# Appendix

## Mathematical Appendix

### A.1 FOURIER SERIES AND FOURIER TRANSFORM

If $f(x)$ is a periodic function with a fundamental period $L$, then it can be expanded in a Fourier series:

$$f(x) = \sum_{n=-\infty}^{\infty} a_n e^{ik_n x} \tag{A.1}$$

where $k_n = 2\pi n/L$. The coefficients $a_n$ of the series are given by

$$a_n = \frac{1}{L}\int_0^L f(x) e^{-ik_n x}\, dx \tag{A.2}$$

The Fourier transform of a function $f(x)$ is defined as

$$F(k) = F[f(x)] = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x) e^{-ikx}\, dx \tag{A.3}$$

while the inverse Fourier transform is

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} F(k) e^{ikx}\, dk \tag{A.4}$$

Notice that in quantum mechanics we define the transformations slightly differently, as follows:

$$\Psi(k) = F[\psi(x)] = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} \psi(x) e^{-ipx/\hbar}\, dx \tag{A.5}$$

and

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} \Psi(k) e^{ipx/\hbar}\, dk \tag{A.6}$$

Two formulas of Fourier transform theory are especially relevant.

*Identity of norms:*

$$\int_{-\infty}^{\infty} |f(x)|^2\, dx = \int_{-\infty}^{\infty} |F(k)|^2\, dk \tag{A.7}$$

*Parseval's theorem:*

$$\int_{-\infty}^{\infty} f(x)\, g^*(x)\, dx = \int_{-\infty}^{\infty} F(k) G^*(k)\, dk \tag{A.8}$$

## A.2 THE DIRAC δ-FUNCTION

The Dirac δ-function is defined by the relation

$$\int_{-\infty}^{\infty} f(x)\,\delta(x-x_0)\,dx = f(x_0) \tag{A.9}$$

Some important and useful properties of the δ-function are given below:

$$\delta(-x) = \delta(x) \tag{A.10}$$

$$\delta(cx) = \frac{1}{c}\delta(x) \quad \text{for} \quad c>0 \tag{A.11}$$

$$x\,\delta(x-x_0) = x_0\,\delta(x-x_0) \tag{A.12}$$

Note that $x\,\delta(x) = 0$. Also,

$$f(x)\,\delta(x-x_0) = f(x_0)\,\delta(x-x_0) \tag{A.13}$$

$$\delta(x^2-c^2) = \frac{1}{2c}\left[\delta(x-c) + \delta(x+c)\right] \text{ for } c>0 \tag{A.14}$$

$$\delta[f(x)] = \sum_i \frac{1}{f'(x_i)}\delta(x-x_i) \tag{A.15}$$

where $x_i$ are simple zeros of the function $f(x)$.

$$\int_{-\infty}^{\infty} \delta(x-x_1)\,\delta(x-x_2)\,dx = \delta(x_1-x_2) \tag{A.16}$$

We define $\delta'(x)$ by the relation

$$\int_{-\infty}^{\infty} f(x)\,\delta'(x)\,dx = -f'(0) \tag{A.17}$$

Some properties that are connected to $\delta'(x)$ are given below:

$$\delta'(-x) = -\delta'(x) \tag{A.18}$$

$$\delta^{(n)}(-x) = (-1)^n\,\delta^{(n)}(x) \tag{A.19}$$

$$x\,\delta^{(n)}(x) = -n\,\delta^{(n-1)}(x) \tag{A.20}$$

$$\int_{-\infty}^{\infty} f(x)\,\delta^{n}(x)\,dx = (-1)^n f^{(n)}(0) \tag{A.21}$$

The δ-function in three-dimensional space is defined by

$$\int f(\mathbf{r})\,\delta(\mathbf{r}-\mathbf{r}_0)\,dx\,dy\,dz = f(\mathbf{r}_0) \tag{A.22}$$

where $\delta(\mathbf{r}-\mathbf{r}_0) = \delta(x-x_0)\,\delta(y-y_0)\,\delta(z-z_0)$. In spherical coordinates $(r, \theta, \phi)$ we have

$$\begin{aligned}\delta(\mathbf{r}-\mathbf{r}_0) &= \frac{1}{r^2\sin\theta}\,\delta(r-r_0)\,\delta(\theta-\theta_0)\,\delta(\phi-\phi_0) \\ &= \frac{1}{r^2}\,\delta(r-r_0)\,\delta(\cos\theta-\cos\theta_0)\,\delta(\phi-\phi_0)\end{aligned} \tag{A.23}$$

