

# Appendix

*Many have written of the experience of mathematical beauty as being comparable to that derived from the greatest art.*

S. Zeki, J.P. Romaya, D.M.T. Benincasa, M.F. Atiyah [1]  
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## A.1 Harmonic Functions

The Laplacian is defined in the D-dimensional Cartesian space as

$$\Delta = \sum_{j=1}^D \frac{\partial^2}{\partial x_j^2}.$$

The Laplacian eigenproblem

$$\Delta f = -\lambda f$$

is solved by harmonics, on a finite interval.

## A.2 Laplacian in Orthogonal Coordinates

In general, coordinates can be expressed by n-tuples of values. For instance, the Cartesian coordinates are  $(x_1, x_2, \dots)$  and coordinates of another coordinate systems are  $(u_1, u_2, \dots)$ , and both describe the location of a point in a space depending on a finite number of dimensions. Each location of the space should be accessible by both

coordinate systems and there should be a bijective mapping between both systems, e.g.  $u_j = u_j(x_1, x_2, \dots)$ . A single differentiation with regard to the component  $x_i$ , for instance, is described by the chain rule and consists of the sum of weighted partial differentials with regard to  $u_j$ :

$$\frac{\partial}{\partial x_i} = \sum_j \frac{\partial u_j}{\partial x_i} \frac{\partial}{\partial u_j}. \quad (\text{A.1})$$

Written in terms of vectors, the (Cartesian) gradient  $\nabla = \frac{\partial}{\partial \mathbf{x}}$  with  $\frac{\partial}{\partial \mathbf{u}}$  yields:

$$\nabla = \frac{\partial \mathbf{u}^T}{\partial \mathbf{x}} \frac{\partial}{\partial \mathbf{u}} := \mathbf{J}_{\partial \mathbf{u} / \partial \mathbf{x}} \frac{\partial}{\partial \mathbf{u}}, \quad (\text{A.2})$$

for which the Jacobian matrix  $\mathbf{J}_{\partial \mathbf{u} / \partial \mathbf{x}} = \left[ \frac{\partial u_j}{\partial x_i} \right]_{ij}$  that is either written in dependency of  $\mathbf{x}$  or  $\mathbf{u}$  represents all the partial derivatives of the mapping between the coordinate systems. For bijective mappings also Jacobian of the inverse mapping exists  $\mathbf{J}_{\partial \mathbf{x} / \partial \mathbf{u}} = \left[ \frac{\partial x_i}{\partial u_j} \right]_{ji}$ . The coordinate systems are equivalent if the determinant of the Jacobian is non-zero  $|\mathbf{J}| \neq 0$ .

Orthogonal coordinate systems have the interesting property that the rows of the Jacobian (or its columns) are orthogonal, so that  $\mathbf{J}^T \mathbf{J}$  yields a diagonal matrix. With  $\mathbf{J}_{\partial \mathbf{x} / \partial \mathbf{u}} = \frac{\partial \mathbf{x}^T}{\partial \mathbf{u}}$  the meaning of this property becomes easier to understand: the differential changes in the location  $\partial \mathbf{x} / \partial u_j$  of each Cartesian coordinate into the direction of each individual non-Cartesian coordinate  $u_j$  describes an orthogonal set of motion directions in space, whose orientation depends on the location and whose individual lengths may vary.

To obtain a description of the Laplacian in the Helmholtz equation  $\Delta = \sum_i \frac{\partial^2}{\partial x_i^2}$  is our goal here, and it can be obtained with the chain rule, now calculating from  $x_i$  to  $u_j$ ,

$$\begin{aligned} \Delta &= \sum_i \frac{\partial}{\partial x_i} \left( \frac{\partial}{\partial x_i} \right) = \sum_i \frac{\partial}{\partial x_i} \left( \sum_j \frac{\partial u_j}{\partial x_i} \frac{\partial}{\partial u_j} \right) \\ &= \sum_{i,j} \frac{\partial^2 u_j}{\partial x_i^2} \frac{\partial}{\partial u_j} + \sum_{i,j,k} \frac{\partial u_j}{\partial x_i} \frac{\partial u_k}{\partial x_i} \frac{\partial^2}{\partial u_j \partial u_k}, \end{aligned} \quad (\text{A.3})$$

$$\text{with } \sum_{i,j,k} \frac{\partial u_j}{\partial x_i} \frac{\partial u_k}{\partial x_i} \frac{\partial^2}{\partial u_j \partial u_k} = \mathbf{1}^T \left[ \underbrace{(\mathbf{J}^T \mathbf{J})}_{\text{ortho:diag}} \circ \left( \frac{\partial}{\partial \mathbf{u}^T} \frac{\partial}{\partial \mathbf{u}} \right) \right] = \sum_{i,j} \left( \frac{\partial u_j}{\partial x_i} \right)^2 \frac{\partial^2}{\partial u_j^2},$$

with  $\circ$  denoting the element-wise, i.e. Hadamard product. Orthogonal coordinates largely simplify the Laplacian (see last line) and make it consist of first- and second-order differentials with regard to the new coordinates, individually, with all mixed

derivatives canceling. Both first- and second-order differentials are weighted by the partial derivatives of the coordinate mapping. For each  $u_j$ , the Laplacian is composed of those two expressions

$$\Delta = \sum_j \Delta_{u_j}, \quad \text{where } \Delta_{u_j} = \left[ \sum_i \frac{\partial^2 u_j}{\partial x_i^2} \right] \frac{\partial}{\partial u_j} + \left[ \sum_i \left( \frac{\partial u_j}{\partial x_i} \right)^2 \right] \frac{\partial^2}{\partial u_j^2}. \quad (\text{A.4})$$

### A.3 Laplacian in Spherical Coordinates

The right-handed spherical coordinate systems in ISO31-11, ISO80000-2, [2, 3], uses a radius  $r$ , an azimuth angle  $\varphi$ , and a zenith angle  $\vartheta$ , mapping to Cartesian coordinates  $x = r \cos \varphi \sin \vartheta$ ,  $y = r \sin \varphi \sin \vartheta$ ,  $z = r \cos \vartheta$ , or inversely  $r = \sqrt{x^2 + y^2 + z^2}$ ,  $\varphi = \arctan \frac{y}{x}$ ,  $\vartheta = \arctan \frac{\sqrt{x^2 + y^2}}{z}$ , see Fig. 4.11.

Re-expressing the zenith angle coordinate by  $\zeta = \cos \vartheta = \frac{z}{r}$  reduces the effort in calculation and yields  $x = r \cos \varphi \sqrt{1 - \zeta^2}$ ,  $y = r \sin \varphi \sqrt{1 - \zeta^2}$ ,  $z = r \zeta$ .

In order to obtain solutions along the angular dimensions azimuth and zenith, we first need to re-write the Laplacian from Cartesian to spherical coordinates. For first-order derivative along the  $x$  axis, we get the generalized differential

$$\frac{\partial}{\partial x} = \left[ \frac{\partial r}{\partial x} \right] \frac{\partial}{\partial r} + \left[ \frac{\partial \varphi}{\partial x} \right] \frac{\partial}{\partial \varphi} + \left[ \frac{\partial \zeta}{\partial x} \right] \frac{\partial}{\partial \zeta}.$$

As the Cartesian and spherical coordinates are orthogonal, therefore any mixed second-order derivatives in Cartesian or spherical coordinates vanish. We may derive a second time wrt.  $x$ :

$$\begin{aligned} \frac{\partial}{\partial x} \left[ \frac{\partial}{\partial x} \right] &= \left[ \frac{\partial^2 r}{\partial x^2} + \left( \frac{\partial r}{\partial x} \right)^2 \frac{\partial}{\partial r} \right] \frac{\partial}{\partial r} \\ &\quad + \left[ \frac{\partial^2 \varphi}{\partial x^2} + \left( \frac{\partial \varphi}{\partial x} \right)^2 \frac{\partial}{\partial \varphi} \right] \frac{\partial}{\partial \varphi} + \left[ \frac{\partial^2 \zeta}{\partial x^2} + \left( \frac{\partial \zeta}{\partial x} \right)^2 \frac{\partial}{\partial \zeta} \right] \frac{\partial}{\partial \zeta}. \end{aligned}$$

Obviously, we require all first-order derivatives squared, and all second-order derivatives of the spherical coordinates.

#### A.3.1 The Radial Part

With  $r = \sqrt{x^2 + y^2 + z^2}$  we obtain for the radial part  $\Delta_r = \left[ \frac{\partial^2 r}{\partial x^2} + \left( \frac{\partial r}{\partial x} \right)^2 \frac{\partial}{\partial r} \right] \frac{\partial}{\partial r}$  of the Laplacian

$$\left[\frac{\partial r}{\partial x}\right]^2 = \left[\frac{\partial \sqrt{x^2 + y^2 + z^2}}{\partial x}\right]^2 = \left[\frac{1}{2\sqrt{x^2 + y^2 + z^2}} 2x\right]^2 = \left[\frac{x}{r}\right]^2 = \frac{x^2}{r^2},$$

$$\frac{\partial^2 r}{\partial x^2} = \frac{\partial}{\partial x} \left[\frac{x}{r}\right] = \frac{1}{r} \frac{\partial x}{\partial x} + x \frac{\partial r}{\partial x} \frac{\partial}{\partial r} \frac{1}{r} = \frac{1}{r} - x \frac{x}{r} \frac{1}{r^2} = \frac{r^2 - x^2}{r^3}.$$

For  $x, y, z$  altogether, this is for:

$$\Delta_r = \left[\frac{3r^2 - x^2 - y^2 - z^2}{r^3}\right] \frac{\partial}{\partial r} + \left[\frac{x^2}{r^2} + \frac{y^2}{r^2} + \frac{z^2}{r^2}\right] \frac{\partial^2}{\partial r^2} = \frac{2}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2}. \quad (\text{A.5})$$

**2D.** In two dimensions, there is no  $z$  coordinate, therefore there is just one term fewer:

$$\Delta_{r,2D} = \left[\frac{2r^2 - x^2 - y^2}{r^3}\right] \frac{\partial}{\partial r} + \left[\frac{x^2}{r^2} + \frac{y^2}{r^2}\right] \frac{\partial^2}{\partial r^2} = \frac{1}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2}. \quad (\text{A.6})$$

### A.3.2 The Azimuthal Part

With  $\varphi = \arctan \frac{y}{x}$  and  $\frac{d}{dx} \arctan x = \frac{1}{1+x^2}$ , the azimuthal part  $\Delta_\varphi = \left[\frac{\partial^2 \varphi}{\partial x^2} + \left(\frac{\partial \varphi}{\partial x}\right)^2 \frac{\partial}{\partial \varphi}\right] \frac{\partial}{\partial \varphi}$  of the Laplacian becomes

$$\left[\frac{\partial \varphi}{\partial x}\right]^2 = \left[\frac{\partial \arctan \frac{y}{x}}{\partial x}\right]^2 = \left[\frac{1}{1 + \frac{y^2}{x^2}} \frac{\partial}{\partial x} \frac{y}{x}\right]^2 = \left[-\frac{x^2}{x^2 + y^2} \frac{y}{x^2}\right]^2 = \left[-\frac{y}{r_{xy}^2}\right]^2 = \frac{y^2}{r_{xy}^4},$$

$$\left[\frac{\partial \varphi}{\partial y}\right]^2 = \left[\frac{\partial \arctan \frac{y}{x}}{\partial y}\right]^2 = \left[\frac{x^2}{x^2 + y^2} \frac{\partial}{\partial y} \frac{y}{x}\right]^2 = \left[\frac{x^2}{x^2 + y^2} \frac{1}{x}\right]^2 = \left[\frac{x}{r_{xy}^2}\right]^2 = \frac{x^2}{r_{xy}^4},$$

$$\frac{\partial^2 \varphi}{\partial x^2} = \frac{\partial}{\partial x} \left[-\frac{y}{r_{xy}^2}\right] = -\frac{2xy}{r_{xy}^3},$$

$$\frac{\partial^2 \varphi}{\partial y^2} = \frac{\partial}{\partial y} \left[\frac{x}{r_{xy}^2}\right] = -\frac{2xy}{r_{xy}^3}, \quad \frac{\partial \varphi}{\partial z} = 0.$$

It only depends on  $x$  and  $y$ , and altogether, we obtain

$$\Delta_\varphi = \left[\frac{2xy - 2xy}{r_{xy}^3}\right] \frac{\partial}{\partial \varphi} + \left[\frac{x^2 + y^2}{r_{xy}^4}\right] \frac{\partial^2}{\partial \varphi^2} = \frac{1}{r_{xy}^2} \frac{\partial^2}{\partial \varphi^2} = \frac{1}{r^2(1 - \zeta^2)} \frac{\partial^2}{\partial \varphi^2}. \quad (\text{A.7})$$

**2D.** In two dimensions,  $\zeta = 0$ , therefore

$$\Delta_{\varphi,2D} = \frac{1}{r^2} \frac{\partial^2}{\partial \varphi^2}. \quad (\text{A.8})$$

### A.3.3 The Zenithal Part

The zenith angle is actually  $\vartheta$ , and we define  $\zeta = \cos \vartheta$  as a variable to express it in order to simplify the derivation. With  $\zeta = \frac{z}{\sqrt{x^2+y^2+z^2}} = \frac{z}{r}$ , the zenithal part

$\Delta_{\zeta} = \left[ \frac{\partial^2 \zeta}{\partial x^2} + \left( \frac{\partial \zeta}{\partial x} \right)^2 \frac{\partial}{\partial \zeta} \right] \frac{\partial}{\partial \zeta}$  becomes

$$\begin{aligned} \left[ \frac{\partial \zeta}{\partial x} \right]^2 &= \left[ \frac{\partial}{\partial x} \frac{z}{r} \right]^2 = \left[ -\frac{z}{r^2} \frac{x}{r} \right]^2 = \left[ -\frac{xz}{r^3} \right]^2 = \frac{x^2 z^2}{r^6}, \\ \left[ \frac{\partial \zeta}{\partial z} \right]^2 &= \left[ \frac{\partial}{\partial z} \frac{z}{r} \right]^2 = \left[ \frac{1}{r} - \frac{z}{r^2} \frac{z}{r} \right]^2 = \left[ \frac{r^2 - z^2}{r^3} \right]^2 = \left[ \frac{r_{xy}^2}{r^3} \right]^2 = \frac{r_{xy}^4}{r^6}, \\ \frac{\partial^2 \zeta}{\partial x^2} &= \frac{\partial}{\partial x} \left[ -\frac{xz}{r^3} \right] = -\frac{z}{r^3} + 3xz \frac{1}{r^4} \frac{x}{r} = z \frac{3x^2 - r^2}{r^5}, \\ \frac{\partial^2 \zeta}{\partial z^2} &= \frac{\partial}{\partial z} \left[ \frac{r_{xy}^2}{r^3} \right] = -3 \frac{r_{xy}^2}{r^4} \frac{z}{r} = -z \frac{3r_{xy}^2}{r^5}. \end{aligned}$$

For  $x$ ,  $y$ , and  $z$  altogether, we get

$$\begin{aligned} \Delta_{\zeta} &= z \frac{3x^2 + 3y^2 - 2r^2 - 3r_{xy}^2}{r^5} \frac{\partial}{\partial \zeta} + \frac{(x^2 + y^2)z^2 + r_{xy}^4}{r^6} \frac{\partial^2}{\partial \zeta^2} = -\frac{2r^2}{r^5} \frac{\partial}{\partial \zeta} + \frac{r^2 r_{xy}^2}{r^6} \frac{\partial^2}{\partial \zeta^2} \\ &= -z \frac{2}{r^3} \frac{\partial}{\partial \zeta} + \frac{r^2(1 - \zeta^2)}{r^4} \frac{\partial^2}{\partial \zeta^2} = -\frac{2}{r^2} \zeta \frac{\partial}{\partial \zeta} + \frac{1 - \zeta^2}{r^2} \frac{\partial^2}{\partial \zeta^2}. \end{aligned} \quad (\text{A.9})$$

**2D.** This part does not exist in 2D.

### A.3.4 Azimuthal Solution in 2D and 3D

The azimuth harmonics are found by solving  $\Delta_{\varphi} \Phi = -\lambda r_{xy}^2 \Phi$

$$\frac{d^2}{d\varphi^2} \Phi = -\lambda r_{xy}^2 \Phi. \quad (\text{A.10})$$

We know that  $\cos'' x = -\cos x$  and  $\sin'' x = -\sin x$ , therefore we can insert the solutions

$$\hat{\Phi} = \begin{cases} \cos(a\varphi), & \text{for } a \geq 0, \\ \sin(|a|\varphi), & \text{for } a < 0, \end{cases}$$

and obtain with  $\frac{d^2}{d\varphi^2} \hat{\Phi} = -a^2 \hat{\Phi}$  the characteristic equation that fixes  $a$

$$-a^2 = -\lambda r_{xy}^2.$$

Geometrically, we desire that  $\hat{\Phi}(\varphi) = \hat{\Phi}(\varphi + 2\pi l)$  with  $l \in \mathbb{Z}$ . This is only possible with  $\lambda r_{xy}^2 = m^2$ , and  $m \in \mathbb{Z}$ .

