Laplace's Equation in Spherical Coordinates and Legendre's Equation (II)

1 Associated Legendre's equation and associated Legendre functions

A slightly amended form of Legendre's equation is used very often in physical applications. This is known as the *associated Legendre's equation*, and has the following form:

$$(1-x^2)f^{''}(x) - 2xf^{'}(x) + \left[l(l+1) - \frac{m^2}{1-x^2}\right]f(x) = 0 \tag{1}$$

where, normally , l and m are integer numbers. Its solutions, as one can expect, are strongly correlated to those obtained from Legendre's equation. We could attempt at solving equation (1) just like we have done for Legendre's equation. Instead, another procedure can be used. It avoids expanding the solution in power series and, rather, tries to build them starting from those of Legendre's equation. The calculation carried out for the purpose are quite lengthy and tedious, but it is worth illustrating the method, because it provides us with another technique useful in mathematical physics, i.e. the possibility of solving a differential equation using solutions from a different, but related, equation.
Let us, then, start with,

$$(1-x^2)g^{''}(x) - 2xg^{'}(x) + l(l+1)g(x) = 0,$$

and suppose that $g(x)$ is a solution of this equation. If both members are derived m times,

$$(1-x^2)[g^{(m)}(x)]^{''} - 2x(m+1)[g^{(m)}(x)]^{'} + [l(l+1) - m(m+1)][g^{(m)}(x)] = 0 \tag{2}$$

where,

$$g^{(m)}(x) \equiv \frac{\mathrm{d}^m}{\mathrm{d}x^m}g(x)$$

Now we ask whether it is feasible to find a function y through which $g^{(m)}(x)$ is expressed according to,

$$g^{(m)}(x) = (1-x^2)^r y(x) \tag{3}$$

Given that we do not know r, and do not know of any condition on y, the only reasonable thing to do is to compute the first and second derivative of (3), and replace the obtained expressions into equation (2), hoping to meet with some familiar result. After few simplifications, the following forms for first and second derivative are derived:

$$[g^{(m)}(x)]^{'} = -2rx(1-x^2)^{r-1}y + (1-x^2)^r y^{'}$$

$$[g^{(m)}(x)]'' = (1-x^2)^r y'' - 4rx(1-x^2)^{r-1}y' - 2r(1-x^2)^{r-1}y + 4r(r-1)x^2(1-x^2)^{r-2}y$$

These two expressions, together with the definition of $g^{(m)}$, are to be replaced in equation (2). Eventually, we get,

$$(1-x^2)y'' - 2x(m+1+2r)y' + \left[l(l+1) - m(m+1) - 2r + \frac{4r(r-1)+4r(m+1)}{1-x^2}x^2\right] y = 0$$

Remeber that our initial purpose was to find solutions for the associated Legendre's equation. The above equation does, indeed, coincide with that equation if $r = -m/2$. Therefore, considering definition (3), we have reached the conclusion that those functions y, expressed as,

$$y(x) \equiv (1-x^2)^{m/2} \frac{\mathrm{d}^m}{\mathrm{d}x^m} g(x) \tag{4}$$

with $g(x)$ a solution of Legendre's equation, are solutions of the associated Legendre's equation. We will be, in particular, interested in those solutions derived from Legendre polynomials, known as *associated Legendre functions*. They are defined once two positive integers, say l and m, have been fixed. l refers, as we expect, to the particular Legendre polynomial, while m refers to the number of derivatives to be taken. Using symbol $P_l^m(x)$ for an associated Legendre function, the definition, following (4), will be:

$$P_l^m(x) \equiv (1-x^2)^{m/2} \frac{\mathrm{d}^m}{\mathrm{d}x^m} P_l(x) \tag{5}$$

It goes without saying that $m \leq l$, because all derivatives of a polynomial of l-th degree, with order greater than l, are zero.

