# 1 Topic 4: Laplace Equation in Spherical Co-ordinates and Multipole Expansion

Reading Assignment: Jackson Chapter 3.1-3.5

## 1.1 Laplace Equation in Spherical Coordinates

Review of spherical polar coordinates:

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

The three unit vectors

$$\begin{aligned} \mathbf{e}_r &= (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)\,, \\ \mathbf{e}_\theta &= (\cos\theta\cos\phi, \sin\theta\sin\pi, -\sin\theta)\,, \\ \mathbf{e}_\phi &= (-\sin\phi, \cos\phi, 0)) \end{aligned}$$

form a right handed coordinate system in the sense $(r, \theta, \phi)$. The unit of volume is

$$d^3x = r^2\sin\theta dr\,d\theta\,d\phi = r^2\,dr\,d\Omega \tag{1}$$

where the element of solid angle is

$$d\Omega = d\left(\cos\theta\right)d\phi \tag{2}$$

the delta function in spherical polar coordinates is

$$\delta^3\left(\mathbf{r}-\mathbf{r}'\right) = \frac{1}{r^2\sin\theta}\delta\left(r-r'\right)\delta\left(\theta-\theta'\right)\delta\left(\phi-\phi'\right) \tag{3}$$

and Laplace's equation is

$$\nabla^2\Phi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Phi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Phi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\Phi}{\partial\phi^2} \tag{4}$$

Can the co-ordinates be separated? (not obvious) The answer is yes, this is an important example of a separable coordinate system for the Laplacian.

Let

$$\Phi = R\left(r\right)T\left(\theta\right)P\left(\phi\right) \tag{5}$$

so

$$TP\frac{1}{r^2}\left(\frac{d}{dr}\left(r^2R'\right)\right) + RP\frac{1}{\sin\theta r^2}\frac{d}{d\theta}\left(\sin\theta T'\right) + \frac{RT}{r^2\sin^2\theta}\frac{d^2P}{d\phi^2} = 0 \tag{6}$$

Multiply by $\frac{r^2 \sin^2 \theta}{RTP}$ to get

$$\frac{\sin^2 \theta}{R} \frac{d}{dr} \left( r^2 R' \right) + \frac{1}{T} \sin \theta \frac{d}{d\theta} \left( \sin \theta T' \right) + \frac{1}{P} \frac{d^2 P}{d\phi^2} = 0 \tag{7}$$

So we have

$$\frac{1}{P} \frac{d^2 P}{d\phi^2} = -m^2 \tag{8}$$

choose $m$ real so that $P$ is a sinusoid. If we put this in above and divide by $\sin^2 \theta$

$$\frac{1}{R} \frac{d}{dr} \left( r^2 R' \right) + \frac{1}{T \sin \theta} \frac{d}{d\theta} \left( \sin \theta T' \right) - \frac{m^2}{\sin^2 \theta} = 0 \tag{9}$$

Choose

$$\frac{1}{R} \frac{d}{dr} \left( r^2 R' \right) = const > 0 \tag{10}$$

so that $R$ is not a "wiggly" function. We can imagine that this is going to be applicable to spherical charge distributions where the radial part dies or grows with radius. As an ansatz, take

$$\begin{aligned} R &= r^l \\ R' &= l r^{l-1} \\ r^2 R' &= l r^{l+1} \\ \frac{d}{dr} \left( r^2 R' \right) &= l \left( l+1 \right) r^l \end{aligned}$$

so that

$$\frac{1}{R} \frac{d}{dr} \left( r^2 R' \right) = l \left( l+1 \right) = const = c \geq 0 \tag{11}$$

of $c$ is given then $l^2 + l - c = 0 \rightarrow$

$$\begin{aligned} l_1 &= \frac{-1 + \sqrt{1+4c}}{2} \\ l_2 &= \frac{-1 - \sqrt{1+4c}}{2} \end{aligned}$$

