quad (3.39)$$

That was a little tough. And the result isn't real pretty. But it shows another relation connecting $\sin\theta = \sqrt{1-x^2}$ with in this case, a decrease in the m index. It corresponds to being important for the electric dipole transitions where $\Delta m = -1$.

3.5 Other recurrence relations?

I found only the above 3 recurrence relations, because we know the electric dipole selection rules are $\Delta m = 0, \pm 1$, and these above relations suffice. But it is clear more recurrence relations can be found, that could involve $sin^2\theta$ and $\cos^2\theta$ on the LHS, making connections with $\Delta m = \pm 2$. Different manipulations of the generating function (as with more derivatives w.r.t. t) can be used to get these relations, that would be good for fiding higher order electric and magnetic multipoles. Based on the last relation (3.39) just found, one needs to differentiate w.r.t. t and move the factor $[1-2xt+t^2]$ and its powers around to get what you want. Left as an excercise for the reader!

4 Normalized angular functions $\Theta_l^m(\theta)$ and spherical harmonics $Y_l^m(x,\phi)$

The normalization (3.17) for the associated Legendre functions has been given earlier. It can be used to produce the $\Theta_l^m(\theta)$ functions, such that they are unit normalized over the range of the polar angle θ, or equivalently, over $x = \cos\theta$. Then these have to be defined as

$$\Theta_l^m(x) = \sqrt{\left(\frac{2l+1}{2}\right)\frac{(l-m)!}{(l+m)!}}\, P_l^m(x), \tag{4.1}$$

so that there normalization integrals (for the same values of m) are

$$\int_{-1}^{+1} dx\ \Theta_l^m(x)\,\Theta_{l'}^m(x) = \delta_{ll'}. \tag{4.2}$$

In addition, the spherical harmonics are just the extension of these, with the azimuthal angular dependence $\Phi_m(\phi)$ included,

$$Y_l^m(x,\phi) = \sqrt{\left(\frac{2l+1}{4\pi}\right)\frac{(l-m)!}{(l+m)!}}\, P_l^m(x)\, e^{im\phi}, \qquad \text{from} \quad Y_l^m(x,\phi) = \Theta_l^m(x)\frac{e^{im\phi}}{\sqrt{2\pi}}. \tag{4.3}$$

The spherical harmonics, as constructed, obviously have unit normalization over the surface of a unit sphere. Then based on the recurrence relations found for the P_l^m, they also have similar recurrence relations, as do the $\Theta_l^m(\theta)$.

4.1 Recurrence relations for $\Theta_l^m(\theta)$ functions

One can use the definitions of these functions and combine with the first recurrence relation (3.23) for the associated Legendre functions. It helps to have the definition turned around:

$$P_l^m(x) = \sqrt{\left(\frac{2}{2l+1}\right)\frac{(l+m)!}{(l-m)!}}\, \Theta_l^m(x). \tag{4.4}$$

Then substituting into the recurrence gives

$$\begin{aligned}(2l+1)x\sqrt{\frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}}\,\Theta_l^m &= (l+m)\sqrt{\frac{2}{2(l-1)+1}\frac{(l-1+m)!}{(l-1-m)!}}\,\Theta_{l-1}^m \\ &+ (l-m+1)\sqrt{\frac{2}{2(l+1)+1}\frac{(l+1+m)!}{(l+1-m)!}}\,\Theta_{l+1}^m\end{aligned} \tag{4.5}$$

Cancellations of common terms leads to

$$\boxed{x\,\Theta_l^m = \sqrt{\frac{(l-m+1)(l+m+1)}{(2l+1)(2l+3)}}\,\Theta_{l+1}^m + \sqrt{\frac{(l-m)(l+m)}{(2l-1)(2l+1)}}\,\Theta_{l-1}^m} \tag{4.6}$$

Do the same for the second recurrence relation:

$$
\begin{aligned}
(2l+1)\sqrt{1-x^2}\sqrt{\frac{2}{2l+1}\frac{(l+m-1)!}{(l-(m-1))!}}\,\Theta_l^{m-1} &= \sqrt{\frac{2}{2(l+1)+1}\frac{(l+1+m)!}{(l+1-m)!}}\,\Theta_{l+1}^m \\
&\quad -\sqrt{\frac{2}{2(l-1)+1}\frac{(l-1+m)!}{(l-1-m)!}}\,\Theta_{l-1}^m
\end{aligned}
\tag{4.7}
$$