We can therefore define for  $-\infty \leq m \leq \infty$  the terms of a normalized Fourier series

$$\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} \begin{cases} \sqrt{2} \sin(|m|\varphi), & \text{for } m < 0, \\ 1, & \text{for } m = 0, \\ \sqrt{2} \cos(m\varphi), & \text{for } m > 0. \end{cases} \quad (\text{A.11})$$

The azimuth harmonics are orthogonal: none of the products  $\cos(i\varphi) \sin(j\varphi)$ ,  $\cos(i\varphi) \cos(j\varphi)$ , or  $\sin(i\varphi) \sin(j\varphi)$  produces a constant component unless  $i = j$ , excluding the mixed cosine and sine product. Normalization ensures that the non-zero result is unity

$$\int_0^{2\pi} \Phi_i \Phi_j d\varphi = \delta_{ij} = \begin{cases} 1, & \text{for } i = j, \\ 0, & \text{else,} \end{cases} \quad (\text{A.12})$$

$$\text{by } \int_0^{2\pi} \frac{1}{\sqrt{2\pi^2}} d\varphi = \int_0^{2\pi} \frac{\cos^2 m\varphi}{\sqrt{\pi^2}} d\varphi = \int_0^{2\pi} \frac{\sin^2 m\varphi}{\sqrt{\pi^2}} d\varphi = 1.$$

**2D functions.** With unbounded  $|m| \rightarrow \infty$ , the circular harmonics are complete in the Hilbert space of square-integrable circular polynomials. By their orthonormality, we can derive a transformation integral of a function  $g(\varphi)$  that should be represented as series

$$g = \sum_{j=-\infty}^{\infty} \gamma_j \Phi_j \quad (\text{A.13})$$

by integration of  $g$  over  $\Phi_m \int d\varphi$

$$\int_{-\pi}^{\pi} g(\varphi) \Phi_m d\varphi = \sum_{m=-\infty}^{\infty} \gamma_m \underbrace{\int_{-\pi}^{\pi} \Phi_m \Phi_j d\varphi}_{=\delta_{mj}} = \gamma_m. \quad (\text{A.14})$$

**2D panning functions.** To decompose an infinitely narrow unit-surface Dirac delta function that represents an infinite-order panning function towards the direction  $\varphi_s$ ,

$$\delta(\varphi - \varphi_s) = \begin{cases} \lim_{\varepsilon \rightarrow 0} \frac{1}{2\varepsilon}, & \text{for } |\varphi - \varphi_s| \leq \varepsilon, \\ 0 & \text{otherwise,} \end{cases} \quad (\text{A.15})$$

we obtain the coefficients from the transformation integral

$$\begin{aligned} \gamma_m &= \int_{-\pi}^{\pi} \delta(\varphi - \varphi_s) \Phi_m \, d\varphi = \Phi_m(\varphi_s) \lim_{\varepsilon \rightarrow 0} \int_{-\varepsilon}^{\varepsilon} \frac{1}{2\varepsilon} d\varphi \\ &= \Phi_m(\varphi_s). \end{aligned} \quad (\text{A.16})$$

Typically, a finite-order series will be employed as a panning function

$$g_N = \sum_{m=-N}^N a_m \Phi_m(\varphi_s) \Phi_m(\varphi), \quad (\text{A.17})$$

involving a weight  $a_m = a_{|m|}$  controlling the side lobes. To evaluate the  $E$  measure of loudness, we can write

$$\begin{aligned} E &= \int_{-\pi}^{\pi} g_N^2 \, d\varphi = \int_{-\pi}^{\pi} \left[ \sum_{i=0}^N a_i \Phi_i \right] \left[ \sum_{j=0}^N a_j \Phi_j \right] d\varphi = \sum_{i,j} a_i a_j \int_{-\pi}^{\pi} \Phi_i \Phi_j \, d\varphi \\ &= \sum_{i=0}^N \frac{2 - \delta_i}{2\pi} a_i^2. \end{aligned} \quad (\text{A.18})$$

For  $\varphi_s = 0$ , we obtain an axisymmetric function in terms of a pure cosine series, as  $\sin 0 = 0$ ,

$$g_N(\varphi) = \sum_{m=0}^N a_m \frac{2 - \delta_m}{2\pi} \cos(m\varphi), \quad (\text{A.19})$$

with  $\delta_m = 1$  for  $m = 0$  and 0 elsewhere. The axisymmetric panning function is easier to design.

**2D max- $r_E$ .** For the narrowest-possible spread, we maximize the length of  $r_E$ ,

$$\begin{aligned} r_E &= \frac{\int_{-\pi}^{\pi} g_N^2 \cos \varphi \, d\varphi}{\int_{-\pi}^{\pi} g_N^2 \, d\varphi} = \frac{\int \sum_{i,j=0}^N a_i a_j (2 - \delta_i)(2 - \delta_j) \cos(i\varphi) \cos(j\varphi) \cos(\varphi) \, d\varphi}{(2\pi)^2 E} \\ &= \frac{\sum_{i=1}^N a_i a_{i-1}}{\pi E} =: \frac{\hat{r}_E}{E} \end{aligned} \quad (\text{A.20})$$

where we used  $\cos(i\varphi) \cos(\varphi) = \frac{\cos[(i+1)\varphi] + \cos[(i-1)\varphi]}{2}$ , inserted the orthogonality of the cosine  $\int_{-\pi}^{\pi} \frac{(2-\delta_i) \cos(i\varphi) \cos(j\varphi)}{2\pi} d\varphi = \delta_{ij}$ , and combined  $\sum (a_i a_{i-1} + a_i a_{i+1}) = 2 \sum a_i a_{i-1}$ . To maximize, we zero the derivative to  $a_m$

$$\begin{aligned}
r'_E &= \frac{\hat{r}'_E}{E} - \frac{\hat{r}_E}{E^2} E' = \frac{1}{E} [\hat{r}'_E - E' r_E] = 0 \\
&= a_{m-1} + a_{m+1} - (2 - \delta_m) a_m r_E = 0.
\end{aligned}$$

If we assume that  $a_m = \cos(m\alpha)$ , and we insert this for  $\frac{a_{m+1}+a_{m-1}}{2-\delta_m} = a_m r_E$ , we recognize by inserting the above theorem  $\cos(m\alpha) \cos(\alpha) = \frac{\cos[(m+1)\alpha] + \cos[(m-1)\alpha]}{2-\delta_m}$

$$\frac{\cos[(m+1)\alpha] + \cos[(m-1)\alpha]}{2 - \delta_m} = \cos(m\alpha) r_E = \cos(m\alpha) \cos(\alpha)$$

that  $r_E = \cos \alpha$ . And to maximize  $r_E$  by constraining that  $a_{N+1} = 0$ , we get the smallest-possible spread  $\alpha = \pm \frac{\pi}{2} \frac{1}{N+1} = \pm \frac{90^\circ}{N+1}$

$$a_m = \begin{cases} \cos\left(\frac{\pi}{2} \frac{m}{N+1}\right), & \text{for } 0 \leq m \leq N, \\ 0, & \text{elsewhere.} \end{cases} \quad (\text{A.21})$$

The max- $r_E$  panning function in 2D consequently is

$$g_N(\varphi) = \sum_{m=-N}^N a_m \Phi_m(\varphi_s) \Phi_m(\varphi) = \sum_{m=-N}^N \cos\left(\frac{\pi}{2} \frac{m}{N+1}\right) \Phi_m(\varphi_s) \Phi_m(\varphi). \quad (\text{A.22})$$

### A.3.5 Towards Spherical Harmonics (3D)

The spherical harmonics are harmonics depending only on angular terms. We may superimpose both parts  $\Delta_{\varphi\zeta} = \Delta_\varphi + \Delta_\zeta$  of the Laplacian and solve the eigenproblem  $r^2 \Delta_{\varphi\zeta} Y = -\lambda Y$

$$\frac{1}{1 - \zeta^2} \frac{\partial^2}{\partial \varphi^2} Y - 2\zeta \frac{\partial}{\partial \zeta} Y + (1 - \zeta^2) \frac{\partial^2}{\partial \zeta^2} Y = -\lambda Y.$$

We assume  $Y$  to be a product of the azimuth harmonics  $\Phi_m(\varphi)$  from above and undefined zenith harmonics  $\Theta(\zeta)$

$$Y = \Phi_m \Theta, \quad (\text{A.23})$$

which yields a differential equation ( $\partial \rightarrow d$ ) only in  $\zeta$  after inserting  $\frac{d^2}{d^2\varphi} \Phi_m = -m^2 \Phi_m$

$$\Theta \frac{-m^2}{1 - \zeta^2} \Phi_m - 2\zeta \Phi_m \frac{d}{d\zeta} \Theta + (1 - \zeta^2) \Phi_m \frac{d^2}{d\zeta^2} \Theta = -\lambda \Phi_m \Theta.$$



And after dividing by  $\Phi_m$ , we obtain the *associated Legendre differential equation*

$$\begin{aligned} \frac{-m^2}{1-\zeta^2}\Theta - 2\zeta \frac{d}{d\zeta}\Theta + (1-\zeta^2) \frac{d^2}{d\zeta^2}\Theta &= -\lambda\Theta, \\ \left[ (1-\zeta^2) \frac{d^2}{d\zeta^2} - 2\zeta \frac{d}{d\zeta} + \lambda - \frac{m^2}{1-\zeta^2} \right] \Theta &= 0. \end{aligned} \quad (\text{A.24})$$

### A.3.6 Zenithal Solution: Associated Legendre Differential Equation

The associated Legendre differential equation (written in  $x$  and  $y$  for mathematical simplicity) is

$$(1-x^2)y'' - 2xy' + \left[ \lambda - \frac{m^2}{1-x^2} \right] y = 0,$$

or after gathering the derivatives

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

**Simplifying the differential equation by  $\frac{1}{1-x^2}$ .** In the associated Legendre differential equation, we would like to get rid of the denominator  $\frac{1}{1-x^2}$ . In this case, it is typical to substitute  $y = (1-x^2)^\alpha v$  and try out which  $\alpha$  succeeds. For insertion into the differential equation, the derivative of  $y$  is

$$y' = -\alpha(1-x^2)^{\alpha-1} 2x v + (1-x^2)^\alpha v' = -2\alpha(1-x^2)^{\alpha-1} x v + (1-x^2)^\alpha v',$$

and the second-order derivative term is

$$\begin{aligned} [(1-x^2)y']' &= [-2\alpha(1-x^2)^\alpha x v + (1-x^2)^{\alpha+1} v']' \\ &= 4\alpha^2(1-x^2)^{\alpha-1} x^2 v - 2\alpha(1-x^2)^\alpha v - 2\alpha(1-x^2)^\alpha x v' \\ &\quad - 2(\alpha+1)(1-x^2)^\alpha x v' + (1-x^2)^{\alpha+1} v'' \\ &= (1-x^2)^\alpha \left[ \frac{4\alpha^2}{1-x^2} x^2 v - 2\alpha v - 2(2\alpha+1) x v' + (1-x^2) v'' \right]. \end{aligned}$$

Together with the term  $\left[ \lambda - \frac{m^2}{1-x^2} \right] y$ , the associated Legendre differential equation becomes

$$(1-x^2)^\alpha \left[ \frac{4\alpha^2}{1-x^2} x^2 v - 2\alpha v + \left( \lambda - \frac{m^2}{1-x^2} \right) v - 2(2\alpha+1)x v' + (1-x^2)v'' \right] = 0$$

$$-m^2 \frac{1-\frac{4\alpha^2}{m^2}x^2}{1-x^2} v + (\lambda-2\alpha)v - 2(2\alpha+1)x v' + (1-x^2)v'' = 0.$$

We see that the term  $\frac{1}{1-x^2}$  entirely cancels by  $\alpha = \frac{m}{2}$ , which fixes the substitution

$$y = \sqrt{1-x^2}^m v. \quad (\text{A.25})$$

Note that for rotational symmetric solutions around the Cartesian  $z$  coordinate, the choice of  $m = 0$  would ensure a constant azimuthal part  $\Phi_m = \text{const.}$  Re-inserting  $x = \zeta = \cos \vartheta$ , the preceding term  $\sqrt{1-\cos^2 \vartheta}^m = \sin^m \vartheta$  is understandably required to represent shapes that aren't rotationally symmetric around  $z$ , but any other, freely rotated axis, for which we also required the sinusoids in 2D. The differential equation for  $v = v(\cos \vartheta)$  is

$$(1-x^2)v'' - 2(m+1)xv' + [\lambda - m(m+1)]v = 0. \quad (\text{A.26})$$

Still, the above equation is singular at  $x \pm 1$ , which means that the second-derivative term multiplied by  $(1-x^2)$  vanishes there, rendering the differential equation into a first-order differential equation, locally. Instead of the more comprehensive Frobenius method we keep it simple: Desired spherical polynomials

$Y_n^m = \Phi_m \Theta_n^m = \mathcal{P}_n(\theta_x, \theta_y, \theta_z)$  with  $\Phi_m(\varphi) \propto \frac{1}{\sqrt{1-\theta_z^2}} \begin{pmatrix} \theta_x & -\theta_y \\ \theta_y & \theta_x \end{pmatrix}^{m-1} \begin{pmatrix} \theta_x \\ \theta_y \end{pmatrix} = \frac{\mathcal{P}_m(\theta_x, \theta_y)}{\sqrt{1-\theta_z^2}}$  imply that  $\Theta_n^m$  must contain  $\sqrt{1-\theta_z^2}^m \mathcal{P}_{n-m}(\theta_z)$  to be polynomial and  $n$ th-order: in condensed notation this is  $y = \sqrt{1-x^2}^m \sum_{k=0}^{n-m} a_k x^k$ , see also [4].

