Spherical Harmonics

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1 Introduction

Simply put, spherical harmonics are the angular components of the solutions to Laplace's equation in spherical coordinates. Spherical harmonics play an active role in many different fields such as quantum mechanics and computer graphics.

I was originally introduced to spherical harmonics in my quntum mechanics course. As parts of the solutions to the spherical Laplace equation, it makes sense that spherical harmonics would also arise as solutions to the Schrodinger equation in spherical coordinates when we seperate the radial and the angular variables. While working on a related assignment question, I found myself opening up a whole can of very tedious calculations. In these notes I intend to introduce the spherical harmonics from a the physical perspective and then write out many of the very tedious calculations that I had to go through. Writing out these tedious calculations might seem like a big waste of time. However, I think it will be useful for anyone who wants to know where the explicit form of spherical harmonics actually comes from, which can only be seen by reading through these tedious calculations. These notes also serve as a place to keep these calculations as a reference so that I never, ever have to perform these calculations ever again.

In addition to the tedious calculations, I will present the much more interesting approach to spherical harmonics. It seems ever since I learned about group theory and representation theory, I have been looking for applications of it in everything that I do. Luckily, the spherical harmonics can be realized through a gorup theoretic approac as well, which I will develop here.

At the end I would like to talk about where else we will see spherical harmonics other than in physics.

2 Deveopment from the Physical Persepctive

Spherical harmonics pop up naturally in quantum mechanics when we discuss the position-space representations of angular momentum. When we find these representations, we notice that there is a distinct radial symmetry present. That is, we find that the angular momentum operators in position-space spherical coordinates are completely independent of the radial vector r, and *only* dependent on the angular variables θ and ϕ. A fairly detaield derivation of the position-space representations of the angular momenta can be found in [3]. For now we will just quote the equations from that reference as

$$\hat{L}_x = \frac{\hbar}{i}\left(-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right) \tag{1}$$

$$\hat{L}_y = \frac{\hbar}{i}\left(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right) \tag{2}$$

$$\hat{L}_z = \frac{\hbar}{i}\left(\frac{\partial}{\partial\phi}\right) \tag{3}$$

It is interesting to note that out of all of the above representations, $\hat{L}_z$ is by far the simplest. However, this is just a result of our following the conventional defintion of the spherical cooredintes. We could redefine our spherical coordinates so that either $\hat{L}_y$ or $\hat{L}_x$ had the simplest form. NOTE: IT MIGHT BE NICE TO HAVE DIFFERENT TIKZ DIAGRAMS HERE SHOWING HOW THE SPHERICAL COORDINATES ACTUALLY HAVE BEEN DEFINED.

We can combine the equations in 1 to find a position-space representation for the square of the total angular momentum, given by

$$\hat{\mathbf{L}}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \tag{4}$$

So we see that neither the components of the angular momentam, nor the square of the total angular momentum depend on the variable r. In this case, r is the magnitude of the poisition vector for a point in space. So if the angular momentum is completely independent of r, it means that rotating the position eigenstates changes the direction of the position vector but not the megnitude. This allows us to isolate the angular dependence (OF THE WAVEFUNCTION?) and determine the amplitude for the state of the definite angular momentum to be at the angles θ and ϕ, which we denote by

$$\langle\theta,\phi|l,m\rangle = Y_l^m(\theta,\phi) \tag{5}$$

So in this notation, our energy eigenfunctions are given by

$$\langle r,\theta,\phi|E,l,m\rangle = R(r)Y_l^m(\theta,\phi) \tag{6}$$

3 Computing the Genereal form of the Spherical Harmonics

The most natural question to ask after developing this theory is: what do these spherical harmonics $Y_l^m(\theta,\phi)$ actually look like in their general form?

We start by intruducing the raising and lowering operators, which are written in their position-space representation as

$$\hat{L}_\pm = \frac{\hbar}{i}e^{\pm i\phi}\left(\pm i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\right) \tag{7}$$

The raising and lowering operators, collectively called the ladder operators, are operators which raise (respectively, lower) the eigenvalue of the operator on which they are acting. Basically, if the raising operator $\hat{L}_+$ acts on a spherical harmonic Y_l^m, the result is some eigenvalue multiple of Y_l^{m+1}. Similarely, the lowering operator $\hat{L}_-$ acting on a spherical harmonic Y_l^m yields some eigenvalue multiple of Y_l^{m-1}. Now, in the basis where the $\hat{L}^2$ eigenvalue is l, we know that the values of the $\hat{L}_z$ eigenvalues must be $m = 0, \pm 1, \ldots, \pm l$. In other words, the spherical harmonic Y_l^{l+1} is just equal to zero in the his basis. Thus, we have the equation

$$\langle \theta, \phi | \hat{L}_+ | l, l \rangle = \frac{\hbar}{i} e^{i\phi} \left(\frac{\partial}{\partial \theta} - \cot \theta \frac{\partial}{\partial \phi} \right) \langle \theta, \phi | l, l \rangle = 0 \tag{8}$$