It reduces to

$$
\boxed{\sqrt{1-x^2}\,\Theta_l^{m-1} = \sqrt{\frac{(l+m)(l+m+1)}{(2l+1)(2l+3)}}\,\Theta_{l+1}^m - \sqrt{\frac{(l-m)(l-m+1)}{(2l-1)(2l+1)}}\,\Theta_{l-1}^m}
\tag{4.8}
$$

And, do the same for the third recurrence relation,

$$
\begin{aligned}
&(2l+1)\sqrt{1-x^2}\sqrt{\frac{2}{2l+1}\frac{(l+m+1)!}{(l-(m+1))!}}\,\Theta_l^{m+1} \\
&= (l+m)(l+m+1)\sqrt{\frac{2}{2(l-1)+1}\frac{(l-1+m)!}{(l-1-m)!}}\,\Theta_{l-1}^m \\
&-(l-m)(l-m+1)\sqrt{\frac{2}{2(l+1)+1}\frac{(l+1+m)!}{(l+1-m)!}}\,\Theta_{l+1}^m
\end{aligned}
\tag{4.9}
$$

Carefully do the cancellations, leads to

$$
\boxed{\sqrt{1-x^2}\,\Theta_l^{m+1} = -\sqrt{\frac{(l-m)(l-m+1)}{(2l+1)(2l+3)}}\,\Theta_{l+1}^m + \sqrt{\frac{(l+m)(l+m+1)}{(2l-1)(2l+1)}}\,\Theta_{l-1}^m}
\tag{4.10}
$$

That is very similar to the previous result, but only with the overall sign reversed and the m's negated in the factors on the RHS.

4.2 Recurrences for the spherical harmonics

These are almost the same as for the associated Legendre functions. The only difference is to include the dependences on the azimuthal angles. That means multiply the three recurrence relations by $e^{im\phi}$ and adjust the indeces appropriately. The first relation is identical to that for the Θ_l^m,

$$
\boxed{x\,Y_l^m = \sqrt{\frac{(l-m+1)(l+m+1)}{(2l+1)(2l+3)}}\,Y_{l+1}^m + \sqrt{\frac{(l-m)(l+m)}{(2l-1)(2l+1)}}\,Y_{l-1}^m}
\tag{4.11}
$$

The second relation has some shifting with applying $\Theta_l^m = Y_l^m\,\sqrt{2\pi}e^{-im\phi}$,

$$
\boxed{\sqrt{1-x^2}\,e^{i\phi}\,Y_l^{m-1} = \sqrt{\frac{(l+m)(l+m+1)}{(2l+1)(2l+3)}}\,Y_{l+1}^m - \sqrt{\frac{(l-m)(l-m+1)}{(2l-1)(2l+1)}}\,Y_{l-1}^m}
\tag{4.12}
$$

Finally the third relation gets a similar effect, in the opposite sense,

$$
\boxed{\sqrt{1-x^2}\,,e^{-i\phi}Y_l^{m+1} = -\sqrt{\frac{(l-m)(l-m+1)}{(2l+1)(2l+3)}}\,Y_{l+1}^m + \sqrt{\frac{(l+m)(l+m+1)}{(2l-1)(2l+1)}}\,Y_{l-1}^m}
\tag{4.13}
$$

It's obvious in these last two relations, the extra factor of $e^{\pm i\phi}$ causes the azimuthal dependences to match on the two sides of the equations.

4.2.1 Quality check: Do they work?

As a check, consider the effects of this operations on the $l = 1$ spherical harmonics, and see the expression are valid. Use them first with $l = 1$ and $m = 0$. The first gives

$$\cos\theta \cdot Y_1^0 = \sqrt{\frac{(2)(2)}{(3)(5)}} Y_2^0 + \sqrt{\frac{(1)(1)}{(1)(3)}} Y_0^0 = \sqrt{\frac{4}{15}} Y_2^0 + \sqrt{\frac{1}{3}} Y_0^0. \tag{4.14}$$