**Power-series for  $v$ .** With  $v = \sum_{k=0}^{\infty} a_k x^k$ , we get after inserting and deriving

$$(1-x^2) \sum_{k=2}^{\infty} k(k-1) a_k x^{k-2} - 2(m+1)x \sum_{k=1}^{\infty} k a_k x^{k-1} + [\lambda - m(m+1)] \sum_{k=0}^{\infty} a_k x^k = 0,$$

$$\sum_{k=2}^{\infty} k(k-1) a_k x^{k-2} - \sum_{k=2}^{\infty} k(k-1) a_k x^k - 2(m+1) \sum_{k=1}^{\infty} k a_k x^k + [\lambda - m(m+1)] \sum_{k=0}^{\infty} a_k x^k = 0.$$

For  $k \geq 2$ , all sum terms are present and the comparison of coefficients for the  $k$ th power yields:

$$(k+1)(k+2)a_{k+2} = [k(k-1) + 2(m+1)k - [\lambda - m(m+1)]]a_k$$

$$a_{k+2} = \frac{k(k+2m+1) + m(m+1) - \lambda}{(k+1)(k+2)} a_k.$$

Typically for such a two-step recurrence, two starting conditions  $a_0 = 1$ ,  $a_1 = 0$  and  $a_0 = 0$ ,  $a_1 = 1$  yield a pair of linearly independent solutions (even and odd).

If the series in  $x$  should converge, it will most certainly do so when  $v$  is *polynomial* and stops at some order. To design  $y$  to be of some arbitrary finite order  $n \in \mathbb{Z}$ , we take into account that  $\sqrt{1-x^2}^m$  is of  $m$ th order already, so the polynomial  $v$  must be  $(n-m)$ th order, and  $|m| \leq n$ . The series is forced to stop the coefficient  $a_k$  for  $k = n-m$  if the numerator is forced to become zero by a suitably chosen  $\lambda$ , thus  $\lambda = (n-m)(n+m+1) + m(m+1) = n(n+1)$ . Corresponding to the termination either at an even or odd  $k = n-m$ , even  $a_0 = 1$ ,  $a_1 = 0$  or odd  $a_0 = 0$ ,  $a_1 = 1$  starting conditions must be chosen. The otherwise wrong-parity solution is an infinite series [5, Eq. 3.2.45] whose convergence radius  $R$  indicates singularities at  $x = \pm 1$ ,

$$R = \lim_{k \rightarrow \infty} \frac{a_k}{a_{k+2}} = \lim_{k \rightarrow \infty} \frac{(k+1)(k+2)}{k(k+2m+1) - m(m+1) - n(n+1)} = \lim_{k \rightarrow \infty} \frac{k^2 + \dots}{k^2 + \dots} = 1. \quad (\text{A.27})$$

Using  $\lambda = n(n+1)$  and writing the differentials in condensed form, the defining differential equations for associated Legendre functions  $P_n^m$  ( $m$  is no exponent but a second index) and their polynomial part  $v_n^m$  become

$$\frac{d}{dx} \left[ (1-x^2) \frac{d}{dx} P_n^m \right] + \left[ n(n+1) - \frac{m(m+1)}{1-x^2} \right] P_n^m = 0, \quad (\text{A.28})$$

$$(1-x^2)^{-m} \frac{d}{dx} \left[ (1-x^2)^{m+1} \frac{d}{dx} v_n^m \right] + [n(n+1) - m(m+1)] v_n^m = 0. \quad (\text{A.29})$$

**Orthogonality of associated Legendre functions.** The resulting associated Legendre differential equation

$$\left[ (1-x^2) [P_n^m]' \right]' + \left[ n(n+1) - \frac{m^2}{1-x^2} \right] P_n^m = 0,$$

yields a sequence of finite-order functions  $P_n^m$  with the order  $n \in \mathbb{N}_0$  and  $|m| \leq n$ . Before even defining these functions, we can prove their orthogonality  $\int_{-1}^1 P_n^m P_l^m dx = 0$  for  $n \neq l$ . This means no product of a pair of associated Legendre functions of different indices  $n \neq l$  produces any constant part on  $x \in [-1; 1]$ , and  $P_n^m$  and  $P_l^m$  do not contain shapes of the respective other function. This is important to uniquely decompose shapes and to define transformation integrals. We multiply the differential equation with  $P_l^m$  and integrate it over  $x$

$$\int_{-1}^1 \left[ (1-x^2) [P_n^m]' \right]' P_l^m dx + \int_{-1}^1 \left[ n(n+1) - \frac{m^2}{1-x^2} \right] P_n^m P_l^m dx = 0.$$

Integration by parts of the first integral yields

$$\int_{-1}^1 \left[ (1-x^2) [P_n^m]' \right]' P_l^m dx = \underbrace{(1-x^2) [P_n^m]' P_l^m}_{=0} \Big|_{-1}^1 - \int_{-1}^1 (1-x^2) [P_n^m]' [P_l^m]' dx, \quad (\text{A.30})$$

where the vanishing part is because of  $(1-x^2) = 0$  at the endpoints  $x = \pm 1$  where  $[P_n^m]'$  and  $P_l^m$  are finite. We get

$$\int_{-1}^1 (1-x^2) [P_n^m]' [P_l^m]' dx = \int_{-1}^1 \left[ n(n+1) - \frac{m^2}{1-x^2} \right] P_n^m P_l^m dx.$$

We could have arrived at an alternative expression, with the only difference in  $l(l+1)$  instead of  $n(n+1)$ ,

$$\int_{-1}^1 (1-x^2) [P_l^m]' [P_n^m]' dx = \int_{-1}^1 \left[ l(l+1) - \frac{m^2}{1-x^2} \right] P_l^m P_n^m dx,$$

if we had started integrating the differential equation of  $P_l^m$  over  $P_n^m$ , instead. The difference of both equations is

$$[n(n+1) - l(l+1)] \int_{-1}^1 P_n^m P_l^m dx = 0,$$

and the scalar in brackets only vanishes for  $n = l$ . For the equation to hold at other  $n \neq l$ , we conclude that the associated Legendre functions  $\int_{-1}^1 P_n^m P_l^m dx = 0$  must be orthogonal. (Orthogonality needs not hold for different  $m$ , as  $\Phi_m$  achieves this orthogonality in azimuth.)

**Solving for polynomial part of associated Legendre functions.** To solve the differential equation for the polynomial part  $v_n^m$  in a way to arrive at the elegant Rodrigues formula, we first play with a test function

$$u_n = (1-x^2)^n, \quad \text{differentiated} \quad u_n' = -2n x (1-x^2)^{n-1} = -2n (1-x^2)^{-1} x u_n.$$

We may write its derivative as differential equation

$$(1-x^2)u_n' + 2n x u_n = 0$$

and derive it  $l$  times by the Leibniz rule  $(f g)^{(n)} = \sum_{k=0}^n \binom{n}{k} f^{(k)} g^{(n-k)}$  for repeated differentiation of products, with the binomial coefficient  $\binom{n}{k} = \frac{n!}{k!(n-k)!}$  and  $f^{(k)} = \frac{d^k f}{dx^k}$  for simplicity. The few non-zero derivatives of  $x$  and  $(1-x^2)$  simplify differentiation,  $x' = 1$ ,  $[(1-x^2)' = -2x]' = -2$ ,

$$\begin{aligned} (1-x^2)u_n^{(l+1)} + l(-2x)u_n^{(l)} + \frac{(l-1)l}{2}(-2)u_n^{(l-1)} + 2nxu_n^{(l)} + 2nl u_n^{(l-1)} &= 0, \\ (1-x^2)u_n^{(l+1)} - 2(l-n)xu_n^{(l)} + l(2n-l+1)u_n^{(l-1)} &= 0. \end{aligned}$$

This equation matches  $(1-x^2)v_n^{(m)} - 2(m+1)xv_n^{(m)} + [n(n+1) - m(m+1)]v_n^{(m)} = 0$  by matching the coefficients  $l-n = m+1$ , hence  $l = m+n+1$ , which nicely implies  $l(2n-l+1) = n(n+1) - m(m+1)$ ,

$$(1-x^2)u_n^{(m+n+2)} - 2(m+1)xu_n^{(m+n+1)} + [n(n+1) - m(m+1)]u_n^{(m+n)} = 0.$$

We therefore find the solutions  $v_n^m = u_n^{(n+m)} = \frac{d^{n+m}}{dx^{n+m}}(1-x^2)^n$  yielding  $y_n^m = \sqrt{1-x^2} \frac{d^{n+m}}{dx^{n+m}}(1-x^2)^n$ .

**Rodrigues formula.** By of the above, the Rodrigues formula for the associated Legendre functions  $P_n^m$  becomes

$$P_n^m = \frac{(-1)^{n+m}}{2^n n!} \sqrt{1-x^2}^m \frac{d^{n+m}}{dx^{n+m}}(1-x^2)^n \quad (\text{A.31})$$

$$\text{or } P_n^m = (-1)^m \sqrt{1-x^2}^m \frac{d^m}{dx^m} P_n, \quad \text{with } P_n = \frac{(-1)^n}{2^n n!} \frac{d^n}{dx^n}(1-x^2)^n.$$

and  $P_n = P_n^0$  are the Legendre polynomials. The Legendre polynomials are normalized to  $P_n(1) = 1$  by the factor  $\frac{(-1)^n}{2^n n!}$ . Because  $(1-x^2)$  is zero at  $x = 1$  with any positive integer exponent, only the part of its  $n$ -fold derivative that exclusively affects the power of  $(1-x^2)^n$  for  $n$  times is responsible for its value there:  $n!(-2x)^n(1-x^2)^0|_{x=1} = n!2^n(-1)^n$ . The scaling of the associated Legendre functions with  $m > 0$  is somewhat more arbitrary in sign and value.

**Indices  $n$  and  $m$ .** The boundaries for the index  $m$  of the Legendre functions  $m \in \mathbb{Z}$  are typically  $-n \leq m \leq n$ , however due to the shift of the eigenvalue by  $\frac{m^2}{1-x^2}$ , functions for positive and negative  $m$  are linearly dependent. We observe this by inspecting the highest-order terms in [6]

$$\begin{aligned} 2^n n! \sqrt{1-x^2}^m P_n^m &= (-1)^{n+m} (1-x^2)^m \frac{d^{n+m}(1-x^2)^n}{dx^{n+m}} \\ &= x^{2m} \frac{d^{n+m}}{dx^{n+m}} \left[ x^{2n} - \dots \right] = x^{2m} \left[ \frac{(2n)!}{(n-m)!} x^{n-m} - \dots \right] \\ 2^n n! \sqrt{1-x^2}^m P_n^{-m} &= (-1)^{n+m} \frac{d^{n-m}(1-x^2)^n}{dx^{n-m}} \end{aligned}$$

$$\begin{aligned}
&= (-1)^m \frac{d^{n-m}}{dx^{n-m}} \left[ x^{2n} - \dots \right] = (-1)^m \left[ \frac{(2n)!}{(n+m)!} x^{n+m} - \dots \right] \\
\Rightarrow P_n^{-m} &= (-1)^m \frac{(n-m)!}{(n+m)!} P_n^m \quad (\text{A.32})
\end{aligned}$$

and to avoid confusion, it convenient to only use  $m \geq 0$ , or  $|m|$  to evaluate the associated Legendre functions.

**Alternative definition: three-term recurrence.** Any polynomial  $\mathcal{P}_n$  of the order  $n$  can be decomposed into Legendre polynomials  $\mathcal{P}_n = \sum_{i=0}^n c_i P_i$ , and the Legendre polynomial  $P_j$  is orthogonal to all those Legendre polynomials  $\int_{-1}^1 \mathcal{P}_n P_j dx = 0$  if  $j > n$ . With this knowledge it is interesting to describe  $\int_{-1}^1 (x P_i) P_j dx$ . As  $(x P_i)$  is of  $(i+1)$ th order, the integral must vanish for  $j > i+1$ . Because of commutativity,  $\int_{-1}^1 P_i (x P_j) dx$ , and  $(x P_j)$  being  $(j+1)$ th order, it also vanishes for  $i > j+1$ . Hereby, re-expansion of  $x P_n$  can maximally use three terms,  $x P_n = \alpha P_{n-1} + \gamma P_n + \beta P_{n+1}$ . In fact only two terms remain as  $P_{2k}$  are even functions on  $x \in [-1; 1]$  and  $P_{2k+1}$  are odd, thus orthogonal. The product  $x P_n$  changes the parity of  $P_n$ , leaving  $x P_n = \alpha P_{n-1} + \beta P_{n+1}$ . At  $x = 1$  all polynomials were normalized to  $P_i(1) = 1$ , therefore evaluation at  $x = 1$  leaves  $1 = \alpha + \beta$ , so  $\alpha = 1 - \beta$ , hence

$$x P_n = \beta_n P_{n+1} + (1 - \beta_n) P_{n-1}.$$

As also the associated Legendre functions  $P_n^m$  for a specific  $m$  are orthogonal, the recurrence is more general

$$x P_n^m = \beta_n^m P_{n+1}^m + (1 - \beta_n^m) P_{n-1}^m.$$

To determine the coefficient  $\beta_n^m$ , we only need to find out how the highest-power coefficients  $x^{n-m+1}$  of the polynomial parts in  $x P_n^m$  and  $P_{n+1}^m$  are related. We see this after inserting  $P_n = \sqrt{1-x^2}^m \frac{(-1)^{n+m}}{2^n n!} \frac{d^{n+m}}{dx^{n+m}} (1-x^2)^n$  and division by  $\sqrt{1-x^2}^m \frac{(-1)^{n+m}}{2^n n!}$ , which leaves a recurrence for the polynomial part

$$\underbrace{x v_n^m}_{O=n-m+1} = - \underbrace{\frac{\beta_n^m}{2(n+1)} v_{n+1}^m}_{O=n-m+1} - \underbrace{2(n+1)(1-\beta_n^m) v_{n-1}^m}_{O=n-m-1}.$$

Of the highest powers  $x^{n-m+1}$  in both  $x v_n^m$  and  $v_{n+1}^m$  the coefficients  $c_{n,n-m}^m$  and  $c_{n+1,n-m+1}^m$  define

$$\beta_n^m = -2(n+1) \frac{c_{n,n-m}^m}{c_{n+1,n-m+1}^m}.$$

To find it, we binomially expand  $(1-x^2)^n$  to  $(1-x^2)^n = (-1)^n \sum_{k=0}^n (-1)^k \binom{n}{k} x^{2(n-k)}$

$$\frac{v_n^m}{(-1)^n} = \frac{d^{n+m}}{dx^{n+m}} \sum_{k=0}^n \binom{n}{k} (-1)^k x^{2(n-k)} = \sum_{k=0}^{\lfloor \frac{n-m}{2} \rfloor} \binom{n}{k} \frac{(2n-2k)!(-1)^k}{(n-m-2k)!} x^{n-m-2k},$$

so that with  $k=0$  we can find  $c_{n,n-m}^m = \frac{(-1)^n n!}{n!} \frac{(2n)!}{(n-m)!} = \frac{(-1)^n (2n)!}{(n-m)!}$  for the highest-power coefficient of  $v_n^m$ . Accordingly, coefficient of the recurrence is

$$\beta_n^m = 2(n+1) \frac{(n-m+1)}{(2n+1)(2n+2)} = \frac{n-m+1}{2n+1},$$

hence with  $1 - \beta_n^m = \frac{n+m}{2n+1}$ , and  $x P_n^m = \frac{n-m+1}{2n+1} P_{n+1}^m + \frac{n+m}{2n+1} P_{n-1}^m$ , we can construct  $P_n^m$  recursively by

$$P_{n+1}^m = \frac{2n+1}{n-m+1} x P_n^m - \frac{n+m}{n-m+1} P_{n-1}^m. \quad (\text{A.33})$$

The start value is  $P_n^n = \frac{(-1)^{2n}}{2^n n!} \sqrt{1-x^2}^n \frac{d^{2n}}{dx^{2n}} (1-x^2)^n = \frac{(-1)^n (2n)!}{2^n n!} \sqrt{1-x^2}^n$ , and for  $n=m$ , the term  $P_{n-1}^m$  is excluded.

