Week 9

PHY 303 Quantum Mechanics
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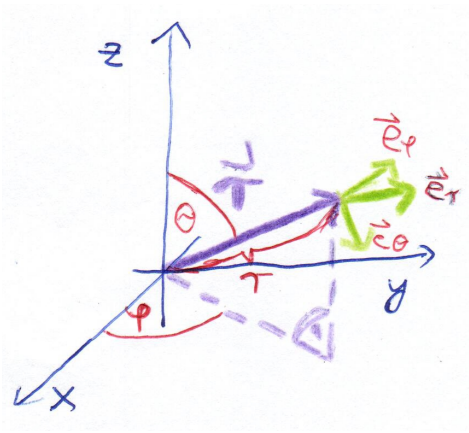
4.2 Spherically symmetric potentials

The 3D potentials we had discussed in the previous week were all such that the problem is separable, due to (4.9). In that case the TISE can frequently be solved analytically even if the potential is not symmetric (such as (4.8) with the $\omega_k \neq \omega_\ell$ for $k \neq \ell$). We shall now look at cases that are not easily separable, but in which the potential is spherically symmetric:

$$V(\mathbf{r}) = V_r(r), \tag{4.29}$$

with $r = \sqrt{x^2+y^2+z^2}$. We have used the radial coordinate from

Spherical polar coordinates:



left: We express our position vector as

$$\mathbf{r} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} r\sin\theta\cos\varphi \\ r\sin\theta\sin\varphi \\ r\cos\theta \end{bmatrix} \tag{4.30}$$

in terms of a radius $r = |\mathbf{r}| = \sqrt{x^2+y^2+z^2}$, a polar angle (co-latidude) θ and an azimuthal angle (longitude) φ, as sketched on the left. We can find the latter two from the cartesian coordinates via $\theta = \arccos(z/r)$ and $\varphi = \text{atan2}(y,x)$. The latter is $\arctan(y/x)$ for $x, y > 0$.

We also have to change our set of unit vectors, from the cartesian ones $\mathbf{e}_x = [1,0,0]^T$, $\mathbf{e}_y = [0,1,0]^T$, $\mathbf{e}_z = [0,0,1]^T$ to spherical polar unit vectors (green in the figure).

$$\mathbf{e}_r = \begin{bmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{bmatrix}, \quad \mathbf{e}_\theta = \begin{bmatrix} \cos\theta\cos\varphi \\ \cos\theta\sin\varphi \\ -\sin\theta \end{bmatrix}, \quad \mathbf{e}_\varphi = \begin{bmatrix} -\sin\varphi \\ \cos\varphi \\ 0 \end{bmatrix}. \tag{4.31}$$

Note that $\mathbf{e}_\theta = \frac{\partial}{\partial\theta}\mathbf{e}_r$ and $\mathbf{e}_\varphi \parallel \frac{\partial}{\partial\varphi}\mathbf{e}_r$.

For setting up the coordinates above, we can for the moment freely chose what we call the z-axis. We shall get back to this subtle point at the end of week 10.

Example 30, Coulomb potential: The obvious example for a spherically symmetric potential is the Coulomb potential V_{coul} felt by a particle of charge q near another one of charge Q, where we place the latter at the origin:

$$V_{\text{coul}}(\mathbf{r}) = \frac{1}{4\pi\epsilon_0}\frac{qQ}{r} = \frac{1}{4\pi\epsilon_0}\frac{qQ}{\sqrt{x^2+y^2+z^2}}, \tag{4.32}$$

where ϵ_0 is the vacuum permittivity. We have written the potential in spherical polar coordinates and cartesian coordinates, to highlight how much simpler it looks in polar ones, and how it can not be separated in the form (4.9) using cartesian coordinates.