The integral representation of the δ-function is obtained by using the definition of Fourier transform [see Section A.1], so that

$$\delta(x - x_0) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik(x - x_0)}\, dx \tag{A.24}$$

The *step function* $\theta(x)$ (also called the *Heaviside function*) is defined as

$$\theta(x) = \begin{cases} 1 & \text{for} \quad x > 0 \\ 0 & \text{for} \quad x < 0 \end{cases} \tag{A.25}$$

The relation between $\delta(x)$ and $\theta(x)$ is

$$\delta(x) = \frac{d\theta(x)}{dx} \tag{A.26}$$

Finally, we mention an important relation for $\delta(\mathbf{r})$:

$$\nabla^2\left(\frac{1}{r}\right) = -4\pi\,\delta(\mathbf{r}) \tag{A.27}$$

## A.3 HERMITE POLYNOMIALS

The *Hermite polynomials* $H_n(x)$ are defined by the relation

$$H_n(x) = (-1)^n e^{x^2}\left(\frac{d^n}{dx^n} e^{-x^2}\right) \qquad n = 0, 1, 2, \ldots \tag{A.28}$$

The $H_n(x)$ are the solutions to the *differential equation*

$$\frac{d^2 H_n(x)}{dx^2} - 2x\frac{dH_n(x)}{dx} + 2nH_n(x) = 0 \tag{A.29}$$

The *orthogonality relation* for $H_n(x)$ is

$$\int_{-\infty}^{\infty} e^{-x^2} H_m(x) H_n(x)\, dx = \sqrt{\pi}\, 2^n n!\, \delta_{mn} \tag{A.30}$$

Two important *recurrence relations* for $H_n(x)$ are

$$\frac{dH_n(x)}{dx} = 2nH_n(x) \qquad\qquad H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$$

The first few Hermite polynomials are given below:

$$H_0(x) = 1 \qquad H_1(x) = 2x \qquad H_2(x) = 4x^2 - 2$$

$$H_3(x) = 8x^3 - 12x \qquad H_4(x) = 16x^4 - 48x^2 + 12$$

## A.4 LEGENDRE POLYNOMIALS

Legendre polynomials $P_l(x)$ are given by *Rodrigue's formula*,

$$P_l(x) = \frac{(-1)^l}{2^n n!}\frac{d^l}{dx^l}(x^2 - 1)^l \tag{A.31}$$

The first few Legendre polynomials are given below:

$$P_0(x) = 1 \qquad P_1(x) = x \qquad P_2(x) = \frac{1}{2}(3x^2 - 1)$$

$$P_3(x) = \frac{1}{2}(5x^3 - 3x) \qquad P_4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3)$$

In terms of $\cos\theta$ the first few Legendre polynomials are

$$P_0(\cos\theta) = 1 \qquad P_1(\cos\theta) = \cos\theta$$

$$P_2(\cos\theta) = \frac{1}{4}(1 + 3\cos 2\theta) \qquad P_3(\cos\theta) = \frac{1}{8}(3\cos\theta + 5\cos 3\theta)$$

The orthogonality relation of the Legendre polynomials is

$$\int_{-1}^{1} P_l(x)\, P_{l'}(x)\, dx = \frac{2}{2l+1}\delta_{ll'} \tag{A.32}$$

## A.5 ASSOCIATED LEGENDRE FUNCTIONS

Associated Legendre functions $P_l^m(x)$ are defined as

$$P_l^m(x) = \sqrt{(1-x^2)^m}\,\frac{d^m}{dx^m} P_l(x) \qquad \text{for } -1 \le x \le 1 \tag{A.33}$$

where $m \ge 0$. $P_l(x)$ are the Legendre polynomials. Note that

$$P_l^0(x) = P_l(x) \qquad P_l^m(x) = 0 \quad \text{for} \quad m > l \tag{A.34}$$

The differential equation that $P_l^m(x)$ satisfies is

$$\left[(1-x^2)\frac{d^2}{dx^2} - 2x\frac{d}{dx} + \left(l(l+1) - \frac{m^2}{1-x^2}\right)\right] P_l^m(x) = 0 \tag{A.35}$$

The first few associated Legendre functions are given below:

$$P_1^1(x) = \sqrt{1-x^2} \qquad P_2^1(x) = 3x\sqrt{1-x^2} \qquad P_2^2(x) = 3(1-x^2)$$

$$P_3^1(x) = \frac{3}{2}(5x^2-1)\sqrt{1-x^2} \qquad P_3^2(x) = 15x(1-x^2) \qquad P_3^3(x) = 15\sqrt{(1-x^2)^3}$$