**Normalization.** A unity square integral (orthonormalization) simplifies the definition of transform integrals. We would like to obtain the corresponding factor  $N_n^m$  with

$$\int_{-1}^1 (P_n^m N_n^m)^2 dx = 1.$$

Normalization for  $m=0$  is easy to find by repeated integration by parts

$$\begin{aligned} \frac{2^{2n} n!^2}{(N_n)^2} &= 2^{2n} n!^2 \int_{-1}^1 (P_n)^2 dx = \underbrace{\left[ (1-x^2)^n \right]^{(n-1)} \left[ (1-x^2)^n \right]^{(n)} \Big|_{-1}}_{=0} \\ &\quad - \int_{-1}^1 \left[ (1-x^2)^n \right]^{(n-1)} \left[ (1-x^2)^n \right]^{(n)} dx \\ &= \dots = (-1)^n \int_{-1}^1 (1-x^2)^n \left[ (1-x^2)^n \right]^{(2n)} dx \\ &= \int_{-1}^1 (1-x^2)^n (2n)! dx = (2n)! \int_0^\pi \sin^{2n} \vartheta \sin \vartheta d\vartheta. \end{aligned}$$

With the integral  $\int_0^\pi \sin^{2n+1} \vartheta d\vartheta = 2 \frac{(2n)!!}{(2n+1)!!} = 2 \frac{2^{2n} n!^2}{(2n+1)!}$ , this is  $(N_n)^{-2} = \frac{2(2n)!}{(2n+1)!} = \frac{2}{2n+1}$ . For  $N_n^m$ , a trick to insert the relation between  $P_n^m$  and  $P_n^{-m}$  is used [6], and integration by parts until the differentials are of the same order

$$\frac{1}{(N_n^m)^2} = \int_{-1}^1 P_n^m P_n^m dx = \int_{-1}^1 P_n^m \frac{(-1)^m (n-m)!}{(n+m)!} P_n^{-m} dx$$

$$\begin{aligned}
&= \frac{1}{2^{2n} n!^2} \frac{(-1)^m (n-m)!}{(n+m)!} \int_{-1}^1 [(1-x^2)]^{(n+m)} [(1-x^2)]^{(n-m)} dx = \dots \\
&= \frac{(n-m)!}{(n+m)!} \underbrace{\int_{-1}^1 \frac{1}{2^{2n} n!^2} [(1-x^2)]^{(n-m)} [(1-x^2)]^{(n-m)} dx}_{=1/(N_n)^2} = \frac{2}{2n+1} \frac{(n+m)!}{(n-m)!} \\
\Rightarrow N_n^m &= (-1)^m \sqrt{\frac{(2n+1)}{2} \frac{(n-m)!}{(n+m)!}} \quad (\text{A.34})
\end{aligned}$$

The  $(-1)^m$  can be excluded if not used in the Rodrigues formula. (*It is always a wise idea to check and compare signs as conventions may differ ... in practice  $(-1)^m$  is a rotation around  $z$  by  $180^\circ$ .*)

### A.3.7 Spherical Harmonics

With all the above definitions, we obtain the fully normalized spherical harmonics

$$Y_n^m(\varphi, \vartheta) = N_n^{|m|} P_n^{|m|}(\cos \vartheta) \Phi_m(\varphi) \quad (\text{A.35})$$

**Orthonormality.** They are *orthonormal* when integrated over the sphere

$$\int_{\mathbb{S}^2} Y_n^m Y_{n'}^{m'} d \cos \theta d\varphi = \delta_{nn'} \delta_{mm'}. \quad (\text{A.36})$$

**Transform integral.** Because of their completeness in the Hilbert space, any square-integrable function  $g(\varphi, \vartheta)$  can be decomposed by

$$g(\varphi, \vartheta) = \sum_{n=0}^{\infty} \sum_{m'=-n'}^{n'} \gamma_{n'm'} Y_{n'}^{m'}(\varphi, \vartheta). \quad (\text{A.37})$$

From a known function  $g(\varphi, \vartheta)$ , the coefficients are obtained by integrating  $g$  with another spherical harmonic  $Y_n^m$  over the unit sphere  $\mathbb{S}^2$ ,  $\int_{-1}^1 d \cos \vartheta \int_0^{2\pi} d\varphi$ . For a simple notation, we gather the two variables in a direction vector  $\boldsymbol{\theta} = [\cos \varphi \sin \vartheta, \sin \varphi \sin \vartheta, \cos \vartheta]^T$  and write

$$\int_{\mathbb{S}^2} g(\boldsymbol{\theta}) Y_n^m d\boldsymbol{\theta} = \sum_{n'=0}^{\infty} \sum_{m'=-n'}^{n'} \gamma_{n'm'} \underbrace{\int_{\mathbb{S}^2} Y_{n'}^{m'} Y_n^m d\boldsymbol{\theta}}_{\delta_{nn'} \delta_{mm'}} = \gamma_{nm}. \quad (\text{A.38})$$



**Parseval's theorem.** Due to orthonormality, the integral norm of any pattern  $g(\boldsymbol{\theta})$  composed as  $\sum_{n=0}^{\infty} \sum_{m=-n}^n \gamma_{nm} Y_n^m(\boldsymbol{\theta})$  is equivalent to

$$\int_{\mathbb{S}^2} |g(\boldsymbol{\theta})|^2 d\boldsymbol{\theta} = \sum_{n=0}^{\infty} \sum_{m=-n}^n |\gamma_{nm}|^2 \quad (\text{A.39})$$

because  $\int_{\mathbb{S}^2} \sum_{n,n',m,m'} \gamma_{nm} \gamma_{n'm'}^* Y_n^m(\boldsymbol{\theta}) Y_{n'}^{m'}(\boldsymbol{\theta}) d\boldsymbol{\theta} = \sum_{n,n',m,m'} \gamma_{nm} \gamma_{n'm'}^* \delta_{nn'} \delta_{mm'}$ .

**3D panning functions: Dirac delta on the sphere.** An infinitely narrow range around the desired direction  $\boldsymbol{\theta}_s$  can be described by limiting the dot product  $\boldsymbol{\theta}_s^T \boldsymbol{\theta} > \cos \varepsilon \rightarrow 1$ . A unit-surface Dirac delta distribution  $\delta(1 - \boldsymbol{\theta}_s^T \boldsymbol{\theta})$  can be described as

$$\delta(1 - \boldsymbol{\theta}_s^T \boldsymbol{\theta}) = \frac{1}{2\pi} \begin{cases} \lim_{\varepsilon \rightarrow 0} \frac{1}{1 - \cos \varepsilon}, & \text{for } \arccos \boldsymbol{\theta}_s^T \boldsymbol{\theta} < \varepsilon \\ 0, & \text{otherwise.} \end{cases} \quad (\text{A.40})$$

And its coefficients are found by the transformation integral

$$\gamma_{nm} = \int_{\mathbb{S}^2} Y_n^m(\boldsymbol{\theta}) d\boldsymbol{\theta} = Y_n^m(\boldsymbol{\theta}_s) \int_0^{2\pi} d\varphi \lim_{\varepsilon \rightarrow 0} \int_{\cos \varepsilon}^1 d\zeta = Y_n^m(\boldsymbol{\theta}_s). \quad (\text{A.41})$$

Typically, a finite-order panning function with  $n \leq N$  employs a weight  $a_n$  to reduce side lobes

$$g_N(\boldsymbol{\theta}) = \sum_{n=0}^N \sum_{m=-n}^n a_n Y_n^m(\boldsymbol{\theta}_s) Y_n^m(\boldsymbol{\theta}). \quad (\text{A.42})$$

Assuming the panning direction is  $\boldsymbol{\theta}_s = [0, 0, 1]^T$ , we get the axisymmetric panning function, with  $Y_n^0 = \sqrt{\frac{2n+1}{4\pi}} P_n$ ,

$$g_N(\vartheta) = \frac{1}{2\pi} \sum_{n=0}^N \frac{2n+1}{2} a_n P_n(\cos \vartheta). \quad (\text{A.43})$$

We can evaluate its  $E$  measure by integrating  $g_N^2$  over the sphere

$$\begin{aligned} E &= \underbrace{\int_0^{2\pi} d\varphi}_{2\pi} \int_{-1}^1 g_N(\zeta)^2 d\zeta = \sum_{i,j} \frac{2i+1}{2} \frac{2j+1}{2} a_i a_j \underbrace{\int_{-1}^1 P_i P_j d\zeta}_{\delta_{ij} \frac{2}{2i+1}} \\ &= \sum_{n=0}^N \frac{2n+1}{2} a_n^2. \end{aligned} \quad (\text{A.44})$$

The  $r_E$  measure is, because of the axisymmetry, perfectly aligned with  $z$ , therefore, its length is calculated by

$$\begin{aligned}
 r_E &= \frac{\int_{-1}^1 g_N(\zeta) \zeta \, d\zeta}{E} = \frac{\sum_{i,j} \frac{2i+1}{2} \frac{2j+1}{2} a_i a_j \int_{-1}^1 P_i \overbrace{\zeta P_j}^{P_{j+1} + \frac{j}{2j+1} P_{j-1}} \, d\zeta}{E} \\
 &= \frac{\sum_{i,j} \frac{2i+1}{4} a_i a_j \int_{-1}^1 P_i [(j+1)P_{j+1} + jP_{j-1}] \, d\zeta}{E} \\
 &= \frac{\sum_{n=0}^N [n a_n a_{n-1} + (n+1) a_n a_{n+1}]}{2E} = \frac{\sum_{n=1}^N n a_n a_{n-1}}{E}. \quad (\text{A.45})
 \end{aligned}$$

**3D max- $r_E$ .** For the narrowest-possible spread, we maximize  $r_E$ , which we decompose into  $r_E = \frac{\hat{r}_E}{E}$  and we zero its derivative, as for 2D,

$$\begin{aligned}
 r'_E &= \frac{\hat{r}'_E}{E} - \frac{\hat{r}_E}{E^2} E' = \frac{1}{E} [\hat{r}'_E - E' r_E] = 0 \\
 n a_{n-1} + (n+1) a_{n+1} - (2n+1) a_n r_E &= 0. \quad (\text{A.46})
 \end{aligned}$$

If we assume that  $a_n = P_n(\zeta)$ , we see by  $(n+1)P_{n+1} + nP_{n-1} = (2n+1)P_n \zeta$

$$(n+1)P_{n+1} + nP_{n-1} = (2n+1)P_n \zeta = P_n r_E \quad (\text{A.47})$$

that  $r_E = \zeta$  and  $a_n = P_n(\zeta) = P_n(r_E)$ . We maximize  $r_E$  under the constraint that  $P_{N+1}(r_E) = 0$ . Therefore,  $r_E$  must be as close to 1 as possible, and be a zero of the Legendre polynomial  $P_{N+1}$ . It can be discovered by a root-finding algorithm in MATLAB, e.g. Newton–Raphson, when the function  $P_n$  is implemented. In [7], the useful approximation  $r_E = \cos \frac{2.4062}{N+1.51} = \cos \frac{137.9^\circ}{N+1.51}$  was given.

**Squared norm mirror/rotation invariance.** The norm of any pattern  $a(\theta)$  is invariant under orthogonal coordinate transform (rotation/mirror)  $\hat{\theta} = \mathbf{R} \theta$  with  $\mathbf{R}^T \mathbf{R} = \mathbf{I}$ ,

$$\int_{\mathbb{S}^2} a^2(\theta) \, d\theta = \int_{\mathbb{S}^2} b^2(\theta) \, d\theta, \quad \text{with } b(\theta) = a(\mathbf{R} \theta). \quad (\text{A.48})$$

The norm equivalence of the corresponding spherical harmonics coefficients  $\alpha_{nm}$  and  $\beta_{nm}$  follows from Parseval's theorem

$$\sum_{n=0}^{\infty} \sum_{m=-n}^n |\alpha_{nm}|^2 = \sum_{n=0}^{\infty} \sum_{m=-n}^n |\beta_{nm}|^2. \quad (\text{A.49})$$

In vector notation of the coefficients, i.e.  $\boldsymbol{\alpha} = [\alpha_{00}, \dots, \alpha_{NN}]^T$  and  $\boldsymbol{\beta} = [\beta_{00}, \dots, \beta_{NN}]^T$ , this is  $\|\boldsymbol{\alpha}\|^2 = \|\boldsymbol{\beta}\|^2$ . To fulfill this equivalence, both vectors are related by an orthogonal matrix  $\boldsymbol{\beta} = \mathbf{Q} \boldsymbol{\alpha}$  with  $\mathbf{Q}^T \mathbf{Q} = \mathbf{I}$ , and hence  $\|\mathbf{b}\|^2 = \boldsymbol{\beta}^T \boldsymbol{\beta} = \boldsymbol{\alpha}^T \mathbf{Q}^T \mathbf{Q} \boldsymbol{\alpha} =$

$\alpha^T \alpha = \|\alpha\|^2$ . Moreover, rotation/mirroring neither creates components of higher nor lower orders, so that  $\mathbf{Q}$  must be block structured

$$\mathbf{Q} = \begin{bmatrix} \mathbf{Q}_0 & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{Q}_1 & \mathbf{0} & \vdots \\ \vdots & \ddots & \ddots & \ddots \end{bmatrix}. \quad (\text{A.50})$$

