Spherical harmonics

In our earlier article "Angular momentum in quantum mechanics," we calculated the eigenvalues of angular momentum operator. In this article, we will find the eigenvectors. In particular, we will use spherical coordinates i.e.,

$$x = r \sin\theta \cos\phi \tag{1}$$

$$y = r \sin\theta \sin\phi \tag{2}$$

$$z = r \cos\theta \tag{3}$$

In other words,

$$r^2 = x^2 + y^2 + z^2 \tag{4}$$

$$\cos\theta = \frac{z}{r}, \qquad \tan\phi = \frac{y}{x} \tag{5}$$

We will first express the angular momentum operators in terms of spherical coordinates. To this end, we need to do some exercises first:

Problem 1. Show

$$\frac{\partial r}{\partial z} = \frac{x}{r}, \qquad \frac{\partial r}{\partial y} = \frac{y}{r}, \qquad \frac{\partial r}{\partial z} = \frac{z}{r} \tag{6}$$

Problem 2. From (5) and (6), show

$$-\sin\theta \frac{\partial \theta}{\partial x} = -\frac{zx}{r^3} \tag{7}$$

Problem 3. From (1), (3) and (7), show that

$$\frac{\partial \theta}{\partial x} = \frac{\cos\phi \cos\theta}{r} \tag{8}$$

Problem 4. Show similarly,

$$\frac{\partial \theta}{\partial y} = \frac{\sin\phi \cos\theta}{r}, \qquad \frac{\partial \theta}{\partial z} = -\frac{\sin\theta}{r} \tag{9}$$

Problem 5. From (5), show

$$\frac{\partial \phi}{\partial x} = -\frac{y\cos^2\phi}{x^2}, \qquad \frac{\partial \phi}{\partial y} = \frac{\cos^2\phi}{x}, \qquad \frac{\partial \phi}{\partial z} = 0 \tag{10}$$

Now, we are ready to derive the following formulas for angular momentum in terms of spherical coordinate:

$$L_x = i\hbar \left(\sin\phi \frac{\partial}{\partial\theta} + \cot\theta\cos\phi \frac{\partial}{\partial\phi} \right) \tag{11}$$

$$L_y = i\hbar \left(-\cos\phi \frac{\partial}{\partial\theta} + \cot\theta\sin\phi \frac{\partial}{\partial\phi} \right) \tag{12}$$

$$L_z = -i\hbar \frac{\partial}{\partial\phi} \tag{13}$$

These can be derived by using chain-rules. For example,

$$\begin{aligned} L_x &= -i\hbar \left[y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \right] \\ &= -i\hbar \left[y\left(\frac{\partial r}{\partial z}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial z}\frac{\partial}{\partial\theta} + \frac{\partial\phi}{\partial z}\frac{\partial}{\partial\phi} \right) - z\left(\frac{\partial r}{\partial y}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial y}\frac{\partial}{\partial\theta} + \frac{\partial\phi}{\partial y}\frac{\partial}{\partial\phi} \right) \right] \end{aligned}$$

Problem 6. Derive (11) and (13).

The form of (13) is not surprising, considering that the rotation around z axis generates rotation in the angle ϕ. (Recall our earlier article "Noether's theorem.")

Is it a coincidence that r doesn't appear in (11), (12), and (13)? No. Let me make a long argument. First, recall that angular momentum generates the rotation, which doesn't change the distance from the center, which is given by $r = \sqrt{x^2+y^2+z^2}$. In other words, the rotation doesn't change the distance squared ($r^2 = x^2+y^2+z^2$). Thus, we have

$$[L_x, r^2] = [L_y, r^2] = [L_z, r^2] = 0 \tag{14}$$

If you recall our earlier article "Angular momentum in quantum mechanics," another way of seeing this is that scalars such as r^2 do not change under a rotation.

