PHYS 632: Quantum Mechanics II (Winter 2021)

Course Notes: Angular Momentum in Coordinate Space

Reading/Exercises for 12 January 2021 (Tuesday, Week 2)
Due Monday, 18 January 2021

1 Preamble

Remember that this exercise set replaces one lecture for this week. I'll be available at the usual class time to answer questions, and you can set up extra meetings later in the week for questions, just let me know.

To reiterate how this works from last term, you should:

- Work through these notes, taking notes if it helps and working through the exercises throughout.
- Submit your exercises via the web site as usual.
- The homework problems associated with this material are also included in Homework #2.

2 Orbital Angular Momentum: Definition

In classical mechanics, angular momentum is defined by

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}. \tag{1}$$

In quantum mechanics, we will use the same definition, and mostly we will work in the position representation:

$$\boxed{\mathbf{L} = \mathbf{r} \times \mathbf{p} = \mathbf{r} \times \frac{\hbar}{i}\nabla.} \tag{2}$$

(orbital angular momentum)

We will call this angular-momentum operator **orbital angular momentum** to distinguish it from other types we will introduce later (spin, composite).

Exercise #2. Usually, observables involving products of x and p must have some kind of symmetric ordering. But the definition $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ does *not* have a symmetric ordering. Why does the order not matter here?

3 Make Your Life 10× Easier By (Not) Doing This One Weird Trick

If you are still working out vector cross products using a determinant mnemonic like

$$\mathbf{a} \times \mathbf{b} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ a_x & a_y & a_z \\ b_x & b_y & b_z \end{vmatrix}, \tag{3}$$

then **now is the time to rid yourself of this bad habit forever!** Seriously, nobody who is really good at physics uses this trick, and I *know* some of you are still doing this. (If you already avoid this mnemonic, you can move on to the next section.)

The good way to write out a cross product is to remember it will involve a bunch of terms that look kind of like $\hat{x}a_y b_z$. Focus on the x, y, and z: you have to fill the slots in terms of the form $\hat{\square}a_\square b_\square$ with these three symbols, each appearing exactly once. The one last detail is that if these appear in the order xyz or any cyclic permutation (yzx, zxy), then the term gets a plus sign; any odd permutation of xyz (yxz, xzy, zyx) gets a minus sign. So just writing down the x-component of the cross product gives

$$\mathbf{a} \times \mathbf{b} = \hat{x}a_y b_z - \hat{x}a_z b_y + \cdots . \tag{4}$$

(Look at the order of symbols and the signs!) The other components follow just by cyclicly permuting the symbols:

$$\mathbf{a} \times \mathbf{b} = \hat{x}(a_y b_z - a_z b_y) + \hat{y}(a_z b_x - a_x b_z) + \hat{z}(a_x b_y - a_y b_x). \tag{5}$$

That is, just permute the symbols in the first term $\hat{x}a_y b_z$ to get the other first terms, and then swap the order of the a and b subscripts to get the corresponding negative term.

This is the fast way to do the cross product, and usually when you do a calculation involving a cross product like this (or lots of vector calculations), you can just work out one component and then get the others by permuting indices. (Pay attention to how we do this in the following.) The cross-product rule also follows of course from the definition $\mathbf{a} \times \mathbf{b} = \epsilon_{ijk}\hat{e}_i a_j b_k$ (repeated indices summed), where ϵ_{ijk} is the Levi-Civita symbol.

4 Commutation Rules

Now we want to establish that $\mathbf{L}$ is indeed an angular-momentum operator in the sense that we have already defined it, and so we will need to work out a bunch of commutators. To start, consider

$$[L_x, y] = [yp_z - zp_y, y] = -z[p_y, y] = -z(-i\hbar) = i\hbar z. \tag{6}$$

By the same argument, we have

$$[L_x, x] = 0. \tag{7}$$

Other cases follow by cyclic permutation of indices in the above two commutators, as well as in $[L_y, x] = -i\hbar z$. Together, we can write this as

$$[L_\alpha, r_\beta] = i\hbar\epsilon_{\alpha\beta\gamma}r_\gamma. \tag{8}$$

(commutator with position)

Exercise #3. In a similar way, show that

$$[L_\alpha, p_\beta] = i\hbar\epsilon_{\alpha\beta\gamma}p_\gamma. \tag{9}$$

(commutator with momentum)

Now we are in a position to compute commutators of angular-momentum operators.