EXAMPLE 1.
Starting from $P_3(x) = (1/2)(5x^3 - 3x)$, build all possible associated Legendre functions.
Solution.
The assigned Legendre polynomial is of degree 3. Therefore we can only build the associated functions P_3^0, P_3^1, P_3^2 and P_3^3. This is easily done using definition (5):

$$\begin{aligned} P_3^0(x) &= \frac{1}{2}(5x^3 - 3x) \\ P_3^1(x) &= \frac{3}{2}(5x^2 - 1)\sqrt{1-x^2} \\ P_3^2(x) &= 15x(1-x^2) \\ P_3^3(x) &= 15(1-x^2)\sqrt{1-x^2} \end{aligned}$$

From definition (5) it would appear that it is only possible to build associated Legendre functions with positive values of m, because we do not know how to compute derivatives of negative index. This is not true, as negative m's can be used, as long as $-l \leq m \leq l$. Let us, in fact, re-write definition (5) with $P_l(x)$ defined through Rodrigues' formula (see Lecture 8):

$$P_l^m(x) = (1-x^2)^{m/2} \frac{\mathrm{d}^m}{\mathrm{d}x^m}\left[\frac{1}{2^l l!}\frac{\mathrm{d}^l}{\mathrm{d}x^l}(x^2-1)^l\right] = \frac{1}{2^l l!}(1-x^2)^{m/2}\frac{\mathrm{d}^{l+m}}{\mathrm{d}x^{l+m}}(x^2-1)^l$$

Re-writing now the above formula with m replaced by $-m$ yields,

$$P_l^{-m}(x) = \frac{1}{2^l l!}(1-x^2)^{-m/2}\frac{\mathrm{d}^{l-m}}{\mathrm{d}x^{l-m}}(x^2-1)^l$$

This expression is always computable, because $l - m$ is always greater or equal to zero. We have, thus, shown that it is feasible to define associated Legendre functions with negative values of m.

The formula just defined, though, is not normally used. It is, rather, preferred to compute P_l^m for positive values of m (through formula (5)) and then apply the following relation,

$$P_l^{-m}(x) = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(x) \tag{6}$$

To derive this relation is not straightforward. The demonstration makes use of Rodrigues' formula and of Leibniz' rule for multiple derivatives of a product of functions. It is not appropriate to work out the derivation here, as the important bit of information to remember is formula (6) itself.

<u>EXAMPLE 2</u>.
Write the five associated Legendre functions with $l = 2$, as functions of θ.
<u>Solution</u>.
We need, first of all, the P_2 legendre polynomial, $P_2(x) = (1/2)(3x^2 - 1)$. Then we start calculating the associated Legendre functions with positive $m \leq 2$, i.e. for $m = 0, 1, 2$, using formula (5):

$$\begin{aligned}
P_2^0(x) &= P_2(x) = \frac{1}{2}(3x^2 - 1) \\
P_2^1(x) &= \sqrt{1-x^2}\frac{\mathrm{d}}{\mathrm{d}x}P_2(x) = 3x\sqrt{1-x^2} \\
P_2^2(x) &= (1-x^2)\frac{\mathrm{d}^2}{\mathrm{d}x^2}P_2(x) = 3(1-x^2)
\end{aligned}$$

From P_2^1 and P_2^2, P_2^{-1} and P_2^{-2} are readily calculated using formula (6):

$$\begin{aligned}
P_2^{-1}(x) &= -\frac{(2-1)!}{(2+1)!}P_2^1(x) = -\frac{1}{2}x\sqrt{1-x^2} \\
P_2^{-2}(x) &= \frac{(2-2)!}{(2+2)!}P_2^2(x) = \frac{1}{8}(1-x^2)
\end{aligned}$$