Due to the simplicity of a spherically symmetric potential in spherical polar coordinates, we want to rewrite the TISE (4.6) for those cases entirely in those coordinates. The main challenge is to change the Laplacian, which is a nasty technical operation, the result of which we take from mathematics courses:

Laplacian in spherical polar coordinates:

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}. \tag{4.33}$$

Inserting this into (4.6), for a particle of mass m, we now want to solve the time-independent

Schrödinger equation for spherically symmetric potentials

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]\phi_n(r,\theta,\varphi)$$
$$+ V(r)\phi_n(r,\theta,\varphi) = E_n\phi_n(r,\theta,\varphi). \tag{4.34}$$

In order to get this tidied up a bit, we can be guided by our knowledge of classical mechanics: We know, for example from the treatment of the Kepler problem, that for a spherically symmetric potential (central force), angular momentum is conserved. This motivates us to attempt to re-express parts of (4.34) using the angular momentum operator (4.17). To do that, we first express it also in spherical polar coordinates. This is easy for the position operator, which just becomes $\hat{\mathbf{r}} = \hat{r}\mathbf{e}_r$. For the momentum operator we need the

Three dimensional gradient: in spherical polar coordinates

$$\boldsymbol{\nabla} = \mathbf{e}_r\frac{\partial}{\partial r} + \mathbf{e}_\theta\frac{1}{r}\frac{\partial}{\partial\theta} + \mathbf{e}_\varphi\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi} \tag{4.35}$$

with unit vectors defined in (4.31).

Inserting this for the momentum operator in (4.17) you can convince yourself (exercise/Griffith)

that we get the following

Position space representation of the angular momentum operator For the operator itself, we find

$$\hat{\mathbf{L}} = -i\hbar \left(\mathbf{e}_\varphi \frac{\partial}{\partial \theta} - \mathbf{e}_\theta \frac{1}{\sin\theta} \frac{\partial}{\partial \varphi} \right) \tag{4.36}$$

and for the angular momentum square consequently

$$\hat{\mathbf{L}}^2 = -\hbar^2 \left(\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \varphi^2} \right) \tag{4.37}$$

Note, that to get from (4.36) to (4.37) you need to be careful that derivatives in the left operator of $\hat{\mathbf{L}}^2 = \mathbf{L} \cdot \mathbf{L}$ act on angles within the unit vectors (4.31) of the right one.
Finally using $\hat{L}_z = \mathbf{e}_z \cdot \hat{\mathbf{L}}$, Eq. (4.36) and Eq. (4.31) we have

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \varphi}, \tag{4.38}$$

for the z-component of angular momentum.

Comparing (4.37) with (4.34) we spot, that we can write the latter (somewhat more tidily) as:

$$\underbrace{\left[-\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{\hat{\mathbf{L}}^2}{2mr^2} + V(r) \right]}_{=\hat{H}} \phi_n(r,\theta,\varphi) = E_n \phi_n(r,\theta,\varphi). \tag{4.39}$$

- You can easily show that $\left[\hat{H}, \hat{L}\right] = 0$. According to Eq. (3.50), this means that angular momentum is conserved, as we know it has to be in a central potential.
- According to section 3.8, in quantum mechanics this implies that we can expect the eigenfunctions of the Hamiltonian to simultaneously be eigenfunctions of the angular momentum operator, as we indeed will see shortly.
- Conservation of angular momentum is deeply connected to the spherical symmetry, or in other words rotational invariance of the central force problem. You have learnt (or will learn) in classical mechanics, that for a continuous rotational symmetry Noether's theorem enforces angular momentum to be conserved. Similarly in quantum mechanics, we could show directly from the the rotational symmetry of the Hamiltonian, that angular momentum must be conserved (see Griffith chapter 6 for further reading).

Since only $\hat{L}$ contains derivatives with respect to angles, we can hope to sort r and angles θ, φ apart, and again use our separation of variables trick from section 1.6.5. We make the Ansatz

$$\phi(r,\theta,\varphi) = R(r)Y(\theta,\varphi), \tag{4.40}$$

suppressing the index n. Inserting this into (4.39), we then bring everything with r onto the LHS of the resultant equation, and everything with θ and φ onto the RHS, concluding that both sides

have to be equal to the same constant C (exercise, see Griffith), which we call $C = \ell(\ell+1)$ for reasons that shall become clear later.