Check by the definitions $Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$ and $Y_2^0 = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1)$ and $Y_0^0 = \sqrt{\frac{1}{4\pi}}$. These give $\cos^2\theta = \frac{1}{3}(\sqrt{\frac{16\pi}{5}}Y_2^0 + 1)$, and

$$\cos\theta \cdot Y_1^0 = \cos\theta \cdot \sqrt{\frac{3}{4\pi}}\cos\theta = \sqrt{\frac{3}{4\pi}}\frac{1}{3}\left(\sqrt{\frac{16\pi}{5}}Y_2^0 + 1\right) = \sqrt{\frac{4}{15}} Y_2^0 + \sqrt{\frac{1}{3}} Y_0^0. \tag{4.15}$$

which is correct. Just try one more, the second recurrence relation. There, apply it to $Y_1^{-1} = \sqrt{\frac{3}{8\pi}} e^{-i\phi}\sin\theta$, then it gives

$$\sin\theta \cdot e^{i\phi} Y_1^{-1} = \sqrt{\frac{(1)(2)}{(3)(5)}} Y_2^0 - \sqrt{\frac{(1)(2)}{1)(3)}} Y_0^0 = \sqrt{\frac{2}{15}} Y_2^0 - \sqrt{\frac{2}{3}} Y_0^0 \tag{4.16}$$

For comparison, the known result is

$$\sin\theta \cdot e^{i\phi}\sqrt{\frac{3}{8\pi}} e^{-i\phi}\sin\theta = \sqrt{\frac{3}{8\pi}}(1-\cos^2\theta) = \sqrt{\frac{3}{8\pi}}\frac{1}{3}\left(2 - \sqrt{\frac{16\pi}{5}}Y_2^0\right) \tag{4.17}$$

This actually gives the negative of that from the recurrence. The reason is simple. The usual definition of spherical harmonics in physics includes the Condon-Shortley phase of $(-1)^m$. I have not included it in these recurrence relations. Once it would be included, the second two recurrence relations, where m changes, will get a minus sign, say, added to the RHS. This is really of no great physical importance, just as long as you know ifthat phase is included or not. It is simple to include at the end, however, probably unnecessary since matrix elements tend to get squared to find transition probabilities.

5 Transition matrix elements

Let me conclude here by evaluating the possible transition matrix elements, between an initial state at l, m and a final state at l', m'. It is clear the number of nonzero matrix elements are limited by the selection rules, $\Delta l = \pm 1$, $\Delta m = 0, \pm 1$. Even so, there are quite a few possibilities when the different Cartesian components are also accounted for. In fact, let me account for Cartesian components of $\hat{r}$, and for matrix elements of circular polarization states of the operator.

The approach is now simple. Consider $\hat{r}_x$ and its matrix elements. It requires $\Delta m = \pm 1$. Use (4.12) when $\Delta m = +1$ and use (4.13) when $\Delta m = -1$. Here the Condon-Shortley phase factor of -1 is not included in these expressions. A shift of m is needed to apply those expressions. Then we see that, due to the orthonormalization of the spherical harmonics, integrals of the form wanted are easy. For $\hat{r}_x = \sin\theta\cos\phi$,

$$\langle l'm'|\hat{r}_x|lm\rangle = \frac{1}{2}\int d\Omega\; Y_{l'}^{m'*}(\Omega)\sin\theta(e^{i\phi} + e^{-i\phi})Y_l^m(\Omega) \tag{5.1}$$

Doing the appropriate shifting of m, the recurrrences give

$$\langle l+1, m+1|\hat{r}_x|lm\rangle = +\frac{1}{2}\sqrt{\frac{(l+m+1)(l+m+2)}{(2l+1)(2l+3)}} \qquad \Delta l = +1,\ \Delta m = +1. \tag{5.2}$$

$$\langle l-1,m+1|\hat{r}_x|lm\rangle = -\frac{1}{2}\sqrt{\frac{(l-m-1)(l-m)}{(2l-1)(2l+1)}} \qquad \Delta l=-1,\ \Delta m=+1. \tag{5.3}$$

$$\langle l+1,m-1|\hat{r}_x|lm\rangle = -\frac{1}{2}\sqrt{\frac{(l-m+1)(l-m+2)}{(2l+1)(2l+3)}} \qquad \Delta l=+1,\ \Delta m=-1. \tag{5.4}$$

$$\langle l-1,m-1|\hat{r}_x|lm\rangle = +\frac{1}{2}\sqrt{\frac{(l+m-1)(l+m)}{(2l-1)(2l+1)}} \qquad \Delta l=-1,\ \Delta m=-1. \tag{5.5}$$