These five functions can be re-expressed as functions of θ by using $x = \cos\theta$:

$$\begin{aligned}
P_2^2(\theta) &= 3\sin^2\theta \\
P_2^1(\theta) &= 3\cos\theta\sin\theta \\
P_2^0(\theta) &= \frac{1}{2}(3\cos^2\theta - 1) \\
P_2^{-1}(\theta) &= -\frac{1}{2}\cos\theta\sin\theta \\
P_2^{-2}(\theta) &= \frac{1}{8}\sin^2\theta
\end{aligned}$$

2 Orthogonality of associated Legendre functions

It is possible to prove, although it will not be done here, that the associated Legendre functions satisfy orthogonality relations similar to those for Legendre polynomials. More specifically, we are interested in the following orthogonality integral,

$$\int_{-1}^{1} P_l^m(x)P_{l'}^m(x)\mathrm{d}x = \frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}\delta_{ll'} \tag{7}$$

where $\delta_{ll'}$ is the kroenecker symbol of indices l and l'. It is important to pay attention to the upper indices of the two associated Legendre functions; they need to be the same. An orthogonality

relation exists for associated Legendre functions with same lower indices, but different upper ones; this relation is, though, rarely used for applications.
The orthogonality integral in (7) is expressed with the integration variable x. More often the angular variable θ ($0 \leq \theta \leq \pi$) is used. Integral (7) is, in this case, replaced by,

$$\int_0^\pi P_l^m(\cos\theta) P_{l'}^m(\cos\theta)\sin\theta \mathrm{d}\theta = \frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}\delta_{ll'} \tag{8}$$

3 Spherical harmonics

In many physical problems the angular part of a given equation can be isolated, thus giving origin to a function depending only on angular variables, typically θ and ϕ ($0 \leq \theta \leq \pi$, $0 \leq \phi < 2\pi$). Given the ubiquity of functions depending on angular space variables in all subfields of physics, it is important to have an orthogonal set with which any of these functions can be expanded as a series in an angular range. As θ and ϕ vary on the surface of a sphere (centred at the origin and of arbitrary radius), we will be talking about series expansion "on the sphere".
The orthogonal functions normally used for the expansion on the sphere are called *spherical harmonics*. They are symbolically indicated as $Y_l^m(\theta,\phi)$ and defined as follows,

$$Y_l^m(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta)\exp(im\phi) \quad , \quad \begin{array}{l} l = 0,1,2,3,\dots \\ -l \leq m \leq l \end{array} \tag{9}$$

Sometimes a sign (or phase) factor, $(-1)^m$ is prepended to definition (9). This is known as *Condon-Shortley phase*, and it is a convenient choice for applications related to quantum mechanics.
A simple relation exists between $Y_l^m(\theta,\phi)$ and $Y_l^{-m}(\theta,\phi)$. It is quite straightforward to derive it. We start from definition (9),

$$Y_l^{-m}(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l+m)!}{(l-m)!}} P_l^{-m}(\cos\theta)\exp(-im\phi),$$

then replace P_l^{-m} with (6),

$$Y_l^{-m}(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l+m)!}{(l-m)!}}(-1)^m\frac{(l-m)!}{(l+m)!} P_l^{m}(\cos\theta)\exp(-im\phi)$$

$$\Downarrow$$

$$Y_l^{-m}(\theta,\phi) = (-1)^m\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} P_l^{m}(\cos\theta)\exp(-im\phi) \equiv (-1)^m\, Y_l^{m\,*}(\theta,\phi)$$

We have, thus, proved that,

$$Y_l^{-m}(\theta,\phi) = (-1)^m\, Y_l^{m\,*}(\theta,\phi) \tag{10}$$

EXAMPLE 3.
Write the five spherical harmonics with $l = 2$.
Solution.
First let us calculate Y_2^0, Y_2^1, Y_2^2 using formula (9); then it is easier to compute Y_2^{-1} and Y_2^{-2} through relation (10).