Exercise #4. Use the above commutators to show

$$[L_\alpha, L_\beta] = i\hbar\epsilon_{\alpha\beta\gamma}L_\gamma. \tag{10}$$

(commutator of orbital angular momentum)

Thus, orbital angular momentum satisfies the axiomatic definition of angular momentum.

5 Application to Central-Force Problems

One of the primary applications of the **L** operator is to central potentials of the form

$$H(\mathbf{p}, \mathbf{r}) = \frac{p^2}{2m} + V(r), \tag{11}$$

so that the potential is only a function of $r = |\mathbf{r}|$. To see why this is useful, we will need yet more commutators. Because $[L_x, p_x] = 0$, it follows that

$$[L_x, p_x^2] = 0 \tag{12}$$

as well. Also, from $[L_x, p_y] = i\hbar p_z$, it follows that

$$[L_x, p_y^2] = p_y[L_x, p_y] + [L_x, p_y]p_y = i\hbar(p_y p_z + p_z p_y) = 2i\hbar(p_y p_z) \tag{13}$$

and thus also $[L_x, p_z^2] = -2i\hbar(p_y p_z)$. Putting together the three components of $p^2 = p_x^2 + p_y^2 + p_z^2$, we have

$$[L_x, p^2] = 0, \tag{14}$$

so any component of **L** commutes with the kinetic-energy operator. The same calculations lead to $[L_x, x^2] = 0$, $[L_x, y^2] = 2i\hbar yz$, and $[L_x, z^2] = -2i\hbar yz$, so that

$$[L_x, r^2] = 0. \tag{15}$$

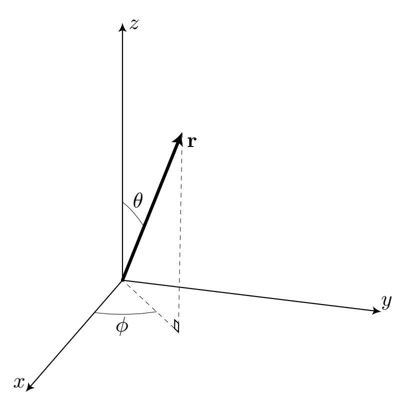
Then any component of **L** also commutes with any *function* of r^2, including $r = \sqrt{r^2}$, and any function of r like $V(r)$. Thus, any component of **L** commutes with the Hamiltonian,

$$[L_x, H] = 0, \tag{16}$$

in the case of a central potential. This is important, because the Hamiltonian will have simultaneous eigenstates with, say, L^2 and L_z. Thus, when we develop these eigenstates $|\ell\ m\rangle$, we will also be developing the angular dependence of the central-force problem.

6 Representation in Spherical Coordinates

Now the goal is to work out the representation of the eigenstates $|\ell\ m\rangle$ in spherical angles (θ, ϕ). Unfortunately, it's going to be something of a long slog to get there. To start, the convention for the spherical angles is shown in the diagram below.



From the diagram we can read off the coordinate transformations

$$\begin{aligned} z &= r\cos\theta \\ x &= r\sin\theta\cos\phi \\ y &= r\sin\theta\sin\phi. \end{aligned} \tag{17}$$

Now we will need the gradient operator in spherical coordinates,

$$\nabla = \hat{r}\partial_r + \frac{\hat{\theta}}{r}\partial_\theta + \frac{\hat{\phi}}{r\sin\theta}\partial_\phi, \tag{18}$$

where the proof of this formula is left as a homework problem.

Homework Problem #3. Derive formula (18) for the gradient operator in spherical coordinates by considering the differential

$$df(r,\theta,\phi) = d\mathbf{r}\cdot\nabla f(\mathbf{r}) \tag{19}$$

for an arbitrary scalar function $f(\mathbf{r})$, and working out the effect of infinitesimal displacements in different directions. Note the suggestive forms of the (equivalent) arguments on both sides.