The orthogonality relation of the associated Legendre functions is

$$\int_{-1}^{1} P_l^m(x)\, P_{l'}^m(x)\, dx = \int_0^{\pi} P_l^m(\cos\theta)\, P_{l'}^m(\cos\theta)\sin\theta\, d\theta = \frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}\delta_{ll'} \tag{A.36}$$

## A.6 SPHERICAL HARMONICS

The spherical harmonics are defined as

$$Y_l^m(\theta, \phi) = (-1)^m \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\, P_l^m(\cos\theta)\, e^{im\phi} \qquad \text{for} \quad m \ge 0 \tag{A.37}$$

and

$$Y_l^{-m}(\theta, \phi) = (-1)^m\,[Y_l^m(\theta, \phi)]^* \tag{A.38}$$

The differential equation that $Y_l^m$ satisfies is

$$\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + l(l+1)\right] Y_l^m(\theta, \phi) = 0 \tag{A.39}$$

The $Y_l^m$ have well-defined parity given as follows:

$$Y_l^m(\pi-\theta,\pi+\phi) = (-1)^l Y_l^m(\theta,\phi) \tag{A.40}$$

The orthonormalization relation of $Y_l^m$ is written as

$$\int_0^{2\pi} d\phi \int_0^{\pi} [Y_{l'}^{m'}(\theta,\phi)]^* Y_l^m(\theta,\phi)\sin\theta d\theta = \delta_{l'l}\delta_{m'm} \tag{A.41}$$

and the closure relation

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_l^m(\theta,\phi)[Y_l^m(\theta',\phi')]^* = \delta(\cos\theta-\cos\theta')\delta(\phi-\phi') = \frac{1}{\sin\theta}\delta(\theta-\theta')\delta(\phi-\phi') \tag{A.42}$$

Some important recurrence relations are given below:

$$e^{i\phi}\left(\frac{\partial}{\partial\theta}-m\cot\theta\right)Y_l^m(\theta,\phi) = \sqrt{l(l+1)-m(m+1)}\,Y_l^{m+1}(\theta,\phi) \tag{A.43}$$

$$e^{-i\phi}\left(-\frac{\partial}{\partial\theta}-m\cot\theta\right)Y_l^m(\theta,\phi) = \sqrt{l(l+1)-m(m-1)}\,Y_l^{m-1}(\theta,\phi) \tag{A.44}$$

$$Y_l^m(\theta,\phi)\cos\theta = \sqrt{\frac{(l+1+m)(l+1-m)}{(2l+1)(2l+3)}}Y_{l+1}^m + \sqrt{\frac{(l+m)(l-m)}{(2l+1)(2l-1)}}Y_{l-1}^m \tag{A.45}$$

The first few $Y_l^m$ are given below:

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}$$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta \qquad Y_1^1 = -\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\phi}$$

$$Y_2^0 = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta-1) \qquad Y_2^1 = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{i\phi} \qquad Y_2^2 = \sqrt{\frac{15}{32\pi}}\sin^2\theta e^{2i\phi}$$

$$Y_3^0 = \sqrt{\frac{7}{16\pi}}(5\cos^3\theta-3\cos\theta) \qquad Y_3^1 = -\sqrt{\frac{21}{64\pi}}\sin\theta(5\cos^2\theta-1)e^{i\phi}$$

$$Y_3^2 = \sqrt{\frac{105}{32\pi}}\sin^2\theta\cos\theta e^{2i\phi} \qquad Y_3^3 = -\sqrt{\frac{35}{64\pi}}\sin^3\theta e^{3i\phi}$$

An important result for spherical harmonics is

$$P_l(\cos\alpha) = \frac{4\pi}{2l+1}\sum_{m=-l}^{l}(-1)^m Y_l^m(\theta_1,\phi_1)\,Y_l^m(\theta_2,\phi_2) \tag{A.46}$$

where $\alpha$ is the angle between the directions $(\theta_1,\phi_1)$ and $(\theta_2,\phi_2)$. This result is known as the *spherical harmonics addition theorem.*

## A.7 ASSOCIATED LAGUERRE POLYNOMIALS

First we shall deal with the Laguerre polynomials given by *Rodrigue's formula,*

$$L_l(x) = e^x\frac{d^l}{dx^l}(x^l e^{-x}) \tag{A.47}$$

The associated Laguerre polynomials are defined as

$$L_l^m(x) = \frac{d^m}{dx^m}L_l(x) \tag{A.48}$$

where $l$ and $m$ are nonnegative integers. Note that

$$L_l^0(x) = L_l(x) \qquad L_l^0(x) = 0 \quad \text{for} \quad m > 1 \tag{A.49}$$