So, why is there no r dependenc in $\vec{L}$? Recall

$$\vec{L} = \vec{r} \times \vec{p} = \vec{r} \times (-i\hbar\nabla) \tag{15}$$

From ∇, we see that each term in $\vec{L}$ must contain the first derivative of coordinates, as each term in the gradient contains the first derivative of coordinate as a factor. That is indeed what we see in (11), (12), (13). Each term has either $\partial/\partial\theta$ or $\partial/\partial\phi$ as a factor. Now, for the sake of argument, let's *assume* that $\vec{L}$ depended on r. In other words, it contained factors such as r or $\partial/\partial r$. (Factors such as $\partial/\partial r^2$ are impossible.) However, if you have the factor $\partial/\partial r$, (14) is not satisfied because of Leibniz rule. Therefore, there should be no partial derivative with respect to r in the angular momentum.

Then, we are left with the case in which "coefficients" for $\partial/\partial\theta$ or $\partial/\partial\phi$ contain r dependence terms. In other words,

$$\vec{L} \sim i\hbar f(r,\theta,\phi)\frac{\partial}{\partial\theta} + i\hbar g(r,\theta,\phi)\frac{\partial}{\partial\phi} \tag{16}$$

However, from the dimensional analysis, $f(r,\theta,\phi)$ and $g(r,\theta,\phi)$ must be *dimensionless*. Then, f and g must not have r dependence, as you can never make a dimensionless quantity out of r. This completes the argument that there is no r dependence in $\vec{L}$.

Back to our story, (11), (12) and (13) yield:

$$L^2 = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right) \tag{17}$$

Now, let's denote the eigenfunctions of angular momentum by Y_ℓ^m, i.e.,

$$Y_\ell^m(\theta,\phi) = \langle\theta,\phi|\ell,\ m\rangle \tag{18}$$

just like $\phi(x) = \langle x|\phi\rangle$. They satisfy

$$L^2 Y_\ell^m(\theta,\phi) = \ell(\ell+1)\hbar^2 Y_\ell^m(\theta,\phi) \tag{19}$$

$$L_z Y_\ell^m(\theta,\phi) = m\hbar Y_\ell^m(\theta,\phi) \tag{20}$$

where L_z and L^2 are given by (13) and (17). They are normalized as

$$\int Y_{\ell'}^{m'*}(\theta,\phi) Y_\ell^m(\theta,\phi)d\Omega = \delta_{\ell\ell'}\delta_{mm'} \tag{21}$$

where $d\Omega = \sin\theta d\theta d\phi$ i.e., the standard measure for 2-sphere.

Now, let's solve (20) first. We have

$$\frac{\partial}{\partial\phi}Y_\ell^m(\theta,\phi) = imY_\ell^m(\theta,\phi) \tag{22}$$

Thus, we see that the spherical harmonics can be expressed as

$$Y_\ell^m(\theta,\phi) = A(\theta)e^{im\phi} \tag{23}$$

for a suitable function $A(\theta)$. Recall now that, in spherical coordinate system, (r,θ,ϕ) and $(r,\theta,\phi+2\pi)$ are the same point. Thus, we need to have

$$Y_\ell^m(\theta,\phi) = Y_\ell^m(\theta,\phi+2\pi) \tag{24}$$

Plugging this into (23), we get

$$e^{2\pi im} = 1 \tag{25}$$

Thus, m must be an integer. Notice that m doesn't admit half-integers such as 1/2, 3/2, 5/2. Therefore, we see that orbital angular momentum (i.e., the angular momentum due to actual movement of particle) can only admit integer m, therefore, only integer l, which means that it cannot admit half-integer l. Spin angular momentum is not due to the actual movement of particle, of which the angular momentum can be described by formulas such as (11), (12) and (13). Otherwise, we won't be able to have spin 1/2 particle, such as electrons, quarks and neutrinos.

Problem 7. From (21), show that

$$Y_0^0(\theta, \phi) = \frac{1}{\sqrt{4\pi}} \tag{26}$$

apart from an arbitrary phase factor which we can choose to be 1.

Problem 8. Show that $Y_\ell^{-m}(\theta, \phi) = cY_\ell^{m*}(\theta, \phi)$ for some phase factor c.