The order subspaces in  $n$  therefore stay de-coupled, so that the coefficient vectors for every order-subspace  $n$  are related and norm equivalent under mirror/rotation operations

$$\|\alpha_n\|^2 = \|\beta_n\|^2, \quad \beta_n = \mathbf{Q}_n \alpha_n, \quad \mathbf{Q}_n^T \mathbf{Q}_n = \mathbf{I}_{2n+1}. \quad (\text{A.51})$$

**Pseudo all-pass character of the Dirac delta.** Dirac delta distributions  $\delta(\theta^T \theta_s - 1)$  yield the coefficients  $Y_n^m(\theta_s)$ , and due to rotation invariance they yield constant energy in every spherical harmonic order  $n$ , regardless of the aiming  $\theta_s$ . One can determine the norm for zenithal aiming  $\vartheta = 0$ , i.e.  $\theta_z = 0, 0, 1^T$ , yielding a non-zero coefficient for  $m = 0$

$$Y_n^m(\theta_z) = \sqrt{\frac{2n+1}{4\pi}} \overbrace{P_n(1)}^{=1} \delta_m = \sqrt{\frac{2n+1}{4\pi}} \delta_m.$$

Because of the rotation invariance we recognize a pseudo-allpass character (Unsöld theorem) of the spherical harmonics of any order  $n$

$$\sum_{m=-n}^n |Y_n^m(\theta_s)|^2 = \sum_{m=-n}^n |Y_n^m(\theta_z)|^2 = \frac{2n+1}{4\pi} = (2n+1) |Y_0^0(\theta_s)|^2.$$

For encoded single-direction Ambisonic signals  $\alpha_{nm}(t)$ , this implies

$$\sum_{m=-n}^n |\alpha_{nm}(t)|^2 = (2n+1) |\alpha_{00}(t)|^2. \quad (\text{A.52})$$

**Expected norm in the diffuse field.** An ideal diffuse sound field is composed of directional signals  $a(\theta_s, t)$  from all directions  $\theta_s$ , with no correlation for signals from different directions  $\mathcal{E}\{a(\theta_1, t) a(\theta_2, t)\} = \sigma_a^2 \delta(\theta_1^T \theta_2 - 1)$ . Its coefficients are obtained by the integral over the directions

$$\alpha_{nm}(t) = \int_{\mathbb{S}^2} a(\theta_s, t) Y_n^m(\theta_s) d\theta_s, \quad (\text{A.53})$$

and we can show that not only the expected directional signals, but also the spherical harmonic coefficients are orthogonal by  $\mathcal{E}\{a(\theta_1, t) a(\theta_2, t)\} = \sigma_a^2 \delta(\theta_1^T \theta_2 - 1)$  and

orthonormality  $\int_{\mathbb{S}^2} Y_n^m Y_{n'}^{m'} d\boldsymbol{\theta} = \delta_{nn'} \delta_{mm'}$  of the spherical harmonics

$$\begin{aligned} \mathcal{E}\{\alpha_{nm}(t) \alpha_{n'm'}(t)\} &= \int_{\mathbb{S}^2} \int_{\mathbb{S}^2} \mathcal{E}\{a(\boldsymbol{\theta}_1, t) a(\boldsymbol{\theta}_2, t)\} Y_n^m(\boldsymbol{\theta}_1) Y_{n'}^{m'}(\boldsymbol{\theta}_2) d\boldsymbol{\theta}_1 d\boldsymbol{\theta}_2 \\ &= \sigma_a^2 \int_{\mathbb{S}^2} Y_n^m(\boldsymbol{\theta}) Y_{n'}^{m'}(\boldsymbol{\theta}) d\boldsymbol{\theta} = \sigma_a^2 \delta_{nn'} \delta_{mm'}. \end{aligned} \quad (\text{A.54})$$

In a perfectly diffuse field, we therefore expect the same norm in every spherical harmonic component per frequency band. We could reformulate this to

$$\mathcal{E}\{|\alpha_{nm}(t)|^2\} = \mathcal{E}\{|\alpha_{00}(t)|^2\},$$

however the temporal disjointness assumption of SDM only invents a drastically thinned out content in the individual higher-order spherical harmonics. To cover the available temporal information from all  $(2n + 1)$  spherical harmonic signals within each order  $n$  and for a similar formulation as for a single-direction component, we may re-formulate

$$\sum_{m=-n}^n \mathcal{E}\{|\alpha_{nm}(t)|^2\} = (2n + 1) \mathcal{E}\{|\alpha_{00}(t)|^2\}. \quad (\text{A.55})$$

**Spherical convolution.** By the argumentation used above to prove rotation invariance, we can argue that isotropic filtering of spherical patterns is invariant under rotation, and must therefore depend only on the order  $n$ . Spherical convolution is defined in [8] by the coefficients  $\beta_{nm}$  of a function  $b(\boldsymbol{\theta})$  convolved with the coefficients  $\alpha_n$  of a rotationally symmetric shape  $a(\boldsymbol{\theta}) = a(\theta_z)$

$$\gamma_{nm} = \alpha_n \beta_{nm}. \quad (\text{A.56})$$

**Spherical cap function.** A rotationally symmetric spherical cap function at  $\pm \frac{\alpha}{2}$  centered around  $\vartheta = 0$ , briefly  $\theta_z$ , can be written in terms of a unit-step. We find the shape coefficients  $w_n$  for its spherical harmonic decomposition by

$$u(\cos \vartheta - \cos \frac{\alpha}{2}) = \sum_{n=0}^{\infty} \sum_{m=-n}^n w_n Y_n^m(\boldsymbol{\theta}) Y_n^m(\boldsymbol{\theta}_z) = \sum_{n=0}^{\infty} w_n P_n(\cos \vartheta) \frac{2n+1}{4\pi}, \quad (\text{A.57})$$

where  $Y_n^m(\boldsymbol{\theta}_z) = \sqrt{\frac{2n+1}{4\pi}} P_n^m(1) = \sqrt{\frac{2n+1}{4\pi}} \delta_m$  and  $P_n^0 = P_n$  was used. The coefficients  $w_n$  are obtained by integration over Legendre polynomials  $d \cos \vartheta \int_{-1}^1 P_{n'}(\cos \vartheta)$  and for the right hand-side using their orthogonality  $\int_{-1}^1 P_{n'}(\zeta) P_n(\zeta) d\zeta = \frac{2}{2n+1} \delta_{nn'}$ , leaving  $w_n \frac{2}{2n+1} \frac{2n+1}{4\pi}$ , so that

$$w_n = 2\pi \int_{\cos \frac{\alpha}{2}}^1 P_n(x) dx.$$

The integral is solved by  $2^n n! P_n = \frac{d^n v^n}{dx^n}$  with  $v = (x^2 - 1)$  after replacing the innermost derivative by  $\frac{d}{dx} = \frac{dv}{dx} \frac{d}{dv} = 2x \frac{d}{dv}$ , and Leibniz' rule for repeated derivatives

$$\begin{aligned} \frac{d^n v^n}{dx^n} &= \frac{d^{n-1} 2x \frac{dv^n}{dv}}{dx^{n-1}} = \frac{d^{n-1} (2x n v^{n-1})}{dx^{n-1}} \\ &= (2n) \left[ \binom{0}{n-1} \frac{d^0 x}{dx^0} \frac{d^{n-1} v^{n-1}}{dx^{n-1}} + \binom{1}{n-1} \frac{d^1 x}{dx^1} \frac{d^{n-2} v^{n-1}}{dx^{n-2}} \right] \\ &= (2n) \left[ x \frac{d^{n-1} v^{n-1}}{dx^{n-1}} + (n-1) \frac{d^{n-2} v^{n-1}}{dx^{n-2}} \right]. \end{aligned}$$

We may increase  $n$  by one, observe that the last expression has one fewer differential, thus is an integrated version, and obtain after re-inserting  $2^n n! P_n = \frac{d^n v^n}{dx^n}$

$$\begin{aligned} 2^{n+1} (n+1)! P_{n+1} &= 2(n+1) \left[ 2^n n! x P_n + n 2^n n! \int P_n dx - n C \right] \\ \int P_n dx &= \frac{P_{n+1} - x P_n}{n} + C \end{aligned} \quad (\text{A.58})$$

With the definite integration limits  $x_0 = \cos \frac{\alpha}{2}$  and 1 and  $\int_{x_0}^1 P_n dx$  only depends on lower boundary as  $P_{n+1}(1) - 1 \cdot P_n(1) = 0$ ,

$$\int_{x_0}^1 P_n(x) dx = - \frac{P_{n+1}(x_0) - x_0 P_n(x_0)}{n} \quad (\text{A.59})$$

$$w_n = -2\pi \frac{P_{n+1}(\cos \frac{\alpha}{2}) - \cos \frac{\alpha}{2} P_n(\cos \frac{\alpha}{2})}{n}, \quad \text{for } n > 0, \quad (\text{A.60})$$

and  $w_0 = 2\pi \int_{\cos \frac{\alpha}{2}}^1 dx = 2\pi(1 - \cos \frac{\alpha}{2})$  for  $n = 0$ .

The recurrence  $(2n+1)xP_n - (n+1)P_{n+1} = nP_{n-1}$  yields alternatively for  $n > 0$

$$w_n = 2\pi \frac{P_{n+1}(\cos \frac{\alpha}{2}) + P_{n-1}(\cos \frac{\alpha}{2})}{2n+1} = 2\pi \frac{P_{n-1}(\cos \frac{\alpha}{2}) - \cos \frac{\alpha}{2} P_n(\cos \frac{\alpha}{2})}{n+1}. \quad (\text{A.61})$$

## A.4 Encoding to SH and Decoding to SH

**Mode-matching decoder:**  $L$  loudspeakers driven by the weights  $g_l$  and given by their directions  $\{\theta_l\}$  produce a pattern  $f(\theta)$  linearly composed of Dirac deltas

$$\begin{aligned}
 f(\boldsymbol{\theta}) &= \sum_{l=1}^L \delta(\boldsymbol{\theta}^T \boldsymbol{\theta}_l - 1) g_l \\
 &= \sum_{n=0}^{\infty} \sum_{m=-n}^n Y_n^m(\boldsymbol{\theta}) \sum_{l=1}^L Y_n^m(\boldsymbol{\theta}_l) g_l = \mathbf{y}(\boldsymbol{\theta})^T \mathbf{Y} \mathbf{g},
 \end{aligned} \tag{A.62}$$

in an order-unlimited representation. The vector  $\mathbf{y} = [Y_n^m(\boldsymbol{\theta})]_{nm}$  contains all the spherical harmonics  $0 \leq n \leq \infty$ ,  $-n \leq m \leq n$ , in a suitable order, e.g. Ambisonic Channel Number (ACN)  $n^2 + m + n$ , and the matrix  $\mathbf{Y} = [\mathbf{y}(\boldsymbol{\theta}_l)]_l$  contains the spherical harmonic coefficient vectors of every loudspeaker. Obviously, the spherical harmonic coefficients synthesized by the loudspeakers are  $\boldsymbol{\phi} = \mathbf{Y} \mathbf{g}$ , so that

$$f(\boldsymbol{\theta}) = \mathbf{y}(\boldsymbol{\theta})^T \mathbf{Y} \mathbf{g} = \mathbf{y}(\boldsymbol{\theta})^T \boldsymbol{\phi}.$$

With  $L$  loudspeakers, at most  $(N + 1)^2 \leq L$  spherical harmonics can be controlled. Therefore control typically restricts to the under-determined  $N$ th-order subspace

$$\boldsymbol{\phi}_N = \mathbf{Y}_N \mathbf{g},$$

in which we can synthesize any coefficient vector  $\boldsymbol{\phi}_N$ . To get a finite and well-determined solution with the exceeding and arbitrary degrees of freedom in  $\mathbf{g}$ , the least-squares solution for  $\mathbf{g}$  is searched under the constraint

$$\begin{aligned}
 &\min \|\mathbf{g}\|^2 \\
 &\text{subject to: } \boldsymbol{\phi}_N = \mathbf{Y}_N \mathbf{g},
 \end{aligned} \tag{A.63}$$

yielding the cost function with the Lagrange multipliers  $\boldsymbol{\lambda}$

$$J(\mathbf{g}, \boldsymbol{\lambda}) = \mathbf{g}^T \mathbf{g} + (\boldsymbol{\phi}_N - \mathbf{Y}_N \mathbf{g})^T \boldsymbol{\lambda}.$$

For the optimum in  $\mathbf{g}$ , its derivative to  $\mathbf{g}$  is zero, and in  $\boldsymbol{\lambda}$  the corresponding derivative:

$$\begin{aligned}
 \frac{\partial J}{\partial \mathbf{g}} &= 2\mathbf{g}_{\text{opt}} - \mathbf{Y}_N^T \boldsymbol{\lambda} = 0, & \frac{\partial J}{\partial \boldsymbol{\lambda}} &= \boldsymbol{\phi}_N - \mathbf{Y}_N \mathbf{g} = 0.
 \end{aligned}$$

For  $\mathbf{g}$  the equation yields  $\mathbf{g}_{\text{opt}} = \frac{1}{2} \mathbf{Y}_N^T \boldsymbol{\lambda}$ , and for  $\boldsymbol{\lambda}$  the original constraint  $\boldsymbol{\phi}_N = \mathbf{Y}_N \mathbf{g}$  that only allows to insert the optimal  $\mathbf{g}$  yielding  $\boldsymbol{\phi}_N = \mathbf{Y}_N (\frac{1}{2} \mathbf{Y}_N^T \boldsymbol{\lambda}_{\text{opt}})$ . Inversion of  $(\frac{1}{2} \mathbf{Y}_N \mathbf{Y}_N^T)^{-1}$  from the left yields the multipliers  $2(\mathbf{Y}_N \mathbf{Y}_N^T)^{-1} \boldsymbol{\phi}_N = \boldsymbol{\lambda}_{\text{opt}}$ , so that

$$\mathbf{g} = \mathbf{Y}_N^T (\mathbf{Y}_N \mathbf{Y}_N^T)^{-1} \boldsymbol{\phi}_N. \tag{A.64}$$

The solution is right-inverse to  $\mathbf{Y}_N$ , i.e.  $\mathbf{Y}_N [\mathbf{Y}_N^T (\mathbf{Y}_N \mathbf{Y}_N^T)^{-1}] = \mathbf{I}$ .

**Best-fit encoder by MMSE:** When given  $M$  samples of a spherical function  $g(\boldsymbol{\theta})$  at the locations  $\{\boldsymbol{\theta}_l\}$ , we can minimize the means-square error (MMSE)

$$\min \sum_{l=1}^L \left[ g(\boldsymbol{\theta}_l) - \sum_{n=0}^N \sum_{m=-n}^n Y_n^m(\boldsymbol{\theta}_l) \gamma_{nm} \right]^2$$

to find suitable spherical harmonic coefficients  $\gamma_{nm}$ . Using the matrix notation from above, this is

$$\min \|\mathbf{e}\|^2 = \min \|\mathbf{g} - \mathbf{Y}_N^T \boldsymbol{\gamma}_N\|^2 \quad (\text{A.65})$$

and we find by zeroing the derivative

$$\begin{aligned} \frac{\partial}{\partial \boldsymbol{\gamma}_N} \mathbf{e}^T \mathbf{e} &= 2 \left( \frac{\partial \mathbf{e}}{\partial \boldsymbol{\gamma}_N} \right)^T \mathbf{e} = 2 \mathbf{Y}_N \mathbf{e} = 2 \mathbf{Y}_N \mathbf{Y}_N^T \boldsymbol{\gamma}_N - 2 \mathbf{Y}_N \mathbf{g} = 0, \\ \implies \boldsymbol{\gamma}_N &= (\mathbf{Y}_N^T \mathbf{Y}_N)^{-1} \mathbf{Y}_N \mathbf{g}. \end{aligned} \quad (\text{A.66})$$

The resulting matrix is left-inverse to the thin matrix  $\mathbf{Y}_N^T$ , and can be written in terms of the more general pseudo inverse  $(\mathbf{Y}_N^T)^\dagger$ .