Using this expression, we can compute the angular momentum operator:

$$\mathbf{L} = -i\hbar\mathbf{r}\times\nabla = -i\hbar\left(\hat{r}\times\hat{\theta}\,\partial_\theta + \frac{1}{\sin\theta}\hat{r}\times\hat{\phi}\,\partial_\phi\right) = i\hbar\left(\frac{1}{\sin\theta}\hat{\theta}\,\partial_\phi - \hat{\phi}\,\partial_\theta\right). \tag{20}$$

More useful will be the projection of this form into Cartesian coordinates:

$$\begin{aligned} L_z &= -i\hbar\partial_\phi \\ L_x &= i\hbar\Big(\cot\theta\cos\phi\,\partial_\phi + \sin\phi\,\partial_\theta\Big) \\ L_y &= i\hbar\Big(\cot\theta\sin\phi\,\partial_\phi - \cos\phi\,\partial_\theta\Big). \end{aligned} \tag{21}$$

Exercise #5. Work out these expressions for the Cartesian components of $\mathbf{L}$.

The idea is to use these to calculate L^2, so we will have spherical representations of the operators L^2 and L_z to diagonalize. First, squaring the z component gives

$$L_z^2 = -\hbar^2\partial_\phi^2, \tag{22}$$

while squaring the x component gives the considerably messier expression

$$L_x^2 = -\hbar^2\Big[\cot^2\theta\cos\phi\,\partial_\phi\cos\phi\,\partial_\phi + \sin^2\phi\,\partial_\theta^2 + \cot\theta\cos\phi\,\partial_\phi\sin\phi\,\partial_\theta + \sin\phi\cos\phi\,\partial_\theta\cot\theta\,\partial_\phi\Big]. \tag{23}$$

Since this is only a step towards computing L^2, we can avoid the pain of writing down a similarly ugly expression for L_y^2 by realizing that $L_x^2 + L_y^2$ is azimuthally symmetric, so that it doesn't change under an average over ϕ. Thus, we can compute $L_x^2 + L_y^2$ by averaging L_x^2 over ϕ and then doubling the result. Making the replacements $\sin\phi\cos\phi \longrightarrow 0$; $\sin^2\phi$, $\cos^2\phi \longrightarrow 1/2$; $\cos\phi\,\partial_\phi\cos\phi\,\partial_\phi = \cos^2\phi\,\partial_\phi^2 - \cos\phi\sin\phi\,\partial_\phi \longrightarrow \partial_\phi^2/2$; and $\cos\phi\,\partial_\phi\sin\phi = \cos^2\phi - \cos\phi\sin\phi\,\partial_\phi \longrightarrow 1/2$, we have

$$L_x^2 + L_y^2 = -\hbar^2\Big[\cot^2\theta\,\partial_\phi^2 + \partial_\theta^2 + \cot\theta\,\partial_\theta\Big]. \tag{24}$$

Combining this result with Eq. (22), we have

$$L^2 = -\hbar^2 \Big[(\cot^2\theta + 1)\partial_\phi^2 + \big(\partial_\theta + \cot\theta\big)\,\partial_\theta\Big]. \tag{25}$$

After a big more algebra, we have

$$\begin{aligned} L^2 &= -\hbar^2 \left[\frac{1}{\sin\theta}\,\partial_\theta\Big(\sin\theta\,\partial_\theta\Big) + \frac{1}{\sin^2\theta}\,\partial_\phi^2\right] \\ L_z &= -i\hbar\partial_\phi, \end{aligned} \tag{26}$$

(operators to diagonalize)

including the operator L_z from Eqs. (21). Remember that the goal is to find simultaneous eigenfunctions of these two operators.

6.1 Azimuthal-Angle Solution

Recalling the general form of the J_z eigenvalue,

$$L_z|\ell\ m\rangle = m\hbar|\ell\ m\rangle, \tag{27}$$

where m must be an integer or half-integer. If we project into the angular representation with $\langle\theta,\phi|$, we have

$$L_z\Phi(\phi) = -i\hbar\Phi'(\phi) = m\hbar\Phi(\phi), \tag{28}$$

where $\Phi(\phi)$ represents the functional dependence on ϕ in $\langle\theta,\phi|\ell\ m\rangle$, and we are dropping the θ dependence since there is no such dependence in L_z This leads to the simple differential equation

$$\Phi'(\phi) = im\Phi(\phi), \tag{29}$$

which has solution

$$\Phi(\phi) = e^{im\phi}. \tag{30}$$

There is also technically an undetermined constant here that we are dropping, because we will normalize the entire state separately later, once the θ dependence is better established.