so $l_1 + 1 = -l_2$. Thus we could alternatively choose $l = l_1$ as the constant rather than $c$ and write the two solutions

$$R = A_l r^l + B_l r^{-l-1} \tag{12}$$

and

$$\begin{aligned} \frac{d}{dr} \left( r^2 R' \right) &= \frac{d}{dr} \left( A_l l r^{l+1} - \left( l+1 \right) B_l r^2 r^{-l-2} \right) \\ &= \left( A_l l \left( l+1 \right) r^l + l \left( l+1 \right) B_l r^{-l-1} \right) \\ &= l \left( l+1 \right) R = CR \end{aligned}$$

So we finally have the equation for $\theta$:

$$l\left(l+1\right)+\frac{1}{T\sin\theta}\frac{d}{d\theta}\left(\sin\theta T'\right)-\frac{m^2}{\sin^2\theta}=0 \tag{13}$$

or

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dT}{d\theta}\right)+\left(l\left(l+1\right)-\frac{m^2}{\sin^2\theta}\right)T=0 \tag{14}$$

The function $T$ for the special case that $l$ and $m$ are integers (and special initial conditions) is called the associated Legendre function $P_l^m\left(\cos\theta\right)$. $P_l^m\left(x\right)$ satisfies

$$\frac{d}{dx}\left(\left(1-x^2\right)\frac{d}{dx}P_l^m\left(x\right)\right)+\left(l\left(l+1\right)-\frac{m^2}{1-x^2}\right)P_l^m\left(x\right)=0 \tag{15}$$

This is the first time in the course that we have seen a non-trivial example of a differential equation of the form

$$\frac{d}{dx}\left(p\left(x\right)\ f_i'\right)+q_{(i)}f_i=0 \tag{16}$$

where $f_i=f_i\left(x\right)$, $i$ can be a collection of indices, *not necessarily integers*, and both $p\left(x\right)$ and $q_{(i)}\left(x\right)$ are given functions. If it is the case that $p\left(x\right)\geq 0$ and $q\left(x\right)\geq 0$ for a range of $x$ (or if both are negative) then the solutions will be oscillatory in that range since if $f>0$, then $\frac{d}{dx}\left(pf'\right)<0$ or $pf'$ is decreasing and since $p>0$, $f'$ is decreasing. Eventually $f'$ will become negative, $f$ will decrease and pass through zero and its sign will change, yielding the inverse of the above argument, so

the general behavior of $f_i$ when $p>0$ and $q_i>0$. The simplest example is $p=const, q=const$ so $p>0$ and $q>0$ we have

$$f_k''+k^2f_k=0\rightarrow f_k\propto e^{\pm ikx} \tag{17}$$

A crucially important property of these oscillatory functions is their orthogonality. We've seen this property for sines and cosines - now look at it more generally. To find the orthogonality condition, write for two different $i$'s – say $i,j$

$$\begin{aligned}\left(pf_i'\right)'+q_{(i)}f_i &= 0\\ \left(pf_j'\right)'+q_{(j)}f_j &= 0\end{aligned}$$

Cross multiply and subtract to get

$$f_j\left(pf_i'\right)'-f_i\left(pf_j'\right)'+\left(q_{(i)}-q_{(j)}\right)f_if_j=0 \tag{18}$$

But the first term is

$$\frac{d}{dx}\left[f_jpf_i'-f_ipf_j'\right] \tag{19}$$

which is trivially integrable

$$\int_a^b dx\frac{d}{dx}\left[f_jpf_i'-f_ipf_j'\right]+\int_a^b\left(q_{(i)}-q_{(j)}\right)f_if_jdx=0 \tag{20}$$

$$p(b)\left[f_j(b)\,f_i'(b) - f_i(b)\,f_j'(b)\right] - p(a)\left[f_j(a)\,f_i'(a) - f_i(a)\,f_j'(a)\right] = \int_a^b \left(q_{(j)} - q_{(i)}\right) f_i f_j dx \tag{21}$$

