PartVI
Appendix

A Separation of Variables for Hel,holtz Equation in Polar Coordinates

Consider the Helmholtz equation:

$$\Delta u + k^2 u = 0$$

We let the polar coordinates be

$$x = r\sin\theta\cos\phi, \quad y = r\sin\theta\sin\phi, \quad x = r\cos\theta$$

from which we express

$$\begin{aligned}
\Delta_{3D} &= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \\
&= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \\
\Delta_{2D} &= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \\
&= \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\phi^2}
\end{aligned}$$

In the three-dimension:

$$u(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$$

Rewrite the Helmholtz equation, we obtain

$$\begin{aligned}
\Delta u + k^2 u &= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \\
&= \frac{1}{r^2}\frac{\partial R}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\Theta\Phi + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\Phi}{\partial\phi^2} + k^2 R\Theta\Phi = 0
\end{aligned}$$

$$\sin^2\theta\left(\frac{\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)}{R} + k^2r^2\right) + \sin\theta\frac{\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)}{\Theta} = -\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}$$

Consider the independent variables, we write:

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -\mu^2 = (constant)$$

$$\frac{\frac{d}{dr}\big(r^2\frac{dR}{dr}\big)}{R} + k^2r^2 = -\frac{1}{\sin\theta}\frac{\frac{d}{d\theta}\big(\sin\theta\frac{d\Theta}{d\theta}\big)}{\Theta} + \frac{\mu^2}{\sin^2\theta}$$

Let both sides of the equation be the constant λ:

$$\begin{aligned}\frac{1}{r^2}\frac{d}{dr}\big(r^2\frac{dR}{dr}\big) + \big(k^2 - \frac{\lambda}{r^2}\big)R &= 0\\ \frac{1}{\sin\theta}\frac{d}{d\theta}\big(\sin\theta\frac{d\Theta}{d\theta}\big) + \big(\lambda - \frac{\mu^2}{\sin^2\theta}\big)\Theta &= 0\end{aligned}$$

Where Φ is $\Phi(\phi) = e^{i\mu\phi}$, its single-valuedness is ensured by $\mu = m = scalar$:

$$\Phi(\phi) = e^{i\mu\phi}, \quad m = \cdots, -2, -1, 0, 1, 2, \cdots$$

Where Θ is $x = \cos\theta$ such that

$$\frac{d}{d\theta} = \frac{dx}{d\theta}\frac{d}{dx} = -\sin\theta\frac{d}{dx}$$

, giving

$$\begin{aligned}\frac{1}{\sin\theta}\frac{d}{d\theta}\big(\sin\theta\frac{d\Theta}{d\theta}\big) &= \frac{d}{dx}\left(\sin^2\theta\frac{d\Theta}{dx}\right)\\ &= \frac{d}{dx}\left((1-x^2)\frac{d\Theta}{dx}\right)\end{aligned}$$

Thus,

$$\frac{d}{dx}\left((1-x^2)\frac{d\Theta}{dx}\right) + \left(\lambda - \frac{m^2}{1-x^2}\right)\Theta = 0$$

This is known as the associated Legendre differential equation, and which is in the form of the Sturm-Liouville equation:

$$\frac{d}{dx}\big(p(x)\frac{du}{dx}\big) + (\lambda\rho(x) - q(x))u = 0$$

In the case of

$$\lambda = \ell(\ell+1), \quad \ell = 0, 1, 2, \cdots$$

there is bounded solutions at $x = \pm 1$, which is expressed by $P_\ell^m(x)$ and known as the associated Legendre function of the first kind.

B Spherical Function

B.1 Legendre Differential Equation

$$\begin{aligned}\frac{d}{dx}\left[(1-x^2)\frac{dP_\ell}{dx}\right] + \lambda P_\ell &= \frac{d}{dx}\left[(1-x^2)\frac{dP_\ell}{dx}\right] + \ell(\ell+1)P_\ell\\ &= (1-x^2)P_\ell'' - 2xP_\ell' + \ell(\ell+1)P_\ell = 0\end{aligned}$$

This is called the Legendre differential equation. On the closed interval $[-1,1]$ the bounded solutions exist at $\ell = 0, 1, 2, 3, \cdots$. The solutions to the equation are the polynomials, and they are known as the Legendre polynomials. The characteristics of the polynomials are described in the followings:

$$\begin{aligned}
P_\ell(x) &= \sum_{n=0}^{\ell} C_n x^n, \quad \left(C_n = \prod_{j=0}^{n-1} \frac{\ell(\ell+1) - j(j+1)}{2(j+1)^2}\right) \\
&= \frac{1}{2^\ell \ell!}\frac{d^\ell}{dx^\ell}(x^2-1)^\ell \\
P_0(x) &= 1 \\
P_1(x) &= x \\
P_2(x) &= \frac{3}{2}x^2 - \frac{1}{2} \\
&\vdots \\
\int_{-1}^{1} dx P_{\ell'}(x) P_\ell(x) &= \delta_{\ell\ell'}\frac{2}{2\ell+1}
\end{aligned}$$

An expansion of the generating function is also valid:

$$\frac{1}{|\vec{r} - \vec{r}'|} = \sum_{\ell=0}^{\infty} P_\ell(\cos\theta)\frac{1}{r_>}\left(\frac{r_<}{r_>}\right)^\ell$$