## A.5 Covariance Constraint for Binaural Ambisonic Decoding

The interaural covariance matrix is related to the expectation value of the auto/cross-covariances of the left and right HRTFs:

$$\mathbf{R}^* = \int_{\mathbb{S}^2} \begin{bmatrix} h_{\text{left}}(\boldsymbol{\theta}, \omega) \\ h_{\text{right}}(\boldsymbol{\theta}, \omega) \end{bmatrix} [h_{\text{left}}(\boldsymbol{\theta}, \omega)^* \ h_{\text{right}}(\boldsymbol{\theta}, \omega)^*] d\boldsymbol{\theta} = \int_{\mathbb{S}^2} \mathbf{h}(\boldsymbol{\theta}, \omega) \mathbf{h}(\boldsymbol{\theta}, \omega)^H d\boldsymbol{\theta}. \quad (\text{A.67})$$

When specified in terms of spherical harmonic coefficients  $\mathbf{h} = \mathbf{y}^T \mathbf{h}_{\text{SH}}$ , the integral  $\int_{\mathbb{S}^2} h_1^* h_2 d\boldsymbol{\theta}$  of any of  $\mathbf{R}$ 's entries vanishes by the orthogonality of the spherical harmonics  $\mathbf{h}_{\text{SH1}}^H \int_{\mathbb{S}^2} \mathbf{y} \mathbf{y}^T d\boldsymbol{\theta} \mathbf{h}_{\text{SH2}} = \mathbf{h}_{\text{SH1}}^H \mathbf{h}_{\text{SH2}}$ , and we obviously only need the inner product between the spherical-harmonic coefficients of the HRTFs.

A very-high-order spherical harmonics HRTF dataset  $\mathbf{H}_{\text{SH}}^H$  of dimensions  $2 \times (M+1)^2$  with the order ( $M \gg N$ ) yields a covariance matrix at every frequency

$$\mathbf{R} = \mathbf{H}_{\text{SH}}^H \mathbf{H}_{\text{SH}} = \mathbf{X}^H \mathbf{X}$$

that can be factored into a quadratic form of a  $2 \times 2$  matrix  $\mathbf{X}$  by Cholesky factorization, which reduces the degrees of freedom involved to the minimum required size.

The Nth-order Ambisonically reproduced, high-frequency modified HRTF dataset  $\tilde{\mathbf{H}}_{\text{SH}}$  of dimensions  $2 \times (M + 1)^2$  also has a  $2 \times 2$  covariance matrix  $\hat{\mathbf{R}}$  that will differ from  $\mathbf{R}$ , and which we also decompose in Cholesky factors  $\hat{\mathbf{X}}$ ,

$$\hat{\mathbf{R}} = \hat{\mathbf{H}}_{\text{SH}}^{\text{H}} \hat{\mathbf{H}}_{\text{SH}} = \hat{\mathbf{X}}^{\text{H}} \hat{\mathbf{X}}. \quad (\text{A.68})$$

To equalize  $\mathbf{R} = \hat{\mathbf{R}}$ , the reproduced HRTF set is corrected by a  $2 \times 2$  filter matrix  $\mathbf{M}$ ,

$$\hat{\mathbf{H}}_{\text{SH,corr}} = \hat{\mathbf{H}}_{\text{SH}} \mathbf{M}. \quad (\text{A.69})$$

This is done properly as soon as

$$\mathbf{X}^{\text{H}} \mathbf{X} = \mathbf{M}^{\text{H}} \hat{\mathbf{X}}^{\text{H}} \hat{\mathbf{X}} \mathbf{M} = \mathbf{M}^{\text{H}} \hat{\mathbf{X}}^{\text{H}} \overbrace{\mathbf{Q}^{\text{H}} \mathbf{Q}}^I \hat{\mathbf{X}} \mathbf{M}, \quad (\text{A.70})$$

and the orthogonal matrix  $\mathbf{Q}$  is used to compensate for degrees of freedom that the Cholesky factors  $\mathbf{X}$  and  $\hat{\mathbf{X}}$  have in sign, phase, mixing, with regard to each other. We recognize the root and hereby the preliminary solution for  $\mathbf{M}$

$$\mathbf{X} = \mathbf{Q} \hat{\mathbf{X}} \mathbf{M}, \quad \Rightarrow \mathbf{M} = \hat{\mathbf{X}}^{-1} \mathbf{Q}^{\text{H}} \mathbf{X}. \quad (\text{A.71})$$

This leaves  $\hat{\mathbf{H}}_{\text{SH,corr}} = \hat{\mathbf{H}}_{\text{SH}} \hat{\mathbf{X}}^{-1} \mathbf{Q}^{\text{H}} \mathbf{X}$  depending on an unspecific orthogonal  $2 \times 2$  matrix  $\mathbf{Q}$ . To obtain a corrected-covariance HRTFs  $\hat{\mathbf{H}}_{\text{corr,SH}}$  of highest-possible phase-alignment and correlation to its uncorrected counterpart  $\hat{\mathbf{H}}_{\text{SH}}$ , we maximize the trace, i.e. the sum of diagonal elements

$$\begin{aligned} \max \Re \text{Tr}\{\hat{\mathbf{H}}_{\text{SH}}^{\text{H}} \hat{\mathbf{H}}_{\text{corr,SH}}\} &= \max \Re \text{Tr}\{\hat{\mathbf{H}}_{\text{SH}}^{\text{H}} \hat{\mathbf{H}}_{\text{SH}} \hat{\mathbf{X}}^{-1} \mathbf{Q}^{\text{H}} \mathbf{X}\} = \\ \max \Re \text{Tr}\{\hat{\mathbf{X}}^{\text{H}} \hat{\mathbf{X}} \hat{\mathbf{X}}^{-1} \mathbf{Q}^{\text{H}} \mathbf{X}\} &= \max \Re \text{Tr}\{\hat{\mathbf{X}}^{\text{H}} \mathbf{Q}^{\text{H}} \mathbf{X}\} = \max \Re \text{Tr}\{\mathbf{Q}^{\text{H}} \hat{\mathbf{X}}^{\text{H}} \mathbf{X}\}. \end{aligned}$$

For the last expression, the property  $\text{Tr}\{\mathbf{AB}\} = \text{Tr}\{\mathbf{BA}\}$  was used. An orthogonal matrix  $\mathbf{Q}^{\text{H}} = \mathbf{V} \mathbf{U}^{\text{H}}$  composed of two orthogonal matrices  $\mathbf{U}$  and  $\mathbf{V}$  would yield  $\text{Tr}\{\hat{\mathbf{X}}^{\text{H}} \mathbf{X} \mathbf{V} \mathbf{U}^{\text{H}}\} = \text{Tr}\{\mathbf{U}^{\text{H}} \hat{\mathbf{X}}^{\text{H}} \mathbf{X} \mathbf{V}\}$ , and it would maximize the trace if  $\mathbf{U}$  and  $\mathbf{V}^{\text{H}}$  diagonalized  $\hat{\mathbf{X}}^{\text{H}} \mathbf{X}$ . This is accomplished by singular-value decomposition (SVD)  $\hat{\mathbf{X}}^{\text{H}} \mathbf{X} = \mathbf{U} \mathbf{S} \mathbf{V}^{\text{H}}$ , when singular values  $\mathbf{S} = \text{diag}\{[s_1, s_2]\}$  are real and positive, as in most SVD implementations. Using  $\mathbf{U}$  and  $\mathbf{V}$ , the desired solution is:

$$\hat{\mathbf{H}}_{\text{corr,SH}} = \hat{\mathbf{H}}_{\text{SH}} \hat{\mathbf{X}}^{-1} \mathbf{V} \mathbf{U}^{\text{H}} \mathbf{X}. \quad (\text{A.72})$$



If the SVD delivers negative or complex-valued singular values, the complex/negative factor just need to be pulled out and factored into either the corresponding left or right singular vector.

## A.6 Physics of the Helmholtz Equation

### A.6.1 Adiabatic Compression

We search for a physical compression equation relating pressure  $p$  and volume  $V$ .

**Ideal gas.** The gas pressure  $p$  inside the volume  $V$  obeys the ideal gas law [9]

$$p V = n R T, \quad (\text{A.73})$$

with  $n$  measuring the amount of substance in moles,  $R$  is the gas constant, and  $T$  is the temperature. This would yield a valid compression equation if the medium of sound propagation was isothermal. However, this is not the case  $T \neq \text{const}$ , and local temperature fluctuations happen too fast to be equalized by thermal dissipation. Isothermal compression would be too soft, the resulting speed of sound off by  $-15\%$ . A compression law involving fluctuations of all three quantities ( $p$ ,  $V$ ,  $T$ ) needs an additional equation.

**First law of thermodynamics.** In thermodynamics [10–12], the enthalpy  $H$  describes the energy required to heat up a freely expanding gas under constant pressure  $p$ . The enthalpy goes to the internal energy  $U$  required to heat up the gas in a constant volume, which is easier, plus the ideal-gas volume work  $p V$  taken by the gas to expand under the constant external pressure

$$H = U + p V, \quad (\text{A.74})$$

$$\text{specifically } n c_p T = n c_v T + n R T, \quad \Rightarrow R = c_p - c_v.$$

The quantities  $c_p$  and  $c_v$  are the specific heat capacities for heating up a gas that is expanding ( $p = \text{const.}$ ) or confined in a fixed volume ( $V = \text{const.}$ ) to a temperature  $T$ , which can be accurately measured or modeled. Obviously, the gas constant  $R$  is the difference between the two. To make sound propagation isenthalpic, the energy must fluctuate between internal energy  $U$  and volume work  $p V$ .

**Adiabatic process.** The above steady-state equations are not useful yet to describe short-term fluctuations of  $p$ ,  $V$ , and  $T$  in time and space. A differential formulation related to the change in enthalpy, internal energy, and volume work  $dH = dU + p dV$  is more useful. Moreover, we regard packages of a constant amount of substance whose internal heat up is just due to compression and not due to external enthalpy sources, it is therefore isenthalpic  $dH = 0$ , see [10, Sect. 3.12.2], [13]

$$0 = n c_V dT + \frac{n R T}{V} dV.$$

We may divide by  $n c_V T$ , replace  $R = c_p - c_V$ , and obtain  $\frac{dT}{T} + (\frac{c_p}{c_V} - 1) \frac{dV}{V} = 0$ , whose integration yields  $\ln T + (\frac{c_p}{c_V} - 1) \ln V = \ln(T V^{\frac{c_p}{c_V} - 1}) = 0$ , hence  $T V^{\frac{c_p}{c_V} - 1} = 1$ , and with the ideal gas equation inserted as  $T = \frac{pV}{nR}$ , the *adiabatic process law* becomes

$$p V^{\frac{c_p}{c_V}} = n R = \text{const}, \quad (\text{A.75})$$

for which the adiabatic exponent is frequently expressed as  $\gamma = \frac{c_p}{c_V}$ . For air, the exponent is  $\gamma = 1.4$ , and we may express a state change as  $(p_0, V_0) \rightarrow (p_0 + p, V_0 + V)$ . The equation  $p_0 V_0^\gamma = (p_0 + p)(V_0 + V)^\gamma$  yields after division by  $p_0 V_0^\gamma$  and by  $(1 + \frac{V}{V_0})^\gamma$ :

$$1 + \frac{p}{p_0} = \left(1 + \frac{V}{V_0}\right)^{-\gamma} \approx 1 - \gamma \frac{V}{V_0}, \quad \text{hence } p = -\gamma p_0 \frac{V}{V_0}.$$

Assuming the Cartesian coordinates  $x, y, z$  measured in the resting gas to define its volume  $V_0 = \Delta x \Delta y \Delta z$ , as well as its deflected coordinates  $\xi(x), \eta(y), \zeta(z)$  after a volume change to  $V$ , we can approximate the volume change well-enough by the three independent volume changes  $\Delta \xi \Delta y \Delta z$ ,  $\Delta x \Delta \eta \Delta z$ , and  $\Delta x \Delta y \Delta \zeta$ , resulting from the superimposed individual elongation into the three coordinates' directions,

$$\lim_{V_0 \rightarrow 0} \frac{\Delta V}{V_0} = \lim_{V_0 \rightarrow 0} \frac{\Delta \xi \Delta y \Delta z + \Delta x \Delta \eta \Delta z + \Delta x \Delta y \Delta \zeta}{\Delta x \Delta y \Delta z} = \frac{\partial \xi}{\partial x} + \frac{\partial \eta}{\partial y} + \frac{\partial \zeta}{\partial z} = \nabla^T \xi.$$

Replacing the bulk modulus  $K = \gamma p_0 = \rho c^2$  of air by more common constants,<sup>1</sup> where  $c = \sqrt{K/\rho}$  and applying the derivative in time  $\frac{\partial}{\partial t}$ , we get the equation of compression in its typical form using the velocities  $\frac{\partial \xi}{\partial t} = \mathbf{v}$ ,

$$\frac{\partial p}{\partial t} = -\rho c^2 \nabla^T \mathbf{v}. \quad (\text{A.76})$$

## A.6.2 Potential and Kinetic Sound Energies, Intensity, Diffuseness

The *potential* energy density or *volume work* stored in the elastic medium that gets compressed by a deformation  $dV$  increases with  $dw_p = p dV$ , while deformation also increases the pressure by  $dp = K dV$ . We may substitute for  $dV = K^{-1} dp$

<sup>1</sup>Typical constants are  $\gamma = 1.4$ ,  $p_0 = 10^5 \text{ Pa}$ ,  $\rho = 1.2 \text{ kg/m}^3$ ,  $c = 343 \text{ m/s}$ .

yielding  $dw_p = K^{-1} p dp$ . The volume work stored by a pressure increase from 0 to  $p$  is

$$w_p = \int_0^p \frac{p dp}{K} = \frac{p^2}{2K} = \frac{p^2}{2\rho c^2}. \quad (\text{A.77})$$

The *kinetic* energy density stored in the motion of the medium along any axis, e.g.  $x$ , increases by acceleration against its mass,  $dw_{v_x} = \rho \frac{dv_x}{dt} dx$ . The velocity is  $v_x = \frac{dx}{dt}$  so that we substitute for  $dx = v_x dt$  to get  $dw_{v_x} = \rho v_x dv_x$ . The total kinetic energy density stored in velocities increasing from 0 to  $v_x, v_y, v_z$  is

$$w_v = \rho \left[ \int_0^{v_x} v_x dv_x + \int_0^{v_y} v_y dv_y + \int_0^{v_z} v_z dv_z \right] = \rho \frac{v_x^2 + v_y^2 + v_z^2}{2} = \frac{\rho \|\mathbf{v}\|^2}{2}. \quad (\text{A.78})$$

**Total energy density and intensity.** The total energy density therefore becomes

$$w = w_p + w_v = \frac{p^2}{2\rho c^2} + \frac{\rho \|\mathbf{v}\|^2}{2}, \quad (\text{A.79})$$

and derived with regard to time, it becomes

$$\frac{\partial w}{\partial t} = \frac{p}{\rho c^2} \frac{\partial p}{\partial t} + \rho \mathbf{v}^T \frac{\partial \mathbf{v}}{\partial t} = p \nabla^T \mathbf{v} + \mathbf{v}^T \nabla p = \nabla^T (p \mathbf{v}) = \nabla^T \mathbf{I}, \quad (\text{A.80})$$

and defines the (time-domain) intensity vector  $\mathbf{I} = p \mathbf{v}$  that describes the energy flow in space. Hereby,  $\frac{\partial w}{\partial t} = \nabla^T \mathbf{I}$  expresses that only a non-zero *divergence* of the intensity causes energy increase (source) or loss (absorption) in the lossless medium.