After separation of variables, we reached a

Separated Schrödinger equation in a central potential. For 3D wavefunction (4.40), the radial part $R(r)$ fulfills the radial Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right) + \underbrace{\left[V(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right]}_{\equiv V_{\text{eff}}(r)} R(r) = ER(r) \tag{4.41}$$

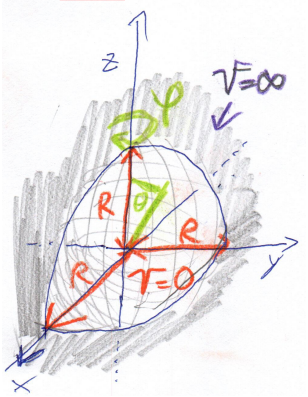
and the angular part $Y(\theta,\varphi)$ fulfills the angular Schrödinger equation

$$-\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)Y(\theta,\varphi) = \hat{\mathbf{L}}^2 Y(\theta,\varphi) = \hbar^2\ell(\ell+1)Y(\theta,\varphi). \tag{4.42}$$

- We see from the second equality in (4.42) that the angular equation tells us that the angular part $Y(\theta,\varphi)$ of the 3D wavefunction is an eigenfunction of the square of angular momentum, with eigenvalue $\hbar^2\ell(\ell+1)$.
- The radial equation (4.41) looks like[11] a 1D Schrödinger equation with an effective potential $V_{\text{eff}}(r)$. Since we can see from (4.42) without having solved anything that $\hbar^2\ell(\ell+1)$ will be the eigenvalue of the angular momentum squared, we recognize this effective potential as exactly the same one that you have encountered in the classical mechanics of the central force problem. We thus interpret that extra part $\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}$ as centrifugal potential.
- The splitting into Eq. (4.41) and Eq. (4.42), can always be done in the form above, independent of the detailed form of $V(r)$ as long as $V(\mathbf{r})$ depends only on the radius $r = |\mathbf{r}|$. We thus see that for this important class of problems, eigenfunctions of the square of the angular momentum operator play a special role. We will thus have to look at these more closely in the next section.

[11] The derivative term is slightly off from our 1D TISE, but that can be cured with a simple substitution (see Griffith or section 4.6 here later).

Example 31, Infinite spherical well: A simple extension of our earlier topic in section 2.2.1 would be to consider the infinite spherical well in three dimensions.



left: We (badly) tried to sketch this on the left. The potential is $V(\mathbf{r}) = 0$ within some radius R, where $r = |\mathbf{r}| < R$, and $V(\mathbf{r}) = \infty$ outside.

The discussion so far applies to this potential, so that we can separately deal with the angular part of the wavefunction (exactly as in the following section), and the radial part (see Griffith if you are interested).

4.3 Angular momentum eigenfunctions

To find all solutions of the angular equation (4.42) (divided by $-\hbar^2$), we can make use of separation of variables one final time. We make the Ansatz

$$Y(\theta, \varphi) = \Theta(\theta)\Phi(\varphi), \tag{4.43}$$

and again (successfully, exercise, Griffith) separate all dependence on θ onto the LHS and all dependence on φ onto the RHS. The two separated equations that we find are:

$$\left[\sin\theta \frac{d}{d\theta}\left(\sin\theta \frac{d\Theta(\theta)}{d\theta}\right)\right] = (m^2 - \ell(\ell+1)\sin^2\theta)\Theta(\theta), \tag{4.44}$$

$$\frac{d^2}{d\varphi^2}\Phi(\varphi) = -m^2\Phi(\varphi) \tag{4.45}$$

This time we have called the separation constant m^2. At this point we do not yet know what m will be, but it has nothing to do with the particle mass. We call it m because everybody does, and you shall see later that there is no real danger of confusion.

To know more about m: The second equation (4.45) is easy to solve and gives us

$$\Phi(\varphi) = e^{im\varphi}. \tag{4.46}$$

From our coordinate definition (4.30) we see that the azimuthal angle φ and $\varphi + 2\pi$ correspond to the same point. For a reasonable wavefunction, we this need $\Phi(\varphi) = \Phi(\varphi + 2\pi)$, which you can reform into $e^{2\pi i m} = 1$, giving us $m = 0, \pm 1, \pm 2, \pm 3$ etc, i.e. m must be an integer. We have thus again found a quantisation rule, even though at this point we are not sure yet what is being quantised (but we shall see that shortly).