Note that the form of this wave function (30) implies a restriction on m. A shift of ϕ by 2π should leave the wave function unchanged; that is to say, since ϕ is an angle, it is subject to periodic boundary conditions. This requires that $e^{2\pi im} = 1$, which in turn requires m to be an integer, *not* a half-integer. This further implies that ℓ is an integer, not a half-integer. Half-integer angular momenta are possible, but do not correspond to orbital angular momentum.

6.2 Polar-Angle Solution: Differential Equation

Note: you can just skim this section. Now for the remainder of the solution for the angular states. Recall that L^2 in Eqs. (26) has no ϕ-dependence (except via the operator ∂_ϕ). Therefore, introducing the notation

$$Y_\ell^m(\theta,\phi) := \langle\theta,\phi|\ell\ m\rangle \tag{31}$$

for the coordinate-space eigenfunction, this function separates into factors for the separate dependences on the two angles:

$$Y_\ell^m(\theta,\phi) = \Theta_\ell^m(\theta)\,\Phi_m(\phi) = \Theta_\ell^m(\theta)\,e^{im\phi}. \tag{32}$$

We have already found the second factor $\Phi_m(\phi)$; what remains is to find the eigenfunction $\Theta_\ell^m(\theta)$ of the L^2 operator (which depends on m via the operator ∂_ϕ).

From the eigenvalue equation for J^2, we already have the eigenvalue equation

$$L^2|\ell\, m\rangle = \ell(\ell+1)\hbar^2|\ell\, m\rangle. \tag{33}$$

Projecting with $\langle\theta,\phi|$ gives

$$-\left[\frac{1}{\sin\theta}\,\partial_\theta\Big(\sin\theta\,\partial_\theta\Big) + \frac{1}{\sin^2\theta}\,\partial_\phi^2\right]\Theta_\ell^m(\theta)\,e^{im\phi} = \ell(\ell+1)\Theta_\ell^m(\theta)\,e^{im\phi}. \tag{34}$$

Carrying out the ϕ derivatives and simplifying leads to

$$\left[\frac{1}{\sin\theta}\,\partial_\theta\Big(\sin\theta\,\partial_\theta\Big) + \ell(\ell+1) - \frac{m^2}{\sin^2\theta}\right]\Theta_\ell^m(\theta) = 0. \tag{35}$$

This can be put into standard form by changing to the variable $\mu := \cos\theta$, so that $\sin^2\theta = 1-\mu^2$ and $\partial_\mu = -(1/\sin\theta)\partial_\theta$. The result is

$$\partial_\mu\Big[(1-\mu^2)\,\partial_\mu\Theta\Big] + \left[\ell(\ell+1) - \frac{m^2}{1-\mu^2}\right]\Theta = 0. \qquad \text{(general Legendre equation)} \tag{36}$$

This differential equation is called the **general Legendre equation**, and the solutions are known as the **associated Legendre polynomials**. The approach here is to assume a power-series solution, show that it truncates, and work out a recursion relation for the coefficients (as was also possible for the Hermite polynomials). However, we will eschew this approach in favor of the more clever, fancy-schmancy method of using the ladder operators to construct solutions.

6.3 Polar-Angle Solution: Ladder Operators for Stretched States

To proceed, then, we will need the usual ladder operators

$$L_\pm := L_x \pm iL_y. \tag{37}$$

Using L_x and L_y from Eqs. (21), we find

$$L_\pm = \hbar e^{\pm i\phi}\Big(i\cot\theta\,\partial_\phi \pm \partial_\theta\Big). \tag{38}$$

Now recall that lowering the lowest state $|\ell\,(-\ell)\rangle$ must lead to a null result:

$$L_-|\ell\,(-\ell)\rangle = 0. \tag{39}$$

In the angular representation, this is a differential equation for the solution $\Theta_\ell^{-\ell}(\theta)$:

$$\hbar e^{-i\phi}\Big(i\cot\theta\,\partial_\phi - \partial_\theta\Big)\Theta_\ell^{-\ell}(\theta)\,e^{-i\ell\phi} = 0. \tag{40}$$

Simplifying a bit, we have

$$\Big(\ell\cot\theta - \partial_\theta\Big)\Theta_\ell^{-\ell}(\theta) = 0, \tag{41}$$

and the solution to this equation is

$$\Theta_\ell^{-\ell}(\theta) = \eta\,(\sin\theta)^\ell \tag{42}$$

for some normalization constant η.