$$Y_2^0(\theta,\phi) \quad = \quad \sqrt{\frac{5}{4\pi}} P_2^0(\cos\theta) = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1)$$

$$
\begin{aligned}
Y_2^1(\theta,\phi) &= \sqrt{\frac{5}{4\pi}\frac{1}{3!}}P_2^1(\cos\theta)\exp(i\phi) = \sqrt{\frac{15}{8\pi}}\cos\theta\sin\theta\exp(i\phi) \\
Y_2^2(\theta,\phi) &= \sqrt{\frac{5}{4\pi}\frac{1}{4!}}P_2^2(\cos\theta)\exp(2i\phi) = \sqrt{\frac{15}{32\pi}}\sin^2\theta\exp(2i\phi)
\end{aligned}
$$

Now Y_2^{-1} and Y_2^{-2} are readily computed as,

$$
\begin{aligned}
Y_2^{-1}(\theta,\phi) &= -\,{Y_2^1}^*(\theta,\phi) = -\sqrt{\frac{15}{8\pi}}\cos\theta\sin\theta\exp(-i\phi) \\
Y_2^{-2}(\theta,\phi) &= {Y_2^2}^*(\theta,\phi) = \sqrt{\frac{15}{32\pi}}\sin^2\theta\exp(-2i\phi)
\end{aligned}
$$

We have said that any function of θ and ϕ (behaving sufficiently well), $f(\theta,\phi)$, can be expanded in spherical harmonics series:

$$
f(\theta,\phi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} a_{lm}Y_l^m(\theta,\phi) \tag{11}
$$

A double summation is needed here because each spherical harmonic is identified by two indices. We know how to compute coefficients a_{lm} only if the spherical harmonics form an orthogonal set. A definition of orthogonality for sets of functions has already been given in Lecture 7 and Lecture 8, for Bessel functions and Legendre polynomials. In those cases the functions were real. The spherical harmonics are complex functions, therefore we need to extend the definition of orthogonality to functions in the complex field of numbers. Given two functions $\alpha(x)$ and $\beta(x)$, with values from $\mathbb{R}$ to $\mathbb{C}$, they are said to be orthogonal if,

$$
\int_{x\in I}\alpha^*(x)\beta(x)p(x)\mathrm{d}x = 0 \tag{12}
$$

where $p(x)$ is the usual weight function, introduced to help the integral to converge, and where the integration is carried out over a certain interval I. For the orthogonality of the spherical harmonics, thus, the following definition seems appropriate,

$$
\int_0^{\pi}\int_0^{2\pi} {Y_l^m}^*(\theta,\phi)Y_{l'}^{m'}(\theta,\phi)\sin\theta\mathrm{d}\theta\mathrm{d}\phi = \delta_{ll'}\delta_{mm'} \tag{13}
$$

It just needs to be proved it is true. Using definition (9) we have,

$$
\int_0^{\pi}\int_0^{2\pi} {Y_l^m}^*(\theta,\phi)Y_{l'}^{m'}(\theta,\phi)\sin\theta\mathrm{d}\theta\mathrm{d}\phi =
$$

$$
\sqrt{\frac{(2l+1)(2l'+1)}{16\pi^2}\frac{(l-m)!(l'-m')!}{(l+m)!(l'+m')!}}\int_0^{\pi}\int_0^{2\pi} P_l^m(\cos\theta)P_{l'}^{m'}(\cos\theta)\exp[i(m'-m)]\sin\theta\mathrm{d}\theta\mathrm{d}\phi =
$$

$$
\sqrt{\frac{(2l+1)(2l'+1)}{4}\frac{(l-m)!(l'-m')!}{(l+m)!(l'+m')!}}\int_0^{\pi} P_l^m(\cos\theta)P_{l'}^{m'}(\cos\theta)\sin\theta\mathrm{d}\theta\left\{\frac{1}{2\pi}\int_0^{2\pi}\exp[i(m'-m)]\mathrm{d}\phi\right\}
$$