The first equation (4.44) is evidently somewhat more complicated. We take its direct solution from the mathematical physics literature for now, and I will show you a tricky way of finding the

answer in the next section 4.4. It turns out (4.45) is solved by $\Theta(\theta) = \mathcal{N} P_\ell^m(\cos\theta)$, where $\mathcal{N}$ is a normalisation factor and we used the

Associated Legendre function: defined by

$$P_\ell^m(x) = (1-x^2)^{|m|/2} \left(\frac{d}{dx}\right)^{|m|} P_\ell(x). \tag{4.47}$$

As seen above, these are in turn obtained via differentiation from P_ℓ, the ℓ'th Legendre polynomial

$$P_\ell(x) = \frac{1}{2^\ell \ell!} \left(\frac{d}{dx}\right)^\ell (x^2-1)^\ell, \tag{4.48}$$

defined for $\ell \geq 0$.

- As the name suggests, the Legendre polynomial P_ℓ is a polynomial of degree ℓ, you can find a few explicit examples in Griffith. I will wait with examples until we have the complete $Y(\theta,\varphi)$ shortly.
- Since Legendre polynomials P_ℓ are of degree ℓ, we see that associated Legendre functions $P_\ell^m(x)$ for $|m| > \ell$ do not exist (or are zero). We thus only need to consider $|m| \leq \ell$.
- Recall that we are on the way of solving the 3D TISE for a wavefunction Ansatz $\phi(r,\theta,\varphi) = R(r)Y(\theta,\varphi)$. For a normalized wavefunction, we require

$$1 = \int d^3\mathbf{r}\, |\phi(r,\theta,\varphi)|^2 = \int_0^\infty dr\, r^2 |R(r)|^2 \underbrace{\int d\Omega}_{\equiv \int_0^\pi d\theta \sin(\theta) \int_0^{2\pi} d\varphi} |Y(\theta,\varphi)|^2, \tag{4.49}$$

  where we have defined the integration $\int d\Omega$ over the 3D solid angle. From the above expression it is clear that it is practical to separately normalize $\int_0^\infty dr\, r^2 |R(r)|^2 = 1$ and

$$\int_0^\pi d\theta \sin(\theta) \int_0^{2\pi} d\varphi |Y(\theta,\varphi)|^2 = 1, \tag{4.50}$$

  which we can use to fix the constant $\mathcal{N}$ in $\Theta(\theta)$ above.

Fixing the normalisation constant and putting it all together, we have now found the

Eigenfunction of the angular motion in a spherically symmetric potential are given by the spherical harmonics

$$Y_\ell^m(\theta,\varphi) = (-1)^m \sqrt{\frac{(2\ell+1)}{4\pi} \frac{(\ell-|m|)!}{(\ell+|m|)!}} e^{im\varphi} P_\ell^m(\cos\theta). \tag{4.51}$$

where the angular momentum quantum number $\ell = 0, 1, 2, 3, \cdots$ is an integer, as is the magnetic quantum number $|m| \leq \ell$.

- We had started off by re-expressing parts of the Hamiltonian in (4.34) using the angular momentum operator, and then we were able to find the angular part of the 3D wavefunction (i.e. its θ and φ dependence) based entirely on the angular momentum operator. The angular part thus exclusively encodes the angular momentum properties of our particle in 3D. Directly from the original equation we already know that $Y_\ell^m(\theta,\varphi)$ is an eigenfunction of $\hat{\mathbf{L}}^2$ with eigenvalue $\hbar^2\ell(\ell+1)$, thus the magnitude of angular momentum is

$$|\hat{\mathbf{L}}| \equiv \hbar\sqrt{\ell(\ell+1)}. \tag{4.52}$$

- From Eq. (4.38) it is also easy to see that we have

$$\hat{L}_z Y_\ell^m(\theta,\varphi) = (-i\hbar\frac{\partial}{\partial\varphi})Y_\ell^m(\theta,\varphi) = (\hbar m)Y_\ell^m(\theta,\varphi), \tag{4.53}$$

  which implies that the spherical harmonics are also eigenfunctions of the z-component of angular momentum, with eigenvalue $\hbar m$.

- Having a fixed value for $\hat{\mathbf{L}}^2$ and $\hat{L}_z$ is the maximum amount of information we can have about the angular momentum, as we have seen in section 4.1.2 (please revisit that now): Since $\left[\hat{L}_n, \hat{L}_m\right] = i\sum_\ell \epsilon_{nm\ell}\hat{L}_\ell$ (Eq. (4.23)), we can know at most one component of the vector without uncertainty. However since $\left[\hat{\mathbf{L}}^2, \hat{L}_n\right] = 0$, we are allowed to additionally know $\hat{\mathbf{L}}^2$.