From now on, I will explain something that I think I never learned at my quantum mechanics class, or if I had, I completely forgot, until I had to look up my references to write this article.

If we plug (23) into (17) and (19), we get

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\frac{\sin^2\theta}{\sin\theta}\frac{dA}{d\theta}\right) + \left(\ell(\ell+1) - \frac{m^2}{\sin^2\theta}\right) A = 0 \tag{27}$$

where we changed the partial derivative into the ordinary derivative, as there is only one variable, namely, θ.

If we let $\mu \equiv \cos\theta$, then the above expression can be re-expressed as

$$\frac{d}{d\mu}\left((1-\mu^2)\frac{dA}{d\mu}\right) + \left(\ell(\ell+1) - \frac{m^2}{1-\mu^2}\right) A = 0 \tag{28}$$

This equation looks too complicated. Let's try to solve it first in a simple case $m = 0$. Let's also assume that we didn't know that the eigenvalues of L^2 operator (19) were $\ell(\ell+1)\hbar^2$. Instead let's just say that the eigenvalue was a number we call $\lambda\hbar^2$. Then, the above equation becomes

$$\frac{d}{d\mu}\left((1-\mu^2)\frac{dA}{d\mu}\right) + \lambda A = 0 \tag{29}$$

This is called "Legendre differential equation." Let's try to solve it by expressing A as a power series as follows

$$A(\mu) = \sum_{n=0}^{\infty} a_n \mu^n \tag{30}$$

Then, we get (**Problem 9.**)

$$(n+2)(n+1)a_{n+2} + (\lambda - n(n+1))a_n = 0 \tag{31}$$

which implies

$$a_{n+2} = \frac{n(n+1) - \lambda}{(n+2)(n+1)} a_n \tag{32}$$

Notice that if a_n where n is odd, and a_n when n is even are unrelated. For example, if we set $a_0 \neq 0$, we can set all $a_{2k+1} = 0$, because a_0 only determines a_{2k}. Similarly, if we set $a_1 \neq 0$, we can set all $a_{2k} = 0$, because a_1 only determines a_{2k+1}. Thus, we see that a "eigen" solution to Legendre's differential equation can be always an even function or an odd function.

Given this, there are two cases for (32). The series terminates as $\lambda = n(n+1)$ for a non-negative integer n, and the series doesn't terminate as $\lambda \neq n(n+1)$ for any non-negative integer. Let's see what happens in the second case first. In such a case, for large n we have

$$a_{n+2} \sim \frac{n}{n+2} a_n \tag{33}$$

which implies, asymptotically,

$$a_n \sim \frac{c}{n} \tag{34}$$

for non-zero a_n (i.e., either n odd or even.) Recalling that $-1 \leq \mu \leq 1$ (i.e., $\mu = \cos\theta$), we see that for large n, (30) becomes something like

$$A(1) \sim \sum_k \frac{1}{2k}, \text{ or } \sum_k \frac{1}{2k+1} \tag{35}$$

which means that it is lograithmically divergent. Similarly, $A(-1)$ is also logarithmically divergent.

Given this, recall what we wanted to do. We were trying to find the wave function. We do not want the wave function to diverge badly; we won't be able to normalize such a wave function. So, we need to discard the case in which the series does't terminate. Therefore, $\lambda = n(n+1)$ for a non-negative integer n. In other words, by solving differential equation, we found out that the eigenvalues of L^2 operator is given by $n(n+1)\hbar^2$ just as we found it alternatively by commutation relations among L_x, L_y, L_z.

Now, notice that $a_{l+2} = 0$, even though $a_\ell \neq 0$ if $\lambda = \ell(\ell+1)$. So, we see that $A(\mu)$ is a degree l polynomial, if $\lambda = \ell(\ell+1)$. In particular, if l is even, it is even function and it is odd function, if l is odd.