This is a simpe differential equation which we solve to yeild

$$Y_l^l(\theta, \phi) = C_l e^{il\phi} \sin^l \theta \tag{9}$$

Now comes the tedious part. We would like to determine the constant C_l. Townsend, hiding many steps, jumps straight to the results. This works well if you're looking for continuity and flow in a textbook, but it hides several pages of tedious manipulations and is a bit misleading in my opinion. Luckily I found the full devlopment in [2] which I am writing here in my own words, mostly for my own understanding. We begin with the normalizaiton contraint on the wavefuntions. Due the seperation of the radial parts and the angular parts of this of the eigenfunctions, we should be able to normalize them seperately. In general, the normalization condition is

$$\int | \langle r, \theta, \phi | E, l, m \rangle |^2 \mathrm{d}^3 r = \int |R(r)|^2 |Y_l^m(\theta, \phi)|^2 \mathrm{d}^3 r \tag{10}$$

In spherical coordinates, we're working with the differential volume element given by

$$\mathrm{d}^3 r = r^2 \mathrm{d}r \sin \theta \mathrm{d}\theta \mathrm{d}\phi \tag{11}$$

Since, as previously stated, we can seperate the radial and the angular components of our wave function, our normalization condition becomes

$$\int_0^\infty r^2 |R(r)|^2 \mathrm{d}r \int_0^\pi \int_0^{2\pi} |Y_l^m(\theta, \phi)|^2 \sin \theta \mathrm{d}\phi \mathrm{d}\theta = 1 \tag{12}$$

The radial componentents should normalize on their own, so that

$$\int_0^\infty r^2 |R(r)|^2 \mathrm{d}r = 1 \tag{13}$$

This, our normalization contraint on the spherical harmonics is given by

$$\int_0^\pi \int_0^{2\pi} |Y_l^m(\theta, \phi)|^2 \sin \theta \mathrm{d}\phi \mathrm{d}\theta = 1 \tag{14}$$

3.1 Computing Y_l^l

We will first compute the eigenstate with the highest possible eigenvalue $m = l$. Plugging our value of $Y_l^l(\theta, \phi)$ given in Equation9 into the above normalization condition, we get

$$\int_0^\pi \int_0^{2\pi} |Y_l^l(\theta, \phi)|^2 \sin \theta \mathrm{d}\phi \mathrm{d}\theta = |C_l|^2 \int_0^\pi \int_0^{2\pi} \sin^{2l} \theta \sin \theta \mathrm{d}\phi \mathrm{d}\theta = 1 \tag{15}$$

Note that the exponentials annihilated each other when we took the complex conjugate. Now, letting

$$I_l = \int_0^\pi \sin\theta \sin^{2l}\theta \mathrm{d}\theta, \tag{16}$$

we can isolate for $|C_l|$ to get

$$|C_l|^2 = \frac{1}{2\pi I_l} \tag{17}$$

Now, to compute I_l, we first make the change of variables $w = \cos\theta$. This gives

$$\begin{aligned}
I_l &= \int_{-1}^{1} \left(1 - w^2\right)^l \mathrm{d}w & (18)\\
&= \int_{-1}^{1} (1 - w^2)(1 - w^1)^{l-1} \mathrm{d}w & (19)\\
&= \int_{-1} 1(1 - w^2)^{l-1} \mathrm{d}w - \int_{-1}^{1} w^2 (1 - w^2)^{l-1} \mathrm{d}w & (20)\\
&= I_{l-1} - \int_{-1}^{1} w^2 (1 - w^2)^{l-1} \mathrm{d}w & (21)
\end{aligned}$$

We can integrate by parts to yield the recurrance relation

$$I_l = I_{l-1} = \frac{1}{2l} I_l \Rightarrow I_l = \frac{2l}{2l+1} I_{l-1}, \tag{22}$$

from which we can derive (Note: this is worked on the assignment that I handed in - I'll add it here when that is returned to me.)

$$I_l = \frac{(2l)!!}{(2l+1)!!} I_0 = \frac{2^{2l+1}(l!)^2}{(2l+1)!} \tag{23}$$

Finally, we can compute C_l form Equation 24 (Again, more details which are on the assignment)

$$C_l = \frac{1}{2^l l!} \sqrt{\frac{(2l+1)!}{4\pi}} \tag{24}$$

Note that this only determines C_l up to an overall phase factor. It is concentional to choose this phase as being -1. This phase convention is known as the Condon-Shortley phase. Thus, we have

$$Y_l^l(\theta, \phi) = \frac{(-1)^l}{2^l l!} \sqrt{\frac{(2l+1)!}{4\pi}} e^{il\phi} \sin^l\theta, \tag{25}$$

just as Townsend derived.