- With the prefactors given in Eq. (4.51), the spherical harmonics are normalized when integrated over the solid angle of all space, see Eq. (4.50):

$$\int d\Omega |Y_\ell^m(\theta,\varphi)|^2 = \int_0^\pi d\theta \sin(\theta) \int_0^{2\pi} d\varphi |Y_\ell^m(\theta,\varphi)|^2 = 1. \tag{4.54}$$

- As all eigenfunctions of a Hermitian operator, they are mutually orthogonal:

$$\int d\Omega \ \left[Y_{\ell'}^{m'}(\theta,\varphi)\right]^* Y_\ell^m(\theta,\varphi) = \int_0^\pi d\theta \sin(\theta) \int_0^{2\pi} d\varphi \ \left[Y_{\ell'}^{m'}(\theta,\varphi)\right]^* Y_\ell^m(\theta,\varphi) = \delta_{\ell\ell'}\delta_{mm'}. \tag{4.55}$$

  Note that here the $*$ is really crucial, since the spherical harmonics are usually complex (unless $m = 0$).

- Like with all eigenfunctions, the $Y_\ell^m(\theta,\varphi)$ are only specified up to a complex phase (in particular up to a factor (-1)), by the equations that define them. For that reason there are unfortunately different sign conventions used in different contexts. Whenever practically making use of them, one thus have to be careful. We gave the sign convention usually used in quantum mechanics for physicists. Already chemists might use different ones. They even might like real spherical harmonics.

- The application of spherical Harmonics is much wider than in quantum mechanics: They are a useful tool whenever one has to expand a function f defined on the surface of a sphere via angles θ and φ:

$$f(\theta,\varphi) = \sum_{\ell,m} c_{\ell,m} Y_\ell^m(\theta,\varphi). \tag{4.56}$$

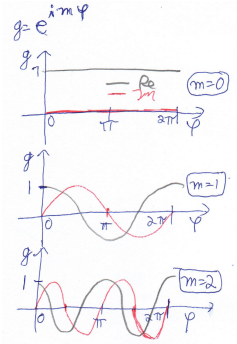
  This surface could be the surface of the earth, or the sky as seen from earth or a spherical object in engineering. Roughly speaking coefficients $c_{0,0}$ with $\ell = 0$ then provide the part of that function that does not vary with angles, while coefficients $c_{\ell,m}$ with higher ℓ and m, the more rapid the variations of that function with angle.

We list the first few spherical harmonics in table 2, you can easily find more in other sources.

	$m=0$	$m=\pm1$	$m=\pm2$
$\ell=0$	$Y_{00}=\frac{1}{\sqrt{4\pi}}$		
$\ell=1$	$Y_{10}=\sqrt{\frac{3}{4\pi}}\cos\theta$	$Y_{1\pm1}=\mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\varphi}$	
$\ell=2$	$Y_{20}=\sqrt{\frac{5}{16\pi}}(3\cos\theta-1)$	$Y_{2\pm1}=\mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{\pm i\varphi}$	$Y_{2\pm2}=\mp\sqrt{\frac{15}{32\pi}}\sin^2\theta e^{\pm 2i\varphi}$
$\ell=3$	$Y_{30}=\sqrt{\frac{7}{16\pi}}(5\cos^3\theta-\cos\theta)$	$Y_{3\pm1}=\mp\sqrt{\frac{21}{64\pi}}\sin\theta(5\cos^2\theta-1)e^{\pm i\varphi}$	$Y_{3\pm2}=\sqrt{\frac{105}{32\pi}}\sin^2\theta\cos\theta e^{\pm 2i\varphi}$
	$m=\pm3$		
	$Y_{3\pm3}=\mp\sqrt{\frac{35}{64\pi}}\sin^3\theta e^{\pm 3i\varphi}$		