Using (32) to find $A(\mu)$ is tedious. Instead we can use Rodrigues' formula. If we denote $A(\mu)$ with $\lambda = l(l+1)$ by $P_\ell(\mu)$, Rodrigues' formula says

$$P_\ell(\mu) = \frac{1}{2^\ell \ell!} \frac{d^\ell}{d\mu^\ell} (\mu^2 - 1)^\ell \tag{36}$$

where the normalization is chosen to satisfy $P_\ell(1) = 1$. $P_\ell(\mu)$ is called "Legendre polynomial."

Problem 10. Show that $P_\ell(-1) = (-1)^\ell$, if $P_\ell(1) = 1$.

Let's check that it indeed satisfies (29). First, let's not worry about the overall normalization factor as we can take care of it later. Let's say $v = (\mu^2 - 1)^\ell$. Then, we want to show that

$$A(\mu) = \frac{d^\ell v}{d\mu^\ell} \tag{37}$$

satisfies (29). To prove this, first notice that

$$(\mu^2 - 1)\frac{dv}{d\mu} = (\mu^2 - 1)\ell(\mu^2 - 1)^{\ell-1}2\mu = 2\ell\mu v \tag{38}$$

If you differentiate this $(\ell + 1)$ times by μ, we get (**Problem 11.**)

$$\begin{aligned}(\mu^2 - 1)\frac{d^{\ell+2}v}{d\mu^{\ell+2}} + (\ell+1)2\mu\frac{d^{\ell+1}v}{d\mu^{\ell+1}} + \frac{(\ell+1)\ell}{2!}\cdot 2\cdot\frac{d^\ell v}{d\mu^\ell}& \\ = 2\ell\mu\frac{d^{\ell+1}v}{d\mu^{\ell+1}} + 2\ell(\ell+1)\frac{d^\ell v}{d\mu^\ell}&\end{aligned} \tag{39}$$

$$(\mu^2 - 1)\frac{d^{\ell+2}v}{d\mu^{\ell+2}} + 2\mu\frac{d^{\ell+1}v}{d\mu^{\ell+1}} = \ell(\ell+1)\frac{d^\ell v}{d\mu^\ell} \tag{40}$$

Now, notice that, when $\lambda = \ell(\ell+1)$, (29) can be re-written as

$$(\mu^2 - 1)\frac{d^2A}{d\mu^2} + 2\mu\frac{dA}{d\mu} = \ell(\ell+1)A \tag{41}$$

Thus, we conclude that (37) is the solution.

Given this, we need to find the normalization factor. (37) can be re-written as

$$A(\mu) = \frac{d^\ell\left((\mu-1)^\ell(\mu+1)^\ell\right)}{d\mu^\ell} \tag{42}$$

Using Leibniz rule, we can express $A(\mu)$ in terms of products of $(\mu - 1)$ and $(\mu + 1)$. However, when we plug in $\mu = 1$, the term involving $(\mu - 1)$ will be zero. (**Problem 12.** Show that $A(1) = \ell!2^\ell$.) Thus, we indeed proved Rodrigues' formula (36).

Now, the orthogonality relation of Legendre polynomials. Recall their origin (23). We see that

$$Y_\ell^0(\theta, \phi) = A(\theta) \tag{43}$$

Apart from normalization, we have $A(\theta) = P_\ell(\cos\theta)$. Thus, by plugging $m = 0$ into (21), we see that

$$\int_0^{2\pi} d\phi \int_{\theta=0}^{\theta=\pi} P_\ell(\cos\theta)P_{\ell'}(\cos\theta)\sin\theta d\theta = \delta_{\ell\ell'}f(\ell) \tag{44}$$

for a suitable $f(\ell)$. Thus, we obtain

$$\int_{-1}^{1} P_\ell(\mu)P_{\ell'}(\mu)d\mu = \delta_{\ell\ell'}g(\ell) \tag{45}$$