B.2 Associated Legendre Differential Equation

$$\left\{(1-x^2)\frac{dP_\ell^m}{dx}\right\} + \left(\ell(\ell+1) - \frac{m^2}{1-x^2}\right)P_\ell^m = 0$$

This is known as the associated Legendre differential equation. The solutions to the equation are obtained through the solutions $P_\ell(x)$ of the Legendre differential equation:

$$P_\ell^m(x) = (1-x^2)^{\frac{m}{2}}\frac{d^m}{dx^m}P_\ell(x)$$

which satisfies the orthogonal relation:

$$\int_{-1}^{1} dx P_\ell^m(x) P_{\ell'}^m(x) = \delta_{\ell\ell'}\frac{2}{2\ell+1}\frac{(\ell+m)!}{(\ell-m)!}$$

B.3 Spherical Function

Here, we define the spherical function $Y_{\ell m}$ as

$$Y_{\ell m}(\theta,\phi) = (-1)^{\frac{m+|m|}{2}}\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}}P_l^m(\cos\theta)e^{im\phi}$$

There are some relations the above spherical function satisfies:

- Orthonormality

$$\langle Y_{\ell' m'} | Y_{\ell m} \rangle \equiv \int d\Omega Y^*_{\ell' m'}(\theta, \phi) Y_{\ell m}(\theta, \phi) = \delta_{\ell, \ell'} \delta_{mm'}$$

- The action of ladder operator

$$L_{\pm} Y_{\ell m} = \hbar \sqrt{(\ell \mp m)(\ell \pm +1)} Y_{\ell m \pm 1}$$

- Addition theorem

$$Y_{\ell m=0}(\cos 0) Y_{\ell m=0}(\omega) = \sum_{m=-\ell}^{\ell} Y^*_{\ell m}(\theta', \phi') Y_{\ell m}(\theta, \phi)$$

  where ω is the angle formed by (θ, ϕ) direction and (θ', ϕ') direction such that

$$\cos \omega = \cos \theta \cos \theta' + \sin \theta \sin \theta' \cos(\phi - phi')$$

To rewrite the above, we have

$$\begin{aligned} P_\ell(\cos \omega) &= P_\ell(\cos \theta) P_\ell(\cos \theta') + 2 \sum_{m=1}^{\ell} \frac{(\ell - m)!}{(\ell + m)!} P_\ell^m(\cos \theta) P_\ell^m(\cos \theta') \cos m(\phi - \phi') \\ &= \frac{4\pi}{2\ell + 1} \sum_m Y^*_{\ell m}(\theta', \phi') Y_{\ell m}(\theta, \phi) \end{aligned}$$

C Spherical Bessel Function

C.1 Spherical Bessel Function

Spherical Bessel equation:

$$\left\{ \left(\frac{d^2}{dx^2} + \frac{2}{x} \frac{d}{dx} \right) + 1 - \frac{\ell(\ell + 1)}{x^2} \right\} R(x) = 0$$

has two independent solutions, which include a canonical solution at origin (spherical Bessel function) $j_\ell(x)$ and a non-canonical solution (spherical Neumann function) $n_\ell(x)$. The two solutions can be further expressed as

$$\begin{aligned} j_\ell(x) &= (-x)^\ell \left(\frac{1}{x} \frac{d}{dx} \right)^\ell \left(\frac{\sin x}{x} \right) \xrightarrow{x \to 0} \frac{x^\ell}{(2\ell + 1)!!} \\ n_\ell(x) &= -(-x)^\ell \left(\frac{1}{x} \frac{d}{dx} \right)^\ell \left(\frac{\cos x}{x} \right) \xrightarrow{x \to 0} - \frac{(2\ell - 1)!!}{x^{\ell + 1}} \end{aligned}$$

In some cases, the Hankel function of the first and the second kinds are defined by

$$\begin{aligned} h_\ell^{(1)}(x) &= j_\ell(x) + i n_\ell(x) \\ h_\ell^{(2)}(x) &= j_\ell(x) - i n_\ell(x) \end{aligned}$$

in which two linearly independent solutions exist. The asymptotic forms for large arguments especially, one obtains:

$$\begin{aligned} j_\ell(x) &\overset{x\to\infty}{\longrightarrow} \frac{1}{x}\sin\left(x - \frac{\ell\pi}{2}\right) \\ n_\ell(x) &\overset{x\to\infty}{\longrightarrow} -\frac{1}{x}\cos\left(x - \frac{\ell\pi}{2}\right) \\ h_\ell^{(1)}(x) &\overset{x\to\infty}{\longrightarrow} (-i)^{\ell+1}\frac{e^{ix}}{x} \\ h_\ell^{(2)}(x) &\overset{x\to\infty}{\longrightarrow} (i)^{\ell+1}\frac{e^{-ix}}{x} \end{aligned}$$

The two important formulas obtained by the above are

$$e^{ikr\cos\theta} = \sum_{\ell=0}^{\infty}(2\ell+1)i^\ell j_\ell(kr)P_\ell(\cos\theta)$$

$$\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} = ik\sum_{\ell=0}^{\infty}(2\ell+1)j_\ell(kr_<)h_\ell^{(1)}(kr_>)P_\ell(\hat{r}\cdot\hat{r}')$$