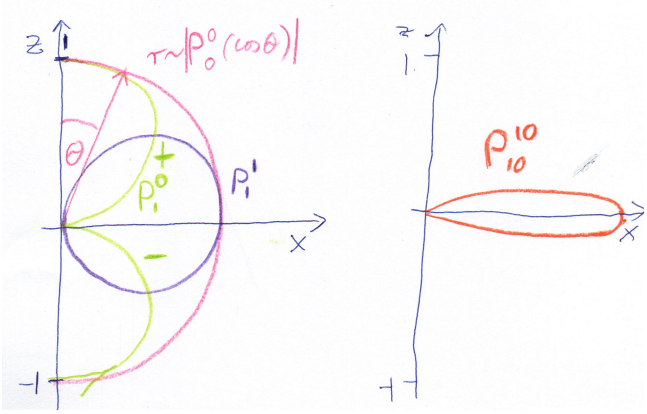
Table 2: List of the lowest few spherical harmonics $Y_\ell^m(\theta,\varphi)$ from (4.51).

Example 32, Sketches of spherical harmonics: In addition to table 2 it is useful to visualize the angular momentum eigenfunctions:



left: The part related to the quantum number m and hence the z-component of the angular momentum is easy to draw, see left. If we compare this with our 1D plane waves e^{ikx} from section 2.1, we realize this corresponds to angular motion with "wavenumber" $k_\varphi = m$.

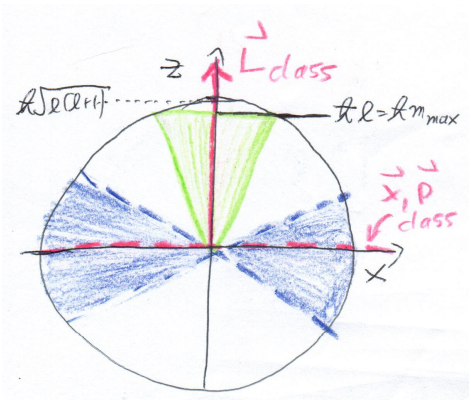
The polar part dependent on θ is more difficult to draw. Me made a "polar graph" below.



left: You have to select an angle θ from the origin, then the distance of the line from the origin is given by $|P_\ell^m(\cos\theta)|$ and the sign is additionally indicated. We can see that for larger ℓ the function changes more rapidly along θ, while m additionally decides in which direction(s) the function is nonzero.

One example that we can understand based on our understanding of classical mechanics is $P_\ell^{m=\ell}$ for large ℓ, e.g. $\ell = 10$. This amounts to a large angular momentum, oriented strongly along the z-axis. Hence motion is mainly (but not quite perfectly) in the $x-y$ plane, see also next example.

Example 33, Angular momentum uncertainty cones:



left: The maximum allowed value of m is $m = \ell$. For that case, if we compare the eigenvalue of $|\hat{\mathbf{L}}|$ which is $\hbar\sqrt{\ell(\ell+1)}$, with that of $\hat{L}_z$ which is $\hbar\ell$, we see that $L_z < |L|$, never quite being equal. This means that for large ℓ the state $m = \ell$ corresponds to the angular momentum pointing almost entirely but not quite along the z-axis. We know from Eq. (4.23) that it cannot point with certainty along the z-axis, since then we would know $L_x = L_y = 0$.

Instead the latter must have some residual uncertainty, which is encoded in the angular momentum lying within the green cone (think of it rotated around the z-axis to form a cone. Classically we know the motion must be in a plane perpendicular to the angular momentum (violet lines). Applied to the uncertainty cone, it must then lie in the blue shaded region (again think 3D, rotated around z)

Most of the above will become clearer when we combine it with the radial wavefunction in the case of Hydrogen, so if you were confused, wait until section 4.6.2 and then refer to the above again.

4.4 Algebraic treatment of angular momentum

Similarly to the harmonic oscillator in section 2.3, we can find the eigenvalue structure of angular momentum entirely without reference to position space wavefunctions, based on commutator algebra and the commutation relation (4.23).