3.2 *Computing Y_l^m*

Now, we know that when $m = l$, m is in its highest possible index - that is, we can only go down from here. That means that in order to compute the general form of Y_l^m, we should just apply the lowering operator to Y_l^l $l - m$ times. In other words, we have

$$(\hat{L}_-) Y_l^l = \hbar\sqrt{(l+m)(l-m+1)} Y_l^{l-1} \tag{26}$$

So in general, we have

$$(\hat{L}_-)^{l-m} Y_l^m = \hbar^{l-m} \sqrt{(2l)(1) \cdot (2l-1)(2) \cdot (2l-2) \ldots (l-m)(l+m+1)} Y_l^{l-(l-m)} \tag{27}$$

$$= (\hbar)^{l-m} \sqrt{\frac{(2l)!(l-m)!}{(l+m)!}} Y_l^m \tag{28}$$

Rearranging this gives us

$$Y_l^m = \sqrt{\frac{(l+m)!}{(2l)!(l-m)!}} \left(\frac{L_-}{\hbar}\right)^{l-m} Y_l^l \tag{29}$$

Now it remains to find a general experssion for the operator $\hat{L}_-$ acting on Y_l^l a total of $l-m$ times. We know that Y_l^l is of the form $Ae^{in\phi}F(\theta)$ and

$$(\hat{L}_-)Ae^{in\phi}F(\theta) = A(\hat{L}_-)e^{in\phi}F(\theta) \tag{30}$$

so all we really need to know is how $\hat{L}_-$ acts on functions of the form $e^{in\phi}F(\theta)$. It can be shown that (show this eventually), that

$$\left(\hat{L}_\pm\right)^p e^{in\phi}F(\theta) = (\mp\hbar)^p \, e^{i(n\pm p)\phi} (\sin\theta)^{p\pm n} \frac{\mathrm{d}^p}{\mathrm{d}(\cos\theta)^p} \left[(\sin\theta)^{\mp n} F(\theta)\right] \tag{31}$$

Substituting this result into Equation 29 and using the value of the coefficient C_l from Equation 24, it is easy to see that

$$Y_l^m(\theta,\phi) = \frac{(-1)^l}{2^l l!} \sqrt{\frac{(2l+1)(l+m)!}{4\pi(l-m)!}} e^{im\phi} (\sin\theta)^{-m} \frac{\mathrm{d}^{l-m}}{\mathrm{d}(\cos\theta)^{l-m}} (\sin\theta)^{2l} \tag{32}$$

Alternatively, we could compute Y_l^m by allowing $(\hat{L}_+)$ to act a total of $l+m$ on Y_l^{-l}, where Y_l^{-l} can be computed my plugging $m = -l$ into Equation 32. This would yeild the slightly different yet equivalent form

$$Y_l^m = \frac{(-1)^{l+m}}{2^l l!} \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} e^{im\phi} (\sin\theta)^m \frac{\mathrm{d}^{l+m}}{\mathrm{d}(\cos\theta)^{l+m}} (\sin\theta)^{2l} \tag{33}$$

4 Explicit Forms and Visualizations

We give explicit forms for the spherical harmonics and the graphs of $|Y_l^m|^2$ for $l = 0, 1, 2$. It is shown in [3] these these graphs are the orbital shells of the atom - i.e. where the electron can be found. This was especially exciting because I remember being told in high school that these were the orbitals and upon pressing for my information, I was always just given the answer "because Quantum Mechanics", but now I have seen it first hand!

References

[1] J. J. Sakurai, J. Napolitano, *Modern Quantum Mechanics*. Addison-Wesley, Massachusetts, 2nd Edition, 2011.

[2] Cohen and Tannoudji

[3] J. S. Townsend, *A Modern Approach to Quantum Mechanics*. University Science Books, 2nd Edition, 2012.

[4] S. Sternberg, *Group Theory and Physics*. Cambridge University Press, Cambridge, UK 1994.