Consider next the results for $\hat{r}_y = \sin\theta\sin\phi$.

$$\langle l'm'|\hat{r}_y|lm\rangle = \frac{1}{2i}\int d\Omega\ Y_{l'}^{m'*}(\Omega)\sin\theta(e^{i\phi}-e^{-i\phi})Y_l^m(\Omega) \tag{5.6}$$

These are equal to the results for $\hat{r}_x$ scaled by factors of $\mp i$ for $\Delta m = \pm 1$, respectively:

$$\langle l+1,m+1|\hat{r}_y|lm\rangle = -\frac{i}{2}\sqrt{\frac{(l+m+1)(l+m+2)}{(2l+1)(2l+3)}} \qquad \Delta l=+1,\ \Delta m=+1. \tag{5.7}$$

$$\langle l-1,m+1|\hat{r}_y|lm\rangle = +\frac{i}{2}\sqrt{\frac{(l-m-1)(l-m)}{(2l-1)(2l+1)}} \qquad \Delta l=-1,\ \Delta m=+1. \tag{5.8}$$

$$\langle l+1,m-1|\hat{r}_y|lm\rangle = -\frac{i}{2}\sqrt{\frac{(l-m+1)(l-m+2)}{(2l+1)(2l+3)}} \qquad \Delta l=+1,\ \Delta m=-1. \tag{5.9}$$

$$\langle l-1,m-1|\hat{r}_y|lm\rangle = +\frac{i}{2}\sqrt{\frac{(l+m-1)(l+m)}{(2l-1)(2l+1)}} \qquad \Delta l=-1,\ \Delta m=-1. \tag{5.10}$$

Finally for $\hat{r}_z = \cos\theta$, only the first recurrence applies,

$$\langle l'm'|\hat{r}_z|lm\rangle = \int d\Omega\ Y_{l'}^{m'*}(\Omega)\cos\theta Y_l^m(\Omega) \tag{5.11}$$

And this gives two results,

$$\langle l+1,m|\hat{r}_z|lm\rangle = \sqrt{\frac{(l-m+1)(l+m+1)}{(2l+1)(2l+3)}} \qquad \Delta l=+1,\ \Delta m=0. \tag{5.12}$$

$$\langle l-1,m|\hat{r}_z|lm\rangle = \sqrt{\frac{(l-m)(l+m)}{(2l-1)(2l+1)}} \qquad \Delta l=-1,\ \Delta m=0. \tag{5.13}$$

Nothing too pretty about these, however, it is the complete set of possibilities for the angular part of the electric dipole matrix elements.

5.1 Matrix elements for circular polarization

If the light is circularly polarized, then one needs to imagine that the electric field of the light waves is expanded as a linear combination of right and left circular polarizations. Really, one is finding matrix elements of an interaction which is a scalar product, $H' = -\mathbf{E}\cdot\mathbf{r}$. For waves travelling in the z-direction, the basis vectors for right and left circular polarizations are [1]

$$\hat{u}_R = \frac{1}{\sqrt{2}}(\hat{x}-i\hat{y}), \qquad \hat{u}_L = \frac{1}{\sqrt{2}}(\hat{x}+i\hat{y}). \tag{5.14}$$

[1] For right circular polarization, with your right thumb pointed towards the source, the electric field vector at a fixed point in space rotates the same direction as your right-hand fingers curl. Vice-versa for left circular polarization.