The integral in braces is a well-known integral. It is always zero, unless $m'=m$, in which case it is 1. Therefore,

$$
\int_0^{\pi}\int_0^{2\pi} {Y_l^m}^*(\theta,\phi)Y_{l'}^{m'}(\theta,\phi)\sin\theta\mathrm{d}\theta\mathrm{d}\phi =
$$

$$\sqrt{\frac{(2l+1)(2l'+1)}{4}\frac{(l-m)!(l'-m')!}{(l+m)!(l'+m')!}}\int_0^\pi P_l^m(\cos\theta)P_{l'}^m(\cos\theta)\sin\theta\mathrm{d}\theta\delta_{mm'}$$

The integral on the right-hand side can be computed with formula (8). We obtain, thus,

$$\int_0^\pi\int_0^{2\pi} Y_l^{m\,*}(\theta,\phi)Y_{l'}^{m'}(\theta,\phi)\sin\theta\mathrm{d}\theta\mathrm{d}\phi =$$

$$\sqrt{\frac{(2l+1)(2l'+1)}{4}\frac{(l-m)!(l'-m')!}{(l+m)!(l'+m')!}}\frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}\delta_{ll'}\delta_{mm'} = \delta_{ll'}\delta_{mm'},$$

that is, result (13). Through property (13) it is possible, quite straightforwardly, to find coefficients a_{lm} in the expansion (11). They are given by the following formula,

$$a_{lm} = \int_0^\pi\int_0^{2\pi} f(\theta,\phi)\,Y_l^{m\,*}(\theta,\phi)\sin\theta\mathrm{d}\theta\mathrm{d}\phi \tag{14}$$

4 The one-particle central-force problem in quantum mechanics

One of the most important applications involving spherical harmonics is found in quantum mechanics. Consider the stationary state of a point-like particle of mass M under the influence of a central force represented by the potential $V(r)$. As it will be shown in any introductory course of quantum mechanics, this process is essentially described by the time-independent *Schrodinger equation*,

$$-\frac{\hbar^2}{2M}\nabla^2\psi(r,\theta,\phi) + V(r)\psi(r,\theta,\phi) = E\psi(r,\theta,\phi) \tag{15}$$

where E is the energy of the particle and $\hbar \equiv h/(2\pi)$, with h the Planck constant. The function ψ is the *wave function*. It is the important quantity to deal with in quantum mechanics. Its square modulus, $|\psi(r,\theta,\phi)|^2$, is equal to the probability density of finding the particle at (r,θ,ϕ). We want to show here that the solution to this equation can be factorised in a radial and an angular part, where the angular part coincides with the spherical harmonics.
Let us, thus, postulate for $\psi(r,\theta,\phi)$ the following factorised expression,

$$\psi(r,\theta,\phi) = R(r)L(\theta,\phi) \tag{16}$$

Let us, also, expand equation (15) using the spherical form of the laplacian,

$$-\frac{\hbar^2}{2M}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}\right] + V(r)\psi - E\psi = 0$$

If we, now, insert the factorised form (16) in this equation, we obtain,

$$-\frac{\hbar^2}{2M}\left[\frac{L}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right) + \frac{R}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial L}{\partial\theta}\right) + \frac{R}{r^2\sin^2\theta}\frac{\partial L^2}{\partial\phi^2}\right] + V(r)RL - ERL = 0$$

(bent derivatives are used for L because it depends on two variables, θ and ϕ) and, multiplying by r^2 and dividing by RL,

$$-\frac{\hbar^2}{2M}\frac{1}{R}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right) + r^2[V(r)-E] = \frac{\hbar^2}{2M}\left[\frac{1}{L\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial L}{\partial\theta}\right) + \frac{1}{L\sin^2\theta}\frac{\partial L^2}{\partial\phi^2}\right] \tag{17}$$