If the points $a\&b$ are chosen in such a way that the left hand side of this equation vanishes (e.g., in Legendre's equation where $p = 1 - x^2$, choose $a = -1, b = +1$) and if the right hand side is a proper integral, then we get

$$\int_a^b (q_{(j)} - q_{(i)}) f_i f_j \, dx = 0 \tag{22}$$

Thus if $q_{(j)} - q_{(i)} \neq 0$, we have that the functions $f_i$ and $f_j$ are orthogonal with the weight function $q_{(j)} - q_{(i)}$

Start with the $m = 0$ case which yields $P_l^0(\cos\theta) \equiv P_l(\cos\theta)$ – the Legendre function, or if $l$ is a positive integer or zero, the *Legendre polynomials*. Then

$$p = 1 - x^2, q_{(i)} = l\,(l+1) \tag{23}$$

We therefore get the result

$$\int_{-1}^{1} P_l P_{l'} \, dx = 0 \quad l \neq l' \tag{24}$$

or

$$\int_{-1}^{1} P_l P_{l'} \, dx = \delta_{ll'} N_{(l)} \tag{25}$$

More generally, if $m \neq 0$ then $q_{lm} = l\,(l+1) - \frac{m^2}{1-x^2}$ and so

$$q_{lm} - q_{l'm} = l\,(l+1) - l'\,(l'+1) \tag{26}$$

so

$$\int_{-1}^{1} P_l^m(x)\, P_{l'}^m(x)\, dx = \delta_{ll'} N_{(l)m} \tag{27}$$

where $N_{lm}$ is a normalization fator;

$$N_{lm} = \int_{-1}^{1} (P_l^m)^2 \, dx \tag{28}$$

and its value is conventional since the differential equation is linear and so any multiple of a solution is a solution. Note that for sinusoids in which $p = 1, q = k^2 > 0$ we can arrange the l.h.s. to vanish by choosing $a\&b$ suitably – e.g. for $k =$ integer$= n$ we have for example

$$\int_0^{2\pi} \sin nx \sin mx \, dx = 0 \text{ if } n \neq m \tag{29}$$

etc.

In general in solving the Sturm-Liouville equation, the points (if any) at which $p\,(x_s) = 0$ are called singular points since at them the $2^{nd}$ derivative term vanishes from the equation. If you were to divide the equation by $p\,(x)$, i.e., write it as

$$f_i'' + \frac{P'}{p} f_i' + \frac{q_{(i)}}{p} f_i = 0 \tag{30}$$

Then $p = 0$ gives trouble – so $x_s$ where $p(x_s)$ are the singular pointsof the equation and except in special cases, the solutions have singularities at these points.

Furthermore, if you make a series expansion for to represent the function about some point (take a Taylor series expansion about some point), the radius of convergence in the complex plane (extend the independent variable $x$ to the complex plane – $z = x + iy$) is a circle from the point of expansion to the nearest singular point in the complex plane. For Legendre's equation with $m = 0$, we have

$$\frac{d}{dx}\left(\left(1-x^2\right)\frac{dP_l}{dx}\right) + l\,(l+1)\,P_l = 0 \tag{31}$$

One finds that if $l$ is an integer that the series solutions (for certain initial conditions) of this form are in fact simple polynomials, ans so $x = \pm 1$ have no problems. As usual, since this is a $2^{nd}$ order differentialequation, we need two initial conditions; e.g. a value and slope at $x = 0$, to get a particular solution. As with sinusoids we take the "cosine-like" function to have

$${}^{c}P_l\,(x=0) = 1 \quad {}^{c}P_l'\,(x=0) = 0 \quad \text{(cosine-like)} \tag{32}$$

and

$${}^{s}P_l\,(x=0) = 0 \quad {}^{s}P_l'\,(x=0) = 1 \quad \text{(sine-like)} \tag{33}$$

The above notation is by the way not conventional (more later).