Exercise #6. Verify this solution.

The normalization convention is to require

$$\int d\Omega \left|Y_\ell^m(\theta,\phi)\right|^2 = 1 \tag{43}$$

for any (ℓ, m), where $d\Omega = \sin\theta\, d\theta\, d\phi$. Putting in Eq. (42) into this condition (the ϕ dependence does not affect the normalization), we find

$$2\pi|\eta|^2 \int_{-1}^{1} d\mu\, (1-\mu^2)^\ell = \frac{4\pi(2^\ell \ell!)^2}{(2\ell+1)!}|\eta|^2 = 1, \tag{44}$$

and thus we have

$$\Theta_\ell^{-\ell}(\theta) = \frac{1}{2^\ell \ell!}\sqrt{\frac{(2\ell+1)!}{4\pi}}\,(\sin\theta)^\ell \tag{45}$$

as the normalized, minimum-m solution, upon choosing a zero global phase angle. Note that the same argument, applying $L_+|\ell\ \ell\rangle = 0$, leads to the same solution for $\Theta_\ell^\ell(\theta)$.

6.4 Polar-Angle Solution: Ladder Operators for Arbitrary States

To construct the rest of the angular-space representations for the eigenstates $|\ell\ m\rangle$, we can iteratively apply the raising operator L_+ to $|\ell\ -\ell\rangle$ to end up with the desired state. The procedure is a little tricky because there is a lot involved, so we will break this into more manageable parts. First, recall that the action of the raising operator on an eigenstate is

$$L_+|\ell\ m\rangle = \hbar\sqrt{(\ell+m+1)(\ell-m)}\ |\ell\ (m+1)\rangle. \tag{46}$$

Shifting $m \longrightarrow m-1$ changes this to

$$L_+|\ell\ (m-1)\rangle = \hbar\sqrt{(\ell+m)(\ell-m+1)}\ |\ell\ m\rangle. \tag{47}$$

We can perform the same shift and then apply the raising operator again using the formula above; the result is

$$(L_+)^2|\ell\ (m-2)\rangle = \hbar^2\sqrt{(\ell+m)(\ell+m-1)(\ell-m+1)(\ell-m+2)}\ |\ell\ m\rangle. \tag{48}$$

Noticing the pattern of the factors, we can continue to k applications of the raising operator:

$$(L_+)^k|\ell\ (m-k)\rangle = \hbar^k\sqrt{\frac{(\ell+m)!}{(\ell+m-k)!}\frac{(\ell-m+k)!}{(\ell-m)!}}\ |\ell\ m\rangle. \tag{49}$$

Setting $k = \ell + m$ gives

$$(L_+)^{\ell+m}|\ell\ (-\ell)\rangle = \hbar^{\ell+m}\sqrt{\frac{(\ell+m)!(2\ell)!}{(\ell-m)!}}\ |\ell\ m\rangle, \tag{50}$$

and then solving for the desired state gives

$$|\ell\ m\rangle = \frac{1}{\hbar^{\ell+m}}\sqrt{\frac{(\ell-m)!}{(\ell+m)!(2\ell)!}}\,(L_+)^{\ell+m}|\ell\ (-\ell)\rangle. \tag{51}$$

Now from Eq. (38) we have

$$L_+ = \hbar e^{i\phi}\Big(i\cot\theta\,\partial_\phi + \partial_\theta\Big), \tag{52}$$

and if we assume this operator to act on $|\ell\; m\rangle$ (or Y_ℓ^m in coordinate space), then we may use the form

$$\begin{aligned} L_+ &= \hbar e^{i\phi}\Big(\partial_\theta - m\cot\theta\Big)\\ &= \hbar e^{i\phi}(\sin\theta)^m\partial_\theta(\sin\theta)^{-m}\\ &= -\hbar e^{i\phi}(1-\mu^2)^{(m+1)/2}\partial_\mu(1-\mu^2)^{-m/2}, \end{aligned} \tag{53}$$

using the same change of variables as before: $\mu = \cos\theta$, $\sin^2\theta = 1-\mu^2$, $\partial_\mu = -(1/\sin\theta)\partial_\theta$. Repeated application of L_+ is complicated somewhat by the observation that m is a moving target: it increases by 1 on each application. Applying it $\ell+m$ times to the edge state has the form

$$(L_+)^{\ell+m}|\ell\;(-\ell)\rangle = (-1)^{\ell+m}\hbar^{\ell+m}e^{i(\ell+m)\phi}(1-\mu^2)^{m/2}\partial_\mu^{\ell+m}(1-\mu^2)^{\ell/2}\,|\ell\;(-\ell)\rangle. \tag{54}$$

