Appendix B

Spherical Harmonics

B.1 The Associated Legendre Functions

In this appendix we restrict ourselves to ℓ and m integers with $|m| \leq \ell \geq 0$, and x real. Given the Legendre polynomials $P_\ell(x)$

$$P_\ell(x) = \frac{1}{2^\ell \; \ell!} \; \frac{d^\ell}{dx^\ell}(x^2 - 1)^\ell, \tag{B.1}$$

we define the associated Legendre functions $P_\ell^m(x)$ as

$$P_\ell^m(x) = (1 - x^2)^{m/2} \; \frac{d^m P_\ell(x)}{dx^m}, \tag{B.2}$$

which satisfy the associated Legendre equation:

$$(1 - x^2)\frac{d^2 P_\ell^m}{dx^2} - 2 \; x \; \frac{dP_\ell^m}{dx} + \left[\ell(\ell + 1) - \frac{m^2}{1 - x^2}\right] P_\ell^m = 0 \tag{B.3}$$

and are finite for $|x| = 1$. The $P_\ell^m(x)$ can be computed efficiently with the following equations:

$$P_0^0(x) \; = \; 1, \quad P_1^0(x) = x, \tag{B.4}$$

$$P_m^m(x) \; = \; (2m - 1)!! \; (1 - x^2)^{m/2} \quad (m \geq 1), \tag{B.5}$$

$$P_{m+1}^m(x) \; = \; x \; (2m + 1) \; P_m^m(x) \qquad (m \geq 1), \tag{B.6}$$

$$(\ell - m) \; P_\ell^m(x) \; = \; x \; (2\ell - 1) \; P_{\ell-1}^m(x) - (\ell + m - 1) \; P_{\ell-2}^m(x), \tag{B.7}$$

$$P_\ell^{-m}(x) \; = \; (-1)^m \; \frac{(\ell - m)!}{(\ell + m)!} \; P_\ell^m(x). \tag{B.8}$$

The notation $n!!$ in equation (B.5) denotes the product of all odd integers less than or equal to n. The stable recurrence relation (B.7) can be used successively with equations (B.5) and (B.6) as a starting point to compute $P_\ell^m(x)$ for $m \geq 0$. For negative m, equation (B.8) can be used first.

The equation

$$(x^2-1)\frac{dP_\ell^m}{dx} = -(\ell+1)\,x\,P_\ell^m + (\ell-m+1)\,P_{\ell+1}^m \tag{B.9}$$

can be used to compute the following useful derivatives:

$$\begin{aligned}\frac{\partial P_\ell^m(\cos\theta)}{\partial\theta} &= \frac{1}{\sin\theta}\Big[-(\ell+1)\cos\theta\;P_\ell^m(\cos\theta)\\ &\qquad +(\ell-m+1)P_{\ell+1}^m(\cos\theta)\Big],\end{aligned} \tag{B.10}$$

$$\begin{aligned}\frac{\partial^2 P_\ell^m(\cos\theta)}{\partial\theta^2} &= (\ell+1)\left[1+(\ell+2)\,\frac{\cos^2\theta}{\sin^2\theta}\right]\;P_\ell^m(\cos\theta)\\ &\quad -2\,(\ell+2)\,(\ell-m+1)\,\frac{\cos\theta}{\sin^2\theta}\;P_{\ell+1}^m(\cos\theta)\\ &\quad +(\ell-m+1)\,(\ell-m+2)\,\frac{1}{\sin^2\theta}\;P_{\ell+2}^m(\cos\theta).\end{aligned} \tag{B.11}$$

B.2 The Spherical Harmonics

We define the spherical harmonics $Y_\ell^m(\theta,\varphi)$ as

$$Y_\ell^m(\theta,\varphi) = (-1)^{(m+|m|)/2}\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}}\;P_\ell^{|m|}(\cos\theta)\;e^{im\varphi} \tag{B.12}$$

for $|m| \leq \ell \geq 0$. This definition is equivalent to another form sometimes given in the literature:

$$Y_\ell^m(\theta,\varphi) \;=\; (-1)^m\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\;P_\ell^m(\cos\theta)\;e^{im\varphi}, \tag{B.13}$$

$$Y_\ell^{-m}(\theta,\varphi) \;=\; (-1)^m\;\overline{Y_\ell^m(\theta,\varphi)}, \tag{B.14}$$

where both equations are valid for $m \geq 0$. The phase factor used in definition (B.12), which disappears for positive even or negative m is sometimes called the Condon phase convention. When $m = 0$, $|m| = \ell$ or $0 \neq |m| < \ell$, the spherical harmonic is called zonal respectively sectoral respectively tesseral. The normalisation factor of the spherical harmonics is chosen so that they form a complete orthonormal set over the surface of a sphere:

$$\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \, \sin\theta \, Y_\ell^m(\theta,\varphi) \, \overline{Y_{\ell'}^{m'}(\theta,\varphi)} = \delta_{\ell,\ell'} \, \delta_{m,m'}. \tag{B.15}$$