The Cartesian unit vectors are expressed with these as

$$\hat{x} = \frac{1}{\sqrt{2}}(\hat{u}_R + \hat{u}_L), \qquad \hat{y} = \frac{i}{\sqrt{2}}(\hat{u}_R - \hat{u}_L). \tag{5.15}$$

Then the dipolar interaction can be expressed as

$$\begin{aligned} H' &= -\mathbf{E}\cdot\mathbf{r} = -(E_R\hat{u}_R + E_L\hat{u}_L)\cdot(x\hat{x} + y\hat{y} + z\hat{z}) \\ &= -\frac{1}{\sqrt{2}}\left[E_R(\hat{x} - i\hat{y}) + E_L(\hat{x} + i\hat{y})\right]\cdot(x\hat{x} + y\hat{y}) \end{aligned} \tag{5.16}$$

Here, E_R and E_L are the amplitudes for the waves being in the two possible polarization states. But I kept the position operator in Cartesian components. This becomes

$$H' = -\left[E_R\left(\frac{x - iy}{\sqrt{2}}\right) + E_L\left(\frac{x + iy}{\sqrt{2}}\right)\right] = -r\left[E_R\left(\frac{\hat{r}_x - i\hat{r}_y}{\sqrt{2}}\right) + E_L\left(\frac{\hat{r}_x + i\hat{r}_y}{\sqrt{2}}\right)\right] \tag{5.17}$$

This was a somewhat round-about way to show that the mixtures of Cartesian components corresponding to right and left circular polarizations, are the objects within parenthesis, following E_R and E_L, respectively. These are in fact the components of the dipole unit vector along the circular polarization "directions." [2]

By simple algebra, the dipole unit operator can be expressed

$$\hat{r}(\Omega) = \hat{x}\sin\theta\cos\phi + \hat{y}\sin\theta\sin\phi + \hat{z}\cos\theta = \frac{1}{\sqrt{2}}\sin\theta\left(\hat{u}_R e^{i\phi} + \hat{u}_L e^{-i\phi}\right) + \hat{z}\cos\theta \tag{5.18}$$

Doing complex scalar products, or the round-about calculation given above, this is composed from the circular polarization components, that give individual spherical harmonics,

$$\hat{r}_R \equiv \frac{1}{\sqrt{2}}(\hat{r}_x - i\hat{r}_y) = \frac{1}{\sqrt{2}}e^{-i\phi}\sin\theta = +\sqrt{\frac{4\pi}{3}}Y_1^{-1}, \tag{5.19}$$

$$\hat{r}_L \equiv \frac{1}{\sqrt{2}}(\hat{r}_x + i\hat{r}_y) = \frac{1}{\sqrt{2}}e^{+i\phi}\sin\theta = -\sqrt{\frac{4\pi}{3}}Y_1^{+1}, \tag{5.20}$$

$$\hat{r}_z = \cos\theta = \sqrt{\frac{4\pi}{3}}Y_1^{0}. \tag{5.21}$$

(These definitions of Y_l^m include the Condon-Shortley phase.) The advantage of using the circular polarization components, is that they are indeed more natural states of a photon, since they have well-defined angular momemtum. This means the list of nonzero matrix elements is smaller. For example, for the left circular polarization, only the second recurrence (4.12) applies, corresponding to $\Delta m = +1$ only.

$$\langle l'm'|\hat{r}_L|lm\rangle = \frac{1}{\sqrt{2}}\int d\Omega\ Y_{l'}^{m'*}(\Omega)\ \sin\theta\, e^{+i\phi}\ Y_l^m(\Omega) \tag{5.22}$$

There are only two nonzero matrix elements. Remembering to shift m up by 1 in (4.12),

$$\langle l+1, m+1|\hat{r}_L|lm\rangle = \sqrt{\frac{(l+m+1)(l+m+2)}{2(2l+1)(2l+3)}}, \qquad \Delta l = +1,\ \Delta m = +1. \tag{5.23}$$

$$\langle l-1, m+1|\hat{r}_L|lm\rangle = -\sqrt{\frac{(l-m-1)(l-m)}{2(2l-1)(2l+1)}}, \qquad \Delta l = -1,\ \Delta m = +1. \tag{5.24}$$

[2] One needs to take care doing these operations because these basis vectors are complex. I am trying to do this in a way where no conjugate operations are needed. If done incorrectly, the right and left parts can get interchanged.