To understand what happens, write

$$P_l\,(x) = \sum_{n=0}^{\infty} a_n x^n \tag{34}$$

Then if you plug this into

$$\frac{d}{dx}\left(\left(1-x^2\right)P_l'\right) + l\,(l+1)\,P_l = 0 \tag{35}$$

and set each coefficient of a power of $x$ to zero, you get

$$a_{m+2} = \frac{m\,(m+1) - l\,(l+1)}{(m+1)\,(m+2)}a_m \tag{36}$$

For the cosine like solution we have $a_o = 1, a_1 = 0$ and the equation for the coefficients gives $a_2, a_4, a_6 ... \neq 0$, $a_1, a_3, a_5 ... = 0$. So

$${}^{c}P_l\,(x) = 1 + \frac{-l\,(l+1)}{2}x^2 + \left(\frac{-l\,(l+1)}{2}\right)\left(\frac{2\cdot 3 - l\,(l+1)}{3\cdot 4}\right)x^4 + ... \tag{37}$$

Clearly ${}^{c}P_l\,(x) = {}^{c}P_l\,(-x)$ an even function about the origin and if l is an even number, the series terminates with the $n = l^{th}$ term since the $n = (l+2)^{th}$ term vanishes and all larger ones do also.

So, if

a) $l =$ even ${}^{c}P\,(x)$ is a polynomial andit is usually notated simply by $C_l P_l\,(x)$

b) $l =$ odd, ${}^cP(x)$ is an infinite series and it can be shown to diverge logarithmically at $x = \pm 1$. These functions are usually called $D_l Q_l(x)$ (even function, $l$ odd).

For the sine-like solutions we have $a_o = 0$ , $a_1 = 1$ and the equation gives $a_2, a_4, a_6... = 0$, $a_1, a_3, a_5... \neq 0$. So

$$ {}^sP_l(x) = x + \frac{1 \cdot 2 - l(l+1)}{2 \cdot 3} x^3 + \left( \frac{1 \cdot 2 - l(l+1)}{2 \cdot 3} \right) \left( \frac{3 \cdot 4 - l(l+1)}{4 \cdot 5} \right) x^5 + ... \tag{38} $$

Clearly ${}^sP_l(x) = -{}^sP_l(x)$, an odd function about $x = 0$ and if l is an odd number, the series terminates and we have a polynomial.

So, if

a) $l =$ odd, ${}^sP_l(x)$ is a polynomial and it is usually simply called $P_l(x)$ which is an odd function when $l$ is odd

b) $l =$ even, ${}^sP_l(x)$ is an infinite series divergent at $x = \pm 1$, usually called $Q_l(x)$ (an odd function where $l$ is even).

Finally, if $l$ is not an integer, the series are infinite and divergent as $x \to \pm 1$.

So, in summary, with the conventional normalization constants chosen to make $P_l(+1) = 1$

$$ \begin{aligned} P_o(x) &= 1 \\ P_1(x) &= x \\ P_2(x) &= \frac{1}{2}\left(3x^3 - 1\right) \\ P_3(x) &= \frac{1}{2}\left(5x^3 - 3x\right) \end{aligned} $$

From the general theory and the fact that there are no difficulties with the integral $\int_{-1}^{1} P_l P_{l'} dx$ we get

$$ \int_{-1}^{1} P_l(x) P_{l'}(x) = \frac{2}{2(l) + 1} \delta_{ll'} \tag{39} $$

Jackson gives recursion relations and examples of expansions.

IMPORTANT FACT: The Legendre polynomials are the *only* solutions allowed in problems in which the points $\theta = 0$ and $\theta = \pi$ are contained in the volume under consideration.

For circumstances which do not include both these points, other solutions to Legendre's equation show up – we won't be concerned with these.