**Direction of arrival and diffuseness:** The intensity vector carries a meaning in its own right: it displays into which direction the energy flows (direction of emission). In the frequency domain, it becomes  $\mathbf{I} = \Re\{p^* \mathbf{v}\}$ , and for a plane-wave sound field  $p = e^{ik \boldsymbol{\theta}_s^T \mathbf{r}}$ , where  $\mathbf{v} = -\frac{\nabla p}{ik\rho c} = -\frac{\boldsymbol{\theta}_s p}{\rho c}$ , it indicates the direction of arrival (DOA)

$$\mathbf{r}_{\text{DOA}} = -\frac{\rho c \mathbf{I}}{|p|^2} = -\frac{\rho c \Re\{p^* \mathbf{v}\}}{|p|^2} = \frac{\rho c |p|^2 \boldsymbol{\theta}_s}{\rho c |p|^2} = \boldsymbol{\theta}_s. \quad (\text{A.81})$$

An ideal, uniformly enveloping diffuse field is composed of uncorrelated plane waves  $E\{\frac{a(\boldsymbol{\theta}_1)^* a(\boldsymbol{\theta}_2)}{4\pi}\} = \frac{a^2}{4\pi} \delta(1 - \boldsymbol{\theta}_1^T \boldsymbol{\theta}_2)$  resulting in the sound pressure  $p = \int \frac{a(\boldsymbol{\theta}_s)}{\sqrt{4\pi}} e^{ik \boldsymbol{\theta}_s^T \mathbf{r}} d\boldsymbol{\theta}_s$ . While the expected sound pressure is non-zero as before  $E\{|p|^2\} = \frac{a^2}{4\pi} = |p|^2$ , the expected intensity of the uniformly surrounding waves vanishes  $-\rho c E\{\mathbf{I}\} = \frac{a^2}{4\pi} \int_{\mathbb{S}^2} \boldsymbol{\theta}_s d\boldsymbol{\theta}_s = \mathbf{0}$ .

Assuming stochastic interference of all sources, the intensity-based DOA estimator  $\mathbf{r}_{\text{DOA}} = -\frac{\rho c \Re\{p^* \mathbf{v}\}}{|p|^2}$  is therefore the physical equivalent to the  $\mathbf{r}_E$  vector measure.

A typical diffuseness measure  $0 \leq \psi \leq 1$  relies on its length between 0 and 1

$$\psi = 1 - \|\mathbf{r}_{\text{DOA}}\|^2. \quad (\text{A.82})$$

The signals  $W = p$  and  $[X, Y, Z]^T = \frac{\sqrt{2}\nabla p}{ik} = -\rho c \sqrt{2}\mathbf{v}$  of a first-order Ambisonic microphone allow to describe a time-domain estimator  $\mathbf{r}_{\text{DOA}}$

$$\mathbf{r}_{\text{DOA}} = -\frac{\rho c E\{\mathbf{I}\}}{E\{p^2\}} = -\frac{\rho c E\{p \mathbf{v}\}}{E\{p^2\}} = \frac{E\{W [X, Y, Z]^T\}}{\sqrt{2} E\{W^2\}}. \quad (\text{A.83})$$

### A.6.3 Green's Function in 3 Cartesian Dimensions

We may compose the Green's function, the solution to the inhomogeneous wave equation

$$\left( \Delta - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) G = -\delta(t)\delta(\mathbf{r}),$$

from products of complex exponentials with regard to time and the Cartesian directions

$$e^{i\omega t + ik_x x + ik_y y + ik_z z} = e^{i\mathbf{k}^T \mathbf{r}} e^{i\omega t}, \quad (\text{A.84})$$

where the position  $x, y, z$  was gathered in a position vector  $\mathbf{r}$ , and the wave numbers  $k_x, k_y, k_z$  of the individual coordinates were gathered in a wave-number vector  $\mathbf{k}$ . From this solution, we compose the Green's function by superimposing all spatial and temporal complex exponentials in  $\mathbf{k}$  and  $\omega$ , weighted by an unknown coefficient  $\gamma$ :

$$G = \iint \gamma e^{i\mathbf{k}^T \mathbf{r}} e^{i\omega t} d\omega d\mathbf{k}. \quad (\text{A.85})$$

Because of  $\Delta e^{i\mathbf{k}^T \mathbf{r}} = (-k_x^2 - k_y^2 - k_z^2) e^{i\mathbf{k}^T \mathbf{r}} = -k^2 e^{i\mathbf{k}^T \mathbf{r}}$  and  $\frac{\partial^2}{\partial t^2} e^{i\omega t} = -\omega^2 e^{i\omega t}$ , insertion into the inhomogeneous wave equation yields

$$-\iint \gamma \left[ k^2 - \frac{\omega^2}{c^2} \right] e^{i\mathbf{k}^T \mathbf{r}} e^{i\omega t} d\omega d\mathbf{k} = -\delta(t)\delta(\mathbf{r}).$$

Multiple transformations  $e^{-i\hat{\mathbf{k}}^T \mathbf{r}} e^{-i\hat{\omega} t} d\mathbf{r} dt$  remove the integrals by orthogonality

$$-\iint \gamma \left( k^2 - \frac{\omega^2}{c^2} \right) \underbrace{\left[ \int e^{i(\mathbf{k}-\hat{\mathbf{k}})^T \mathbf{r}} d\mathbf{r} \right]}_{(2\pi)^3 \delta(\mathbf{k}-\hat{\mathbf{k}})} \underbrace{\left[ \int e^{i(\omega-\hat{\omega})t} dt \right]}_{2\pi \delta(\omega-\hat{\omega})} d\omega d\mathbf{k} = - \underbrace{\int \delta(t) e^{-i\hat{\omega} t} dt}_1 \underbrace{\int \delta(\mathbf{r}) e^{-i\hat{\mathbf{k}}^T \mathbf{r}} d\mathbf{r}}_1,$$

and the unknown coefficient remains  $\gamma = \frac{1}{(2\pi)^{3+1}} \frac{1}{k^2 - \frac{\omega^2}{c^2}}$ . Letting  $G$  in the frequency domain, one  $\frac{1}{2\pi}$  in  $\gamma$  and the integral  $e^{i\omega t} d\omega \int$  are omitted. We transform  $\gamma$  back via  $\mathbf{k}$

$$G = \frac{1}{(2\pi)^3} \iiint \frac{e^{i\mathbf{k}^T \mathbf{r}}}{k^2 - \frac{\omega^2}{c^2}} d\mathbf{k} = \frac{1}{(2\pi)^3} \iiint \frac{e^{ikr\zeta}}{k^2 - \frac{\omega^2}{c^2}} d\mathbf{k}.$$

By re-expressing  $\mathbf{k}^T \mathbf{r} = kr \boldsymbol{\theta}_k^T \boldsymbol{\theta}_r = kr \cos \vartheta = kr\zeta$  we simplify the integral. Now we already see formally that Green's function can only depend on the distance  $r$  between source and receiver location  $G = G(\omega, r)$ .

The book [14, S.110-112] shows a notably compact derivation, which we will use below.

**Derivation for by transforming back from the Fourier domain:** For three dimensions, the transformation back from the Fourier domain is relatively easy to accomplish. Before going into details, we recognize that the substitution of  $\mathbf{k}^T \mathbf{r}$  by  $kr \cos \vartheta$  contains the radius of the wave vector  $k = \|\mathbf{k}\|$  and the cosine of the angle between  $\mathbf{r}$  and  $\mathbf{k}$ . In  $k$  space, we can always define a correspondingly oriented coordinate system for any  $\mathbf{r}$  as to simplify the integral  $\iiint_{-\infty}^{\infty} d\mathbf{k} = \int_0^{\infty} \int_0^{2\pi} \int_0^{\pi} k^2 dk d\varphi d\cos \vartheta = \int_0^{\infty} \int_0^{2\pi} \int_{-1}^1 k^2 dk d\varphi d\zeta$ . After re-arranging the integrals, we get

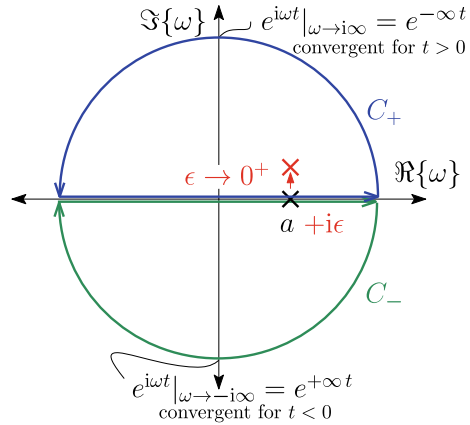
$$\begin{aligned} G &= \frac{\int_0^{2\pi} d\varphi}{(2\pi)^3} \int_0^{\infty} \frac{\int_{-1}^1 e^{ikr\zeta} d\zeta}{k^2 - \frac{\omega^2}{c^2}} k^2 dk = \frac{1}{(2\pi)^2} \int_0^{\infty} \frac{1}{ikr} \frac{e^{ikr} - e^{-ikr}}{k^2 - \frac{\omega^2}{c^2}} k^2 dk \\ &= \frac{1}{(2\pi)^2} \frac{1}{ir} \int_0^{\infty} \frac{e^{ikr} - e^{-ikr}}{k^2 - \frac{\omega^2}{c^2}} k dk = \frac{1}{(2\pi)^2} \frac{1}{ir} \left[ \int_0^{\infty} \frac{e^{ikr} k}{k^2 - \frac{\omega^2}{c^2}} dk - \int_0^{\infty} \frac{e^{-ikr} k}{k^2 - \frac{\omega^2}{c^2}} dk \right] \\ &= \frac{1}{(2\pi)^2} \frac{1}{ir} \left[ \int_0^{\infty} \frac{e^{ikr} k}{k^2 - \frac{\omega^2}{c^2}} dk - \int_0^{-\infty} \frac{e^{-i(-k)r} (-k)}{(-k)^2 - \frac{\omega^2}{c^2}} d(-k) \right] \\ &= \frac{1}{(2\pi)^2} \frac{1}{ir} \left[ \int_0^{\infty} \frac{e^{ikr} k}{k^2 - \frac{\omega^2}{c^2}} dk + \int_{-\infty}^0 \frac{e^{ikr} k}{k^2 - \frac{\omega^2}{c^2}} dk \right] \\ &= \frac{1}{(2\pi)^2} \frac{1}{ir} \int_{-\infty}^{\infty} \frac{e^{ikr}}{k^2 - \frac{\omega^2}{c^2}} k dk. \end{aligned} \tag{A.86}$$

The denominator is expanded in partial fractions  $\frac{1}{k^2 - \frac{\omega^2}{c^2}} = \frac{1}{2k} \frac{1}{k - \frac{\omega}{c}} + \frac{1}{2k} \frac{1}{k + \frac{\omega}{c}}$ , yielding

$$G = \frac{1}{2(2\pi)^2} \frac{1}{ir} \left[ \int_{-\infty}^{\infty} \frac{e^{ikr}}{k - \frac{\omega}{c}} dk + \int_{-\infty}^{\infty} \frac{e^{ikr}}{k + \frac{\omega}{c}} dk \right]. \tag{A.87}$$

To obtain causal temporal solutions, there needs to be a specific solution of the improper and singular integrals.

**Fig. A.1** Closure of improper integration path using  $C_+$  over the positive imaginary half plane for  $t > 0$ , and  $C_-$  for  $t < 0$ , and regularization of pole for causal result, i.e. non-zero only for  $C_+$



**Causal solutions (integral in  $\omega$ ).** Causal responses obeying the transformation

$$h(t) = \int_{-\infty}^{\infty} \frac{e^{i\omega t}}{\omega - a} d\omega \quad (\text{A.88})$$

are obtained by replacing the improper integral  $\int_{-\infty}^{\infty}$  by a closed integration contour, and by introducing vanishing regularization. Jordan's lemma states that improper integration  $\int_{-\infty}^{\infty}$  is equivalent to a closed integration path  $C_+$  of positive orientation involving the additional semi-circle on the upper half of the complex number plane  $\int_{-\infty}^{\infty} = \oint_{C_+} = \lim_{R \rightarrow \infty} [\int_{-R}^R d\omega + \int_0^\pi R d\varphi]$  if the integrand of the semi-circle vanishes, i.e.  $\lim_{R \rightarrow \infty} \frac{e^{i \cos \varphi - \sin \varphi} R t}{R e^{i\varphi - a}} = 0$ . This is the case for positive times  $t > 0$ . For negative times, the integral can be closed using the lower part of the complex number plane,  $\int_{-\infty}^{\infty} = \oint_{C_-} = \lim_{R \rightarrow \infty} [\int_{-R}^R d\omega + \int_0^{-\pi} R d\varphi]$ , if the semi-circular integral vanishes, which is true for negative times  $t < 0$  in our case, see Fig. A.1. We get

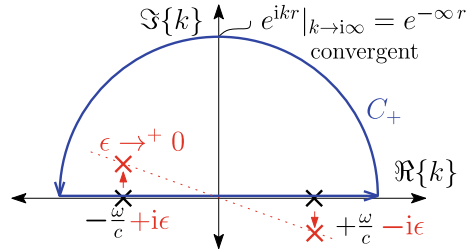
$$h(t) = \begin{cases} \oint_{C_+} \frac{e^{i\omega t}}{\omega - a} d\omega, & \text{if } t > 0, \\ \oint_{C_-} \frac{e^{i\omega t}}{\omega - a} d\omega, & \text{if } t < 0. \end{cases} \quad (\text{A.89})$$

According to Cauchy's integral formula for analytic regular functions  $f(z)$  over a single pole  $\frac{1}{z-a}$ , we obtain

$$\oint_{C_{\pm}} \frac{f(z)}{z-a} dz = \pm 2\pi i \begin{cases} f(a), & \text{if the path } C_{\pm} \text{ surrounds } a, \\ 0, & \text{if } a \text{ lies outside the path } C_{\pm}. \end{cases} \quad (\text{A.90})$$

If a pole on the real axis  $a \in \mathbb{R}$  is slightly shifted by a vanishing imaginary amount to  $\lim_{\epsilon \rightarrow 0^+} \oint_{C_{\pm}} \frac{e^{i\omega t}}{\omega - i\epsilon - a} d\omega$  (regularization) so that it lies within the path  $C_+$  and not in  $C_-$ , the result is perfectly causal and vanishes at negative times:  $h(t) = 2\pi i \lim_{\epsilon \rightarrow 0^+} e^{ia t - \epsilon t} u(t)$ , with the unit step function  $u(t) = 1$  for  $t \geq 0$  and 0 for  $t < 0$ , see Fig. A.1.