This shows more clearly that the photon in this case only raises the z-component of angular momentum of the atom that absorbed it. On the other hand, for the right-circular photon state,

$$\langle l'm'|\hat{r}_R|lm\rangle = \frac{1}{\sqrt{2}}\int d\Omega\; Y_{l'}^{m'*}(\Omega)\;\sin\theta\, e^{-i\phi}\; Y_l^m(\Omega) \tag{5.25}$$

Again, there are only two nonzero matrix elements. In this case shift m down by 1 in (4.13),

$$\langle l+1, m-1|\hat{r}_R|lm\rangle = -\sqrt{\frac{(l-m+1)(l-m+2)}{2(2l+1)(2l+3)}}, \qquad \Delta l = +1,\; \Delta m = -1. \tag{5.26}$$

$$\langle l-1, m-1|\hat{r}_R|lm\rangle = +\sqrt{\frac{(l+m-1)(l+m)}{2(2l-1)(2l+1)}}, \qquad \Delta l = -1,\; \Delta m = -1. \tag{5.27}$$

Now the photon only can lower the z-component of angular momentum of the atom. These are the negatives of those for the left circular polarization, with m reversed inside the formulas.

If one thinks of these matrix elements as being applied to photon absorption, the coupling of left circular to $\Delta m = +1$ makes sense. The left photon is a positive helicity state, meaning, its angular momentum of $\hbar$ is along the propagation direction, or in the $+z$ direction. It can only raise the z-component of angular momentum of the atom, if it is absorbed. On the other hand, the right circular photon has negative helicity, thus its angular momentum aong the z-axis is $-\hbar$. When it gets absorbed, it lowers the z-component of angular momentum of the atom.

5.2 Circular polarization: waves traveling in an arbitrary direction

In the last section the EM waves were assumed to be travelling along the z-direction. That geometry makes sense for some simple situations. But in the most general case, there would be no requirement that the wave vector of the EM waves is aligned with a particular z-axis. So to do this general case, assume the waves travel in some direction with wave vector $\mathbf{k}$, and have the electric field polarized along a vector $\hat{\epsilon}$ that is perpendicular to $\mathbf{k}$. This electric field could be expressed like

$$\mathbf{E}(\mathbf{r},t) = \mathrm{Re}\left\{E\hat{\epsilon}\, e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\right\}, \qquad \text{and}\quad (E_x, E_y, E_z) = E(\epsilon_x, \epsilon_y, \epsilon_z) \tag{5.28}$$

Then the interaction Hamiltonian is now expressed, suppressing the time and space dependence,

$$H' = -\mathbf{E}\cdot\mathbf{r} = -(E\hat{\epsilon})\cdot(x\hat{x}+y\hat{y}+z\hat{z}) = -E\,(x\epsilon_x + y\epsilon_y + z\epsilon_z) \tag{5.29}$$

The polarization vector is given in Cartesian components as $\hat{\epsilon} = (\epsilon_x, \epsilon_y, \epsilon_z)$, where each component is obtaned by $\epsilon_i = \hat{\epsilon}\cdot\hat{x}_i$. Taking out also the radius, the interaction is

$$H' = -\mathbf{E}\cdot\mathbf{r} = -Er\,(\hat{r}_x\epsilon_x + \hat{r}_y\epsilon_y + \hat{r}_z\epsilon_z) = -Er\left[\sin\theta(\epsilon_x\cos\phi + \epsilon_y\sin\phi) + \epsilon_z\cos\theta\right] \tag{5.30}$$

But it makes sense to expand out the ϕ-dependence, which can be done some different ways. The simplest is

$$\begin{aligned}
H' &= -Er\left\{\sin\theta\left[\epsilon_x\frac{1}{2}(e^{i\phi}+e^{-i\phi}) + \epsilon_y\frac{1}{2i}(e^{i\phi}-e^{-i\phi})\right] + \epsilon_z\cos\theta\right\} \\
&= -Er\left\{\sin\theta\left[e^{i\phi}\left(\frac{\epsilon_x - i\epsilon_y}{2}\right) + e^{-i\phi}\left(\frac{\epsilon_x + i\epsilon_y}{2}\right)\right] + \epsilon_z\cos\theta\right\} \\
&= -Er\left\{\sin\theta\left[\frac{e^{i\phi}}{\sqrt{2}}\left(\frac{\epsilon_x - i\epsilon_y}{\sqrt{2}}\right) + \frac{e^{-i\phi}}{\sqrt{2}}\left(\frac{\epsilon_x + i\epsilon_y}{\sqrt{2}}\right)\right] + \epsilon_z\cos\theta\right\}
\end{aligned} \tag{5.31}$$