The left-hand side of this equation depends exclusively on r, while its right-hand side exclusively on θ and ϕ. The equation has non-trivial solutions only if both members are equal to a common constant α. Equating the right-hand side of (17) to α yields,

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

We can, once more, carry out a factorisation, writing $L(\theta,\phi)=T(\theta)F(\phi)$. Replacing this form for L in the above equation leads to,

$$\frac{F}{\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}T}{\mathrm{d}\theta}\right)+\frac{T}{\sin^2\theta}\frac{\mathrm{d}^2F}{\mathrm{d}\phi^2}=\frac{2M}{\hbar^2}\alpha TF$$

or, multiplying both sides by $\sin^2\theta/TF$ and rearranging,

$$\frac{\sin\theta}{T}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}T}{\mathrm{d}\theta}\right)-\frac{2M}{\hbar^2}\alpha\sin^2\theta=-\frac{1}{F}\frac{\mathrm{d}^2F}{\mathrm{d}\phi^2}\tag{18}$$

Again, equation (18) has non-trivial solutions only if both members are equal to a same constant which, has we have learnt, needs to be a positive one, m^2. Two independent solutions for the ϕ-part of the equation are $\cos(m\phi)$ and $\sin(m\phi)$. This time we will choose the equivalent form $\exp(\pm im\phi)$, in order to be able to connect the final solution to the spherical harmonics introduced in the last section. Given that the wave function has to return to the same value after a rotation of 360 degrees around the z-axis, m needs to be an integer number. Equating now the left-hand side of (18) to m^2 we get,

$$\frac{1}{\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}T}{\mathrm{d}\theta}\right)+\left(-\frac{2M\alpha}{\hbar^2}-\frac{m^2}{\sin^2\theta}\right)T=0$$

It is useful, at this stage, to introduce the new variable $x=\cos\theta$, thus obtaining,

$$(1-x^2)\frac{\mathrm{d}^2T}{\mathrm{d}x^2}-2x\frac{\mathrm{d}T}{\mathrm{d}x}+\left(-\frac{2M\alpha}{\hbar^2}-\frac{m^2}{1-x^2}\right)T=0$$

We recognise the above equation as the associated Legendre's equation (1). Finite solutions at ±1 will be obtained only if $2M\alpha/\hbar^2=l(l+1)$, with l a positive or null integer. This leads to,

$$\alpha=-\frac{\hbar^2}{2M}l(l+1)\quad,\quad l=0,1,2,3,\ldots\tag{19}$$

Thus, the solutions of equation (18) are given by,

$$L(\theta,\phi)=T(\theta)F(\phi)=P_l^m(\cos\theta)\exp(\pm im\phi)$$

these, up to constants, are essentially the spherical harmonics (9). We can, therefore, state that solutions of the angular part of Scrodinger equation (15) are the spherical harmonics,

$$L(\theta,\phi)=Y_l^m(\theta,\phi)\quad,\quad\begin{array}{c}l=0,1,2,3,\ldots\\-l\leq m\leq l\end{array}$$

For the radial part of the equation we simply have to equate the left-hand side of (17) to α as given by relation (19),

$$-\frac{\hbar^2}{2M}\frac{1}{R}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right)+r^2[V(r)-E]=-\frac{\hbar^2}{2M}l(l+1)$$

$$\Downarrow$$

$$-\frac{\hbar^2}{2M}\left(\frac{\mathrm{d}^2R}{\mathrm{d}r^2}+\frac{2}{r}\frac{\mathrm{d}R}{\mathrm{d}r}\right)+\frac{l(l+1)\hbar^2}{2Mr^2}R+V(r)R=ER \tag{20}$$

The resolution of equation (20) will be attempted once the potential $V(r)$ is defined (for instance, $V(r)$ is proportional to $1/r$ for the electron in the hydrogen atom). The interesting lesson to be learnt here is that for the class of problems described in this section, the angular solution is always given by the spherical harmonics. This is why they play such a fundamental role in quantum mechanics.