We again start by the definitions of

Ladder operators for angular momentum

$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y. \tag{4.57}$$

Using the basic rules for commutators (3.41), you can show as an easy exercise that

$$\left[\hat{L}_z, \hat{L}_\pm\right] = \pm\hbar\hat{L}_\pm, \tag{4.58}$$

$$\left[\hat{\mathbf{L}}^2, \hat{L}_\pm\right] = 0. \tag{4.59}$$

Now the argumentation proceeds very similar to the one for the harmonic oscillator. Let us assume that f was an eigenfunction of the square of angular momentum $\hat{\mathbf{L}}^2$ and $\hat{L}_z$ with "some" (unknown)

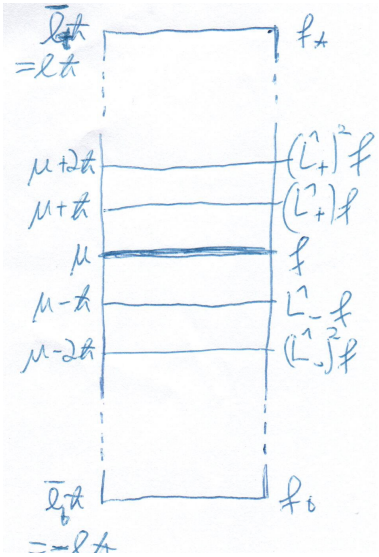
eigenvalue for either, hence $\hat{L}_z f = \mu f$ and $\hat{\mathbf{L}}^2 f = \lambda f$. Then

$$\hat{L}_z(\hat{L}_\pm f) = \hat{L}_z\hat{L}_\pm f \underbrace{-\hat{L}_\pm\hat{L}_z f + \hat{L}_\pm\hat{L}_z f}_{=0} = \underbrace{[\hat{L}_z, \hat{L}_\pm]}_{\overset{Eq.\ (4.58)}{=}\pm\hbar\hat{L}_\pm} f + \hat{L}_\pm \underbrace{\hat{L}_z f}_{=\mu f} = (\mu \pm \hbar)\hat{L}_\pm f. \tag{4.60}$$

We have thus shown, that if the function f has the eigenvalue μ wrt $\hat{L}_z$, then the function $\hat{L}_\pm f$ has the eigenvalue $\mu \pm \hbar$. Similarly

$$\hat{\mathbf{L}}^2(\hat{L}_\pm f) \overset{Eq.\ (4.59)}{=} \hat{L}_\pm \underbrace{\hat{\mathbf{L}}^2 f}_{=\lambda f} = \lambda \hat{L}_\pm f, \tag{4.61}$$

which means that $\hat{L}_\pm f$ remains an eigenfunction of $\hat{\mathbf{L}}^2$ with the same eigenvalue λ that f had.



left: In conclusion, similar to ladder operators for the harmonic oscillator, the ones for angular momentum are climbing up and down "a ladder" of different eigenvalues for $\hat{L}_z$, without changing those of $\hat{\mathbf{L}}^2$, as sketched on the left.
As with the oscillator this cannot go on arbitrarily. It should be intuitive that we require $\langle \hat{L}_z^2 \rangle \leq \langle \hat{\mathbf{L}}^2 \rangle$ (we can proof this, but it is a bit tricky). Hence there shall again be a top and bottom rung of the ladder, such that $\hat{L}_+ f_t = 0$ and $\hat{L}_- f_b = 0$. We expect the maximum and minimal value of $m\hbar$ to be somehow related to ℓ.

To find out how exactly they are related, let us look at $\hat{\mathbf{L}}^2 f_t$. In preparation, we can show (Griffith/exercise), that

$$\hat{\mathbf{L}}^2 = \hat{L}_\pm\hat{L}_\mp + \hat{L}_z^2 \mp \hbar\hat{L}_z. \tag{4.62}$$

Applying the lower sign of Eq. (4.62) to the top state (top rung of the ladder) gives

$$\hat{\mathbf{L}}^2 f_t = \hat{L}_- \underbrace{\hat{L}_+ f_t}_{=0} + \underbrace{\hat{L}_z^2 f_t}_{=(\hbar\bar{\ell}_t)^2 f_t} + \hbar \underbrace{\hat{L}_z f_t}_{=\hbar\bar{\ell}_t f_t} = \hbar^2\bar{\ell}_t(\bar{\ell}_t + 1) f_t. \tag{4.63}$$