This can be seen by writing out the first couple of operations on the initial state, and noticing the pattern of factors (and the cancellation of factors of $(1-\mu^2)$ between the derivative operators):

$$\cdots\Big[(1-\mu^2)^{-(\ell-2)/2}\partial_\mu(1-\mu^2)^{(\ell-1)/2}\Big]\Big[(1-\mu^2)^{-(\ell-1)/2}\partial_\mu(1-\mu^2)^{\ell/2}\Big]\,|\ell\;(-\ell)\rangle. \tag{55}$$

Exercise #7. Write this out in enough detail for you to convince yourself that this works out.

Putting Eq. (54) into Eq. (51) and then projecting into coordinate space, we find

$$\hbar^{\ell+m}\sqrt{\frac{(\ell+m)!(2\ell)!}{(\ell-m)!}}\,Y_\ell^m = (-1)^{\ell+m}\hbar^{\ell+m}e^{i(\ell+m)\phi}(1-\mu^2)^{m/2}\partial_\mu^{\ell+m}(1-\mu^2)^{\ell/2}\,Y_\ell^{-\ell}. \tag{56}$$

Using Eq. (45) with a factor $e^{-i\ell\phi}$ for $Y_\ell^{-\ell}$ and then simplifying everything, we find

$$Y_\ell^m = (-1)^{\ell+m}\frac{1}{2^\ell\ell!}\sqrt{\frac{2\ell+1}{4\pi}}\sqrt{\frac{(\ell-m)!}{(\ell+m)!}}\,(1-\mu^2)^{m/2}\partial_\mu^{\ell+m}(1-\mu^2)^\ell\,e^{im\phi}. \tag{57}$$

To summarize and clean up the notation a little bit, while breaking the result up into simpler factors, we have the **spherical harmonics**

$$\boxed{Y_\ell^m(\theta,\phi) = (-1)^m\sqrt{\frac{2\ell+1}{4\pi}}\sqrt{\frac{(\ell-m)!}{(\ell+m)!}}\,P_\ell^m(\cos\theta)\,e^{im\phi},} \tag{58}$$

(spherical harmonics)

which are the coordinate-space representation of the eigenstates $|\ell\;m\rangle$. Here, it is conventional to define the **associated Legendre polynomials**

$$\boxed{P_\ell^m(\mu) := (1-\mu^2)^{m/2}\partial_\mu^m P_\ell(\mu),} \tag{59}$$

(associated Legendre polynomials)

which are written as derivative of the **Legendre polynomials**

$$\boxed{P_\ell(\mu) := \frac{1}{2^\ell\ell!}\partial_\mu^\ell(\mu^2-1)^\ell.} \tag{60}$$

(Legendre polynomials)

As usual, $\mu = \cos\theta$ here. For handy reference, some of the lower-order spherical harmonics are listed below

$$\begin{aligned} Y_0^0(\theta,\phi) &= \frac{1}{\sqrt{4\pi}} \\ Y_1^0(\theta,\phi) &= \sqrt{\frac{3}{4\pi}}\,\cos\theta \\ Y_1^{\pm1}(\theta,\phi) &= \mp\sqrt{\frac{3}{8\pi}}\,\sin\theta\, e^{\pm i\phi} \\ Y_2^0(\theta,\phi) &= \sqrt{\frac{5}{16\pi}}\,\big(3\cos\theta - 1\big) \\ Y_2^{\pm1}(\theta,\phi) &= \mp\sqrt{\frac{15}{8\pi}}\,\sin\theta\,\cos\theta\, e^{\pm i\phi} \\ Y_2^{\pm2}(\theta,\phi) &= \sqrt{\frac{15}{32\pi}}\,\sin^2\theta\, e^{\pm 2i\phi}. \end{aligned} \tag{61}$$

(example spherical harmonics)

These spherical harmonics will be useful in later calculations.