where $g(l) = f(l)/(2\pi)$ which is to be determined now. From (36), we have

$$\begin{aligned}
\int_{-1}^{1} P_\ell(\mu)P_\ell(\mu)d\mu &= \frac{1}{(2^\ell \ell!)^2}\int_{-1}^{1}\left(\frac{d^\ell}{d\mu^\ell}(\mu^2-1)^\ell\right)\left(\frac{d^\ell}{d\mu^\ell}(\mu^2-1)^\ell\right)d\mu \\
&= \frac{(-1)^\ell}{(2^\ell \ell!)^2}\int_{-1}^{1}\left(\frac{d^{2\ell}}{d\mu^{2\ell}}(\mu^2-1)^\ell\right)(\mu^2-1)^\ell d\mu \qquad (46)\\
&= \frac{(-1)^\ell(2\ell)!}{(2^\ell \ell!)^2}\int_{-1}^{1}(\mu^2-1)^\ell d\mu \qquad (47)\\
&= \frac{(2\ell)!}{(2^\ell \ell!)^2}\int_{0}^{\pi}\sin^{2\ell+1}\theta d\theta = \frac{2}{2\ell+1} \qquad (48)
\end{aligned}$$

where in the last line we used the result of Problem 5. of "Integration by parts."

In other words,

$$\int_{-1}^{1} P_\ell(\mu)P_{\ell'}(\mu)d\mu = \frac{2}{2\ell+1}\delta_{\ell\ell'} \tag{49}$$

Now, I introduce the generating function of Legendre polynomials, which is given by

$$\Phi(\mu, h) = \frac{1}{\sqrt{1-2\mu h+h^2}} \tag{50}$$

and satisfies the property

$$\Phi(\mu, h) = \sum_{l=0}^{\infty} P_\ell(\mu)h^l \tag{51}$$

Problem 13. By expanding (50), check that $P_0(\mu) = 1$, $P_1(\mu) = \mu$, $P_2(\mu) = (3\mu^2-1)/2$.

Checking that $P_\ell(1) = 1$ is eaiser. If we plug $\mu = 1$ to (50), we get

$$\Phi(1, h) = \frac{1}{\sqrt{1-2h+h^2}} = \frac{1}{1-h} = 1 + h + h^2 + h^3 + \cdots \tag{52}$$

Thus, we can conclude $P_\ell(1) = 1$ from (51).

To check that $\Phi(\mu, h)$ indeed generates the Legendre polynomials, we first need to verify the following (**Problem 14.**):

$$(1-\mu^2)\frac{\partial^2\Phi}{\partial\mu^2} - 2\mu\frac{\partial\Phi}{\partial\mu} + h\frac{\partial^2(h\Phi)}{\partial h^2} = 0 \tag{53}$$

If you plug (51) into the above formula, we get

$$(1-\mu^2)\sum_{\ell=0}^{\infty}\frac{d^2P_\ell(\mu)}{d\mu^2}h^\ell - 2\mu\sum_{\ell=0}^{\infty}\frac{dP_\ell(\mu)}{d\mu}h^\ell + \sum_{\ell=0}^{\infty}\ell(\ell+1)P_\ell(\mu)h^\ell = 0 \quad (54)$$

which means

$$(1-\mu^2)\frac{dP_\ell(\mu)}{d\mu^2} - 2\mu\frac{dP_\ell(\mu)}{d\mu} + \ell(\ell+1)P_\ell(\mu) = 0 \quad (55)$$

which is exactly (28) upon the identification $m = 0$. So, why did Legendre come up with Legendre polynomials in 1783? Because he needed it for his astronomial research. We know that, if the distrubition of the density inside the Earth has a perfect spherical symmetry, then outside the Earth, the gravity acts as if all the mass of the Earth were located at the center of the Earth. It is indeed a good approximation, but we know that the Earth is not a perfect sphere but a spheroid, bulging slighlty at the equator due to the daily rotation of the Earth. To calculate more accurately, he needed a better approximation.

See Fig. 1. You are at a position R from the center of the Earth. What is the contribution of the gravitational potential dV at your position due to the one marked with a big black dot that has mass dm and located r from the center of the Earth, and makes an angle θ with the line that connects your position to the center of the Earth?