Similarly, using (4.62) with the upper sign and applying it to the bottom state (bottom rung of the ladder)

$$\hat{\mathbf{L}}^2 f_b = \hat{L}_+ \underbrace{\hat{L}_- f_b}_{=0} + \underbrace{\hat{L}_z^2 f_b}_{=(\hbar\bar{\ell}_b)^2 f_b} - \hbar \underbrace{\hat{L}_z f_b}_{=\hbar\bar{\ell}_b f_b} = \hbar^2\bar{\ell}_b(\bar{\ell}_b - 1) f_b. \tag{4.64}$$

At the same time, we already know from before that $\hat{\mathbf{L}}^2 f_t = \lambda f_t = \hbar^2\ell(\ell+1) f_t$ and $\hat{\mathbf{L}}^2 f_b = \lambda f_b = \hbar^2\ell(\ell+1) f_b$ with the same ℓ, which is the orbital quantum number. We thus have the two equations

$$\ell(\ell+1) = \bar{\ell}_t(\bar{\ell}_t + 1), \qquad \ell(\ell+1) = \bar{\ell}_b(\bar{\ell}_b - 1), \tag{4.65}$$

which come up with four solutions for $\bar{\ell}_t$ and $\bar{\ell}_b$. Out of those only one has the required property that $\bar{\ell}_t > \bar{\ell}_b$ and that is $\bar{\ell}_t = \ell$ and $\bar{\ell}_b = -\ell$. Since we are reaching from $-\ell$ to ℓ in N integer steps, we must have $\ell = N/2$, so ℓ must be an integer or half-integer. The case of integers reproduces the ranges for the azimuthal quantum number m that we had listed near Eq. (4.51). The possibility of half-integer ℓ will be used for spin in section **??**.

4.5 Position representation of angular momentum states

To use the algebraic treatment to also find the position space states in section 4.3, we again mirror what we did for the harmonic oscillator. First we require the

Position space representation of ladder operators

$$\hat{L}_\pm = \pm\hbar e^{\pm i\varphi}\left(\frac{\partial}{\partial\theta} \pm i\cot\theta\frac{\partial}{\partial\varphi}\right). \tag{4.66}$$

- You can show this using Eq. (4.36) and Eq. (4.57).

We now know that $\hat{L}_+ Y_\ell^\ell = 0$, which using (4.66) becomes

$$\hbar e^{\pm i\varphi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right) Y_\ell^\ell(\theta,\varphi) = 0. \tag{4.67}$$

We already know from (4.46) that the φ dependence takes the form $e^{im\varphi}$, which we can use here: Because of it we know that $\frac{\partial}{\partial\varphi}Y_\ell^\ell(\theta,\varphi) = i\ell Y_\ell^\ell(\theta,\varphi)$. Inserting that gives

$$\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right)\underbrace{Y_\ell^\ell(\theta,\varphi)}_{=e^{i\ell\varphi}\Theta_\ell^\ell(\theta)} = 0 \Leftrightarrow \left(\frac{\partial}{\partial\theta} - \ell\cot\theta\right)\Theta_\ell^\ell(\theta) = 0 \tag{4.68}$$

Using $d\sin\theta/d\theta = \cos\theta$ and $\cot\theta = \cos\theta/\sin\theta$, we can reshape this as

$$\begin{aligned}
&\frac{d\Theta_\ell^\ell(\theta)}{\Theta_\ell^\ell(\theta)} = \ell\frac{d(\sin\theta)}{\sin\theta}, \Leftrightarrow \\
&\log\Theta_\ell^\ell(\theta) = \ell\log(\sin\theta) + const, \quad \Leftrightarrow \quad \Theta_\ell^\ell(\theta) = \mathcal{N}(\sin\theta)^\ell.
\end{aligned} \tag{4.69}$$

where $\mathcal{N}$ can be fixed by normalisation. We can now find all the other angular momentum eigenfunctions down to $Y_\ell^{-\ell}$ by repeatedly applying $\hat{L}_-$ as in (4.66). What we find, up to a sign, is (4.51). Unfortunately that is not quite obvious, but if you are sceptical about the statement you can try it out at least for the few examples given in table 2.

We have now worked out all important properties of the eigenfunction of the angular momentum operators $\hat{\mathbf{L}}^2$ and $\hat{L}_z$. These functions describe the angular part of quantum states and quantum dynamics whenever the potential is spherically symmetric. In the next week we finally also sort out the radial part, for which we have to pick a specific potential. We shall of course pick the one for the Hydrogen atom.