The first few associated Laguerre polynomials are given below:

$$L_1^1(x) = -1 \qquad L_2^1(x) = 2x - 4 \qquad L_2^2(x) = 2$$

$$L_3^1(x) = -3x^2 + 18x - 18 \qquad L_3^2(x) = -6x + 18 \qquad L_3^3(x) = -6$$

The orthogonality relation of the associated Laguerre polynomials is

$$\int_0^\infty x^m e^{-x} L_l^m(x) L_{l'}^m(x)\, dx = \frac{(l!)^3}{(l-m)!}\delta_{ll'} \tag{A.50}$$

## A.8 SPHERICAL BESSEL FUNCTIONS

Bessel's differential equation is given as

$$\left[x^2\frac{d^2}{dx^2} + x\frac{d}{dx} + (x^2 - l^2)\right]J_l(x) = 0 \tag{A.51}$$

where $l \geq 0$. The solutions to this equation are called *Bessel functions* of order $l$. $J_l(x)$ are given by the series expansion

$$J_l(x) = \frac{x^l}{2^l\Gamma(l+1)}\left[1 - \frac{x^2}{2(2l+2)} + \frac{x^4}{2\cdot 4(2l+2)(2l+4)}\right] = \sum_{R=0}^{\infty} \frac{(-1)^k (x/2)^{l+2k}}{n!\Gamma(l+k+1)} \tag{A.52}$$

If $l = 0, 1, 2, \ldots, J_{-l}(x) = -1^l J_l(x)$. If $l \neq 0, 1, 2, \ldots, J_l(x)$ and $J_{-l}(x)$ are linearly independent. In this case $J_l(x)$ is bounded at $x = 0$, while $J_{-l}(x)$ is the unbounded Bessel function of the second kind. $N_l(x)$ (also called Neumann functions) are defined by

$$N_l(x) = \frac{J_l(x)\cos(l\pi) - J_{-l}(x)}{\sin(l\pi)} \qquad (l \neq 0, 1, 2, \ldots) \tag{A.53}$$

These functions are unbounded at $x = 0$. The general solution of *(A.51)* is

$$\begin{cases} y(x) = AJ_l(x) + BJ_{-l}(x) & l \neq 0, 1, 2, \ldots \\ y(x) = AJ_l(x) + BN_l(x) & \text{all } l \end{cases} \tag{A.54}$$

where $A$ and $B$ are arbitrary constants. Spherical Bessel functions are related to Bessel functions according to

$$j_l(x) = \sqrt{\frac{\pi}{2x}}J_{l+1/2}(x) \tag{A.55}$$

Also, the Neumann spherical functions are related to the Neumann function $N_l(x)$ by

$$n_l(x) = \sqrt{\frac{\pi}{2x}}N_{l+1/2}(x) \tag{A.56}$$

$j_l(x)$ and $n_l(x)$ are given explicitly as

$$j_l(x) = (-x)^l\left(\frac{1}{x}\frac{d}{dx}\right)^l\left(\frac{\sin x}{x}\right) \tag{A.57}$$

$$n_l(x) = -(-x)^l\left(\frac{1}{x}\frac{d}{dx}\right)^l\left(\frac{\cos x}{x}\right) \tag{A.58}$$

The first few $j_l(x)$ and $n_l(x)$ are given below:

$$j_0(x) = \frac{\sin x}{x} \qquad n_0(x) = -\frac{\cos x}{x}$$

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x} \qquad n_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x}$$

$$j_2(x) = \left(\frac{3}{x^3} - \frac{1}{x}\right)\sin x - \frac{3}{x^2}\cos x \qquad n_2(x) = -\left(\frac{3}{x^3} - \frac{1}{x}\right)\cos x - \frac{3}{x^2}\sin x$$

The asymptotic behavior of the $j_l(x)$ and $n_l(x)$ as $x \to \infty$ and $x \to 0$ is given by

$$\begin{cases} j_l(x)_{x\to 0} \to \dfrac{x^l}{(2l+1)!!} \\ n_l(x)_{x\to 0} \to -\dfrac{(2l-1)!!}{x^{l+1}} \end{cases} \tag{A.59}$$

$$\begin{cases} j_l(x)_{x\to \infty} \to \dfrac{1}{x}\sin\left(x - \dfrac{\pi l}{2}\right) \\ n_l(x)_{x\to \infty} \to -\dfrac{1}{x}\cos\left(x - \dfrac{\pi l}{2}\right) \end{cases} \tag{A.60}$$

where $(2l+1)!! = 1 \cdot 3 \cdot 5 \cdots (2l-1)(2l+1)$.