It is given by

$$dU = -G\frac{dm}{s} = -G\frac{dm}{\sqrt{R^2 - 2Rr\cos\theta + r^2}} \quad (56)$$

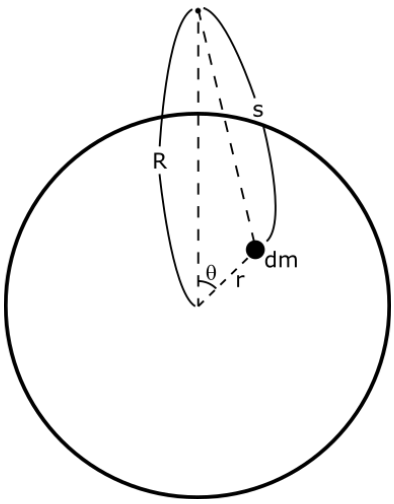

Figure 1: At the point R from the center of the Earth, the gravitational potential contribution from dm is given by $dV = -Gdm/s$

where we used the law of cosines to calculate s. Then, we have

$$dU = -\frac{Gdm}{R}\left(\frac{1}{\sqrt{1 - 2\frac{r}{R}\cos\theta + \frac{r^2}{R^2}}}\right) \tag{57}$$

If we Taylor-expand the expression in the parenthesis in terms of (r/R), we can write

$$dU = -\frac{Gdm}{R}\left(1 + a\left(\frac{r}{R}\right) + b\left(\frac{r}{R}\right)^2 + c\left(\frac{r}{R}\right)^3 + \cdots\right) \tag{58}$$

This is the idea of Legendre polynomial. If you let $h = r/R$, $\mu = \cos\theta$. The term in the parenthesis is exactly the generating function of the Legendre polynomials. In other words,

$$a = P_1(\cos\theta) = \cos\theta, \quad b = P_2(\cos\theta) = \frac{3\cos^2\theta - 1}{2} \tag{59}$$

and so on.

Thus, the total gravitational potential can be obtained by integrating dU over all the regions inside the Earth. Notice that the term $P_1(\cos\theta)$ gives the potential proportional to $1/R^2$. In other words, it gives the gravitational attraction inversely proportional to R^3. Those of you who read "Electric dipole" would recognize this as the dipole moment. Similarly, $P_2(\cos\theta)$ gives the quadrupole moment, and $P_3(\cos\theta)$ give the octupole moment.

Problem 15. Explain why the "gravitational" dipole moment and the "gravitational" octupole of the Earth are zero, at least in very good approximations.

In this article, we talked about the spherical harmonics and Legendre polynomials $P_\ell(\cos\theta)$, which are proportional to $Y_\ell^0(\theta,\phi)$, and are also solutions to Legendre differential equation. Actually, (28) is called "associated Legendre differential equation," and its solution $P_\ell^m(\cos\theta)$ is called "associated Legendre polynomial." Of course, $Y_\ell^m(\theta,\phi)$ is proportional to $P_\ell^m(\cos\theta)e^{im\phi}$. We will not talk more about associated Legendre polynomials, as readers can consult Wikipedia or any other references. Finally, in Appendix, we prove "addition theorem for spherical harmonics."

Summary

- $Y_\ell^m(\theta,\phi)$ is an eigenfunction of the total angular momentum operator L^2 with the eigenvalue $l(l+1)\hbar^2$. It is also an eigenfunction of L_z with the eigenvalue $m\hbar$.

- $Y_\ell^0(\theta,\phi)$ is equal to the Legendre polynomial $P_\ell(\cos\theta)$ up to a normalization constant.

- $P_0(\cos\theta) = 1, P_1(\cos\theta) = \cos\theta$. $P_\ell(\mu)$ is an even function for l even, and $P_\ell(\mu)$ is an odd function for l odd.

- If we Taylor-expand a gravitational or Coulomb force, the dipole moment (i.e., the force inversely proportional to R^3) is given by P_1 and the quadrupole moment (i.e., the force inversely proportional to R^4) is given by P_2.

Appendix

I will add the proof later.