We will often use the following notation for the sake of brevity:

$$N_\ell^m \equiv (-1)^{(m+|m|)/2} \sqrt{\frac{2\ell+1}{4\pi} \frac{(\ell-|m|)!}{(\ell+|m|)!}} \tag{B.16}$$

which has the simple property

$$N_\ell^{-m} = (-1)^m \, N_\ell^m. \tag{B.17}$$

Note also that $N_0^0 = 1/2\sqrt{\pi}$. The spherical harmonics as defined above obey the following useful recursion relations:

$$\sin\theta \, \frac{\partial Y_\ell^m}{\partial\theta} \; = \; \ell \, J_{\ell+1}^m \, Y_{\ell+1}^m - (\ell+1) \, J_\ell^m \, Y_{\ell-1}^m, \tag{B.18}$$

$$\cos\theta \, Y_\ell^m \; = \; J_{\ell+1}^m \, Y_{\ell+1}^m + J_\ell^m \, Y_{\ell-1}^m, \tag{B.19}$$

where we omitted the arguments of the spherical harmonics and where

$$J_\ell^m = \begin{cases} \sqrt{\dfrac{\ell^2-m^2}{4\ell^2-1}} & \text{if } \; |m| < \ell \\ 0 & \text{if } \; |m| \geq \ell \end{cases} \tag{B.20}$$

The terms with $Y_{\ell-1}^m$ in equations (B.18)-(B.19) can be omitted when $|m| \geq \ell - 1$.

Note that the spherical harmonics have an inversion symmetry with respect to the origin:

$$Y_\ell^m(\pi-\theta, \varphi+\pi) = (-1)^\ell \, Y_\ell^m(\theta,\varphi), \tag{B.21}$$

i.e. the parity is positive for even ℓ and negative for odd ℓ.

B.3 The Functions $d^{\ell}_{k,m}(i)$

The spherical harmonic $Y_\ell^m(\theta,\varphi)$ in the (x,y,z) reference frame (see Appendix A) can be written in terms of a linear combination of spherical harmonics $Y_\ell^k(\theta',\varphi')$ in the (x',y',z') reference frame. The transformation formula is:

$$Y_\ell^m(\theta,\varphi) = \sum_{k=-\ell}^{\ell} d^{\ell}_{k,m}(i) \, Y_\ell^k(\theta',\varphi'), \tag{B.22}$$

where the functions $d^\ell_{k,m}(i)$ can be computed with:

$$
\begin{aligned}
d^\ell_{k,m}(i) \;&=\; \sqrt{\frac{(\ell+k)!\,(\ell-k)!}{(\ell+m)!\,(\ell-m)!}}\;\cos(i/2)^{k+m}\;\sin(i/2)^{2\ell-m-k} \\
&\times \sum_{r=r_1}^{r_2} (-1)^{\ell-m-r} \binom{\ell+m}{\ell-k-r} \binom{\ell-m}{r} \left(\frac{\cos(i/2)}{\sin(i/2)}\right)^{2r}, \qquad \text{(B.23)}
\end{aligned}
$$

where $r_1 = \max\{0, -m-k\}$ and $r_2 = \min\{\ell-m, \ell-k\}$ (see e.g. Condon & Odabasi, 1980). For ℓ and i fixed, the square matrices $d^\ell_{k,m}(i)$ obey the following orthonormality relation:

$$\sum_{n=-\ell}^{\ell} d^\ell_{n,k}(i)\; d^\ell_{n,m}(i) = \delta_{k,m}. \qquad \text{(B.24)}$$

For some special arguments in expression (B.23) we have the following reductions:

$$d^\ell_{k,m}(0) \;=\; \delta_{k,m}, \qquad \text{(B.25)}$$

$$d^\ell_{k,\ell}(i) \;=\; \sqrt{\frac{(2\ell)!}{(\ell+k)!\,(\ell-k)!}}\;\cos(i/2)^{\ell+k}\;\sin(i/2)^{\ell-k}, \qquad \text{(B.26)}$$

$$d^\ell_{k,-\ell}(i) \;=\; (-1)^{\ell+k}\sqrt{\frac{(2\ell)!}{(\ell+k)!\,(\ell-k)!}}\;\cos(i/2)^{\ell-k}\;\sin(i/2)^{\ell+k}, \qquad \text{(B.27)}$$

$$d^\ell_{k,0}(i) \;=\; \sqrt{\frac{4\pi}{2\ell+1}}\,N^k_\ell\,P^{|k|}_\ell(\cos i), \qquad \text{(B.28)}$$

$$d^\ell_{0,\ell-1}(i) \;=\; \frac{\sqrt{(2\ell-1)!}}{2^{\ell-1}\,(\ell-1)!}\;\cos i\;(\sin i)^{\ell-1} \quad \text{if } \ell \geq 1. \qquad \text{(B.29)}$$

We also list some important symmetry relations:

$$
\begin{aligned}
d^\ell_{k,m}(-i) \;&=\; (-1)^{k-m}\,d^\ell_{k,m}(i), && \text{(B.30)}\\
d^\ell_{k,m}(i) \;&=\; d^\ell_{-m,-k}(i), && \text{(B.31)}\\
d^\ell_{m,k}(i) \;&=\; d^\ell_{k,m}(-i), && \text{(B.32)}\\
d^\ell_{m,k}(i) \;&=\; (-1)^{k-m}\,d^\ell_{k,m}(i), && \text{(B.33)}\\
d^\ell_{k,m}(\pi-i) \;&=\; (-1)^{\ell-m}\,d^\ell_{-k,m}(i), && \text{(B.34)}\\
d^\ell_{k,m}(\pi+i) \;&=\; (-1)^{\ell-k}\,d^\ell_{-k,m}(i), && \text{(B.35)}\\
d^\ell_{k,m}(2\pi-i) \;&=\; (-1)^{k+m}\,d^\ell_{k,m}(i). && \text{(B.36)}
\end{aligned}
$$