Written this way, one sees that the components of the polarization that are coupled to well-defined angular momenta are factors that resemble the definitions discussed for circular polarization. But one needs to be careful here. The first factors are involved in raising m and are for **left circular** polarization:

$$E_L = E \cdot \left(\frac{\epsilon_x - i\epsilon_y}{\sqrt{2}}\right) = \frac{E_x - iE_y}{\sqrt{2}}, \qquad \hat{r}_L = \frac{1}{\sqrt{2}} e^{+i\phi} \sin\theta = \frac{\hat{r}_x + i\hat{r}_y}{\sqrt{2}}. \tag{5.32}$$

The second factors are involved in lowering m and are for **right circular** polarization:

$$E_R = E \cdot \left(\frac{\epsilon_x + i\epsilon_y}{\sqrt{2}}\right) = \frac{E_x + iE_y}{\sqrt{2}}, \qquad \hat{r}_R = \frac{1}{\sqrt{2}} e^{-i\phi} \sin\theta = \frac{\hat{r}_x - i\hat{r}_y}{\sqrt{2}}. \tag{5.33}$$

You can check that the algebra is correct, and in fact, it has to hold as

$$\hat{r} \cdot \hat{\epsilon} = \hat{r}_x \epsilon_x + \hat{r}_y \epsilon_y + \hat{r}_z \epsilon_z = \left(\frac{\hat{r}_x + i\hat{r}_y}{\sqrt{2}}\right)\left(\frac{\epsilon_x - i\epsilon_y}{\sqrt{2}}\right) + \left(\frac{\hat{r}_x - i\hat{r}_y}{\sqrt{2}}\right)\left(\frac{\epsilon_x + i\epsilon_y}{\sqrt{2}}\right) \tag{5.34}$$

This way of combining gives a real scalar product. One sees that the amplitude for absorption of left circular photons is proportional to E_L and the matrix element of $\hat{r}_L$, as defined here, and for right circular photons, proportional to the product of E_R and the matrix element of $\hat{r}_R$. The particular values of the matrix elements were given in the previous section.

If the electric field moves in such a way that $E_x - iE_y = 0$, then $E_L = 0$ and the wave has a pure right circular polarization.

On the other hand, if the fields behave with $E_x + iE_y = 0$, then $E_R = 0$ and the wave has a pure left circular polarization.

The interaction will probably be expressed in many texts in terms of the spherical harmonics. In this way the expression, if needed, is quite simple,

$$H' = -Er\sqrt{\frac{4\pi}{3}} \left\{ -Y_1^{+1} \left(\frac{\epsilon_x - i\epsilon_y}{\sqrt{2}}\right) + Y_1^{-1} \left(\frac{\epsilon_x + i\epsilon_y}{\sqrt{2}}\right) + Y_1^0 \, \epsilon_z \right\} \tag{5.35}$$

This is also the same as

$$H' = -r\sqrt{\frac{4\pi}{3}} \left\{ -Y_1^{+1} E_L + Y_1^{-1} E_R + Y_1^0 E_z \right\} \tag{5.36}$$

5.2.1 Waves not traveling along z?

Another point is about the z-component. If the waves travel along z, there can be no z-component to the electric field. On the other hand, suppose the waves are traveling, for example in the x-direction, and they could have some aspect of circular polarization. Consider the amplitude as

$$\mathbf{E} = (E_y \hat{y} + E_z \hat{z}) e^{i(kx - \omega t)} = \tag{5.37}$$

If the components have aa relation like $E_y = \pm i E_z$, then the waves are circularly polarized. Now, the matrix elements involving the z-components actually will relate to effects associated with the circular polarization states.

But so far, we put the quantization axis along z, which is somewhat unnatural for this particular problem. Still, the direction chosen for coordinates is arbitrary and has nothing to do with affecting a final answer. A transition rate or matrix element squared, appropriately, will not in the end depend on the coordinate system. But the system starting in an eigenstate of L_z is not the same as starting in an eigenstate of L_x. An eigenstate of L_x, with quantum number m_x, for a chosen l, has to be a linear combination of eigenstates of L_z at its eigenvalues $m_z = 0, \pm 1$. Thus, the comparison between using different coordinate systems takes some care.