**Fig. A.2** Causality-enforcing regularization  $\omega = \lim_{\epsilon \rightarrow 0^+} \omega - i\epsilon$  of the poles in Green's function wrt. wave number  $k$ . For a positive radius  $r \geq 0$ , closure of the improper integration path requires  $C_+$  with semicircle on the positive imaginary half plane (or  $C_-$  for  $r \leq 0$ )



**Integral in  $k$ .** Causality requires specific regularization in frequency as shown above: Replacement of  $\omega$  by  $\lim_{\epsilon \rightarrow 0^+} \omega - i\epsilon$  guarantees causality in the partial-fraction expanded Green's function Eq. (A.87). Jordan's lemma requires to use the path  $C_+$  to close the improper path in  $k$  for a positive radius  $r \geq 0$ , cf. Fig. A.2,

$$G = \frac{1}{2(2\pi)^2} \lim_{\epsilon \rightarrow 0^+} \frac{1}{ir} \left[ \int_{C_+} \frac{e^{ikr} dk}{k - \frac{\omega}{c} + i\epsilon} + \int_{C_+} \frac{e^{ikr} dk}{k + \frac{\omega}{c} - i\epsilon} \right] = \frac{2\pi i e^{-ikr}}{2(2\pi)ir} = \frac{e^{-i\frac{\omega}{c}r}}{4\pi r}. \quad (\text{A.91})$$

## A.6.4 Radial Solution of the Helmholtz Equation

The radial part of the Helmholtz equation in spherical coordinates is characterized by the spherical Bessel differential equation in  $x = kr$

$$y'' + 2x^{-1} y' + [1 - n(n+1)x^{-2}]y = 0. \quad (\text{A.92})$$

**Recursive construction.** For  $n = 0$ , we know that the omnidirectional Green's function is a solution diverging from  $x = 0$ , and it is proportional to  $y \propto \frac{e^{-ix}}{x}$ . We can simplify the equation by inserting  $y = x^{-1} u_n$ , which yields with  $y' = x^{-1} u'_n - x^{-2} u_n$  and  $y'' = x^{-1} u''_n - 2x^{-2} u'_n + 2x^{-3} u_n$  after multiplying with  $x$ :

$$\begin{aligned} u''_n - 2x^{-1} u'_n + 2x^{-2} u_n + 2x^{-1} u'_n - 2x^{-2} u_n + [1 - n(n+1)x^{-2}]u_n &= 0 \\ u''_n + [1 - n(n+1)x^{-2}]u_n &= 0. \end{aligned} \quad (\text{A.93})$$

Moreover, we attempt to find a recursive definition for  $n > 0$  using the approach

$$y_n = x^{-1} u_n, \quad u_n = -x^a [x^{-a} u_{n-1}]'.$$

We evaluate the recursion for the derivatives

$$\begin{aligned}
 u_n &= -u'_{n-1} + a x^{-1} u_{n-1}, \\
 u'_n &= -u''_{n-1} + a x^{-1} u'_{n-1} - a x^{-2} u_{n-1}, \quad \text{with } -u''_{n-1} = [1 - n(n-1)x^{-2}]u_{n-1} \\
 &= a x^{-1} u'_{n-1} + \{1 - [n(n-1) + a]x^{-2}\} u_{n-1} \\
 u''_n &= a x^{-1} u'_{n-1} - a x^{-2} u'_{n-1} + \{1 - [n(n-1) + a]x^{-2}\} u'_{n-1} + 2[n(n-1) + a]x^{-3} u_{n-1} \\
 &= \{1 - [n(n-1) + 2a]x^{-2}\} u'_{n-1} + \{[2n(n-1) + 2a + an(n-1)]x^{-3} - a x^{-1}\} u_{n-1} \\
 &= \{1 - [n(n-1) + 2a]x^{-2}\} u'_{n-1} + \{[n(n-1)(a+2) + 2a]x^{-3} - a x^{-1}\} u_{n-1}
 \end{aligned}$$

The equation  $u''_n + [1 - n(n+1)x^{-2}]u_n = 0$  using the above expressions becomes

$$\begin{aligned}
 \{1 - [n(n-1) + 2a]x^{-2}\} u'_{n-1} + \{[n(n-1)(a+2) + 2a]x^{-3} - a x^{-1}\} u_{n-1} \\
 + [1 - n(n+1)x^{-2}][ -u'_{n-1} + a x^{-1} u_{n-1}] = 0.
 \end{aligned}$$

Comparing coefficients for  $u'_{n-1}$  and  $u_{n-1}$  yields  $a = n$

$$\begin{aligned}
 u'_{n-1} : \quad & 1 - 1 - [n(n-1) + 2a - n(n+1)]x^{-2} = 2(a-n)x^{-2} = 0, \\
 u_{n-1} : \quad & [-a + a]x^{-1} + [n(n-1)(a+2) + 2a - an(n+1)]x^{-3} = 0 \\
 & an(n-1) + 2n(n-1) + 2a(1-n) - an(n-1) = 2(n-a) = 0,
 \end{aligned}$$

and hereby a recurrence for  $y_n$  from  $u_n = -x^n[x^{-n}u_{n-1}]'$  with  $y_n = x^{-1}u_n$ ,  $u_n = x y_n$ ,

$$y_n = -x^{n-1}[x^{-(n-1)}y_{n-1}]' \quad \Rightarrow \quad y_{n+1} = -x^n[x^{-n}y_n]'. \quad (\text{A.94})$$

**Singular and regular solution.** We know from the Green's function that the omnidirectional solution should be proportional to  $g_0 \propto e^{-ix}$ . The typical radial solution for an omnidirectional source field is chosen to be the spherical Hankel function of the second kind<sup>2</sup>

$$h_0^{(2)}(kr) = \frac{e^{-ikr}}{-ikr}, \quad h_{n+1}^{(2)}(kr) = -(kr)^n \frac{d}{d(kr)} \left[ \frac{1}{(kr)^n} h_n^{(2)}(kr) \right]. \quad (\text{A.95})$$

However, this solution is not sufficient to solve problems without singularity at  $r = 0$ . We know that the function  $\frac{\sin(kr)}{kr}$  is finite at  $kr$ , and so are all real parts of the spherical Hankel functions of the second kind, the spherical Bessel functions

$$j_0(kr) = \frac{\sin(kr)}{kr}, \quad j_{n+1}(kr) = -(kr)^n \frac{d}{d(kr)} \left[ \frac{1}{(kr)^n} j_n(kr) \right]. \quad (\text{A.96})$$

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<sup>2</sup>Note that some scholars use the Fourier expansion  $e^{i\omega t}$  with opposite sign  $e^{-i\omega t}$  and require to use the complex conjugate in every expression containing imaginary constants  $h_n^{(1)} = h_n^{(2)*}$ .



The solutions are linearly independent. One check after some calculation that their Wronski determinant is non-zero [15, Eq. 10.50.1]

$$\begin{vmatrix} j_n(kr) & h_n^{(2)}(kr) \\ j'_n(kr) & h_n^{(2)'}(kr) \end{vmatrix} = j_n(kr)h_n^{(2)'}(kr) - j'_n(kr)h_n^{(2)}(kr) = -\frac{i}{(kr)^2}. \quad (\text{A.97})$$

Below, the Frobenius method is shown as alternative way to get these functions.

**Alternative way: Frobenius method.** Given a second-order differential equation with singular coefficients, it can be solved by a generalized infinite power series:

$$y'' + \left( \sum_{l=0}^{\infty} a_l x^l \right) x^{-1} y' + \left( \sum_{l=0}^{\infty} b_l x^l \right) x^{-2} y = 0, \quad \text{solution: } y = \sum_{k=0}^{\infty} c_k x^{k+\gamma}. \quad (\text{A.98})$$

Insertion of the solution yields

$$\sum_{k=0}^{\infty} (k + \gamma - 1)(k + \gamma) c_k x^{k+\gamma-2} + \sum_{k'=0}^{\infty} \sum_{l=0}^{\infty} [(k' + \gamma) a_l + b_l] c_{k'} x^{k'+l+\gamma-2} = 0,$$

an index shift  $k' + l = k$ , and  $l = 0 \dots k$  allows to pull out the common factor  $x^{k+\gamma-2}$

$$\begin{aligned} & \sum_{k=0}^{\infty} \left\{ (k + \gamma - 1)(k + \gamma) c_k + \sum_{l=0}^k [(k - l + \gamma) a_l + b_l] c_{k-l} \right\} x^{k+\gamma-2} = 0 \\ & \sum_{k=0}^{\infty} \left\{ [(k + \gamma + a_0 - 1)(k + \gamma) + b_0] c_k + \sum_{l=1}^k [(k - l + \gamma) a_l + b_l] c_{k-l} \right\} x^{k+\gamma-2} = 0. \end{aligned}$$

The coefficient of every exponent of  $x$  in the above equation must be zero:

$$\text{indical equation for } k = 0 : \quad [(\gamma + a_0 - 1)\gamma + b_0] c_0 = 0, \quad (\text{A.99})$$

$$\text{indical equation for } k = 1 : \quad [(\gamma + a_0)(\gamma + 1) + b_0] c_1 + [a_1 \gamma + b_1] c_0 = 0, \quad (\text{A.100})$$

$$\text{recurrence for } k > 1 : \quad -\frac{\sum_{l=1}^k [(k - l + \gamma) a_l + b_l] c_{k-l}}{(k + \gamma + a_0 - 1)(k + \gamma) + b_0} = c_k. \quad (\text{A.101})$$

Depending on the specific values found for  $\gamma$ , the recurrence, etc. the Frobenius method suggests how to find or construct an independent pair of solutions.

**Spherical Bessel differential equation.** In  $y'' + 2x^{-1} y' + [-n(n+1) + x^2] x^{-2} y = 0$ , all  $a_l$  and  $b_l$  are zero except  $a_0 = 2, b_0 = -n(n+1)$ , and  $b_2 = 1$ . Indical equations and recurrence become

$$[\gamma(\gamma + 1) - n(n + 1)] c_0 = 0, \quad (\text{A.102})$$

$$[(\gamma + 1)(\gamma + 2) - n(n + 1)] c_1 = 0, \quad (\text{A.103})$$

$$(k + \gamma + 1)(k + \gamma) c_k = -c_{k-2}. \quad (\text{A.104})$$

We see that the recurrence is again a two-step recurrence, so that one can choose between an even solution using  $c_0 \neq 0, c_1 = 0$  yielding  $\gamma = n$  or  $\gamma = -(n + 1)$ , [or an odd solution that won't be used, with  $c_0 = 0, c_1 \neq 0$  yielding  $\gamma + 1 = n$  or  $\gamma + 1 = -(n + 1)$ ].

**Spherical Bessel functions.** The choice  $\gamma = n$  yields a solution converging everywhere: Powers of  $x$  are all positive, the recurrences  $c_k = -\frac{c_{k-2}}{(n+k+1)(n+k)} = \frac{(-1)^k c_0}{(n+k+1)!}$  yield a convergence radius  $R = \lim_{k \rightarrow \infty} \left| \frac{c_{k-2}}{c_k} \right| = \lim_{k \rightarrow \infty} (n+k+1)(n+k) = \infty$ . With a starting value  $c_0 = \frac{2^n n!}{(2n+1)!}$ , solutions are called spherical Bessel functions [5, Chap. 3.4]

$$j_n = (2x)^n \sum_{k=0}^{\infty} \frac{(-1)^k (n+k)!}{k! [2(n+k) + 1]!} x^{2k}. \quad (\text{A.105})$$

which are a physical set of regular solutions with  $n$ -fold zero at 0. The spherical Bessel function for  $n = 0$  is

$$j_0(x) = \frac{\sin x}{x}. \quad (\text{A.106})$$

With the above recursive definition iterated [5, Eq. 3.4.15] one could define

$$j_{n+1} = -x^n \frac{d}{dx} \left( \frac{1}{x^n} j_n \right), \quad j_n = (-x)^n \left( \frac{1}{x} \frac{d}{dx} \right)^n j_0. \quad (\text{A.107})$$

**Spherical Neumann functions.** For  $\gamma = -(n + 1)$  and  $c_0 \neq 0, c_1 = 0$ , the recurrences are  $c_k = -\frac{c_{k-2}}{(n-k+1)(n-k)} = \frac{(-1)^k c_0}{(n-k+1)!}$  and yield the spherical Neumann functions with an  $(n + 1)$ -fold pole at 0. They also obey the recursive definition from above,

$$y_0 = -\frac{\cos x}{x}, \quad y_n = (-x)^n \left( \frac{1}{x} \frac{d}{dx} \right)^n y_0. \quad (\text{A.108})$$

**Spherical Hankel functions.** The spherical Neumann and Bessel functions based on either sin or cos are clearly linearly independent. The spherical Bessel functions are useful to representing fields convergent everywhere. Physical source fields (Green's function) diverge at the source location and exhibit a specific way phase radiates, with  $G \propto \frac{e^{-ix}}{x}$ . The spherical Bessel and Neumann functions are asymptotically similar to [15, Eq. 10.52.3]

$$\lim_{x \rightarrow \infty} j_n = (-1)^n \frac{\sin(x)}{x}, \quad \lim_{x \rightarrow \infty} y_n = (-1)^{n+1} \frac{\cos(x)}{x}, \quad (\text{A.109})$$

therefore only their combination to spherical Hankel functions of the second kind

$$h_n^{(2)} = j_n - i y_n \quad (\text{A.110})$$

yields useful physical set of singular solutions. They inherit their  $(n + 1)$ -fold pole from the spherical Neumann functions at 0. Their limiting form for large arguments are

$$\begin{aligned} \lim_{r \rightarrow \infty} h_n^{(2)}(x) &= -x^{n-1} \lim_{r \rightarrow \infty} \frac{d}{dx} \left( \frac{1}{x^{n-1}} h_{n-1}^{(2)} \right) \\ &= -x^{n-1} \lim_{r \rightarrow \infty} \left( -\frac{n-1}{x^n} h_{n-1}^{(2)} + \frac{1}{x^{n-1}} \frac{d}{dx} h_{n-1}^{(2)} \right) = - \lim_{r \rightarrow \infty} \frac{d}{dx} h_{n-1}^{(2)} \\ &= (-1)^n \lim_{r \rightarrow \infty} \frac{d^n}{dx^n} h_0^{(2)} = i^n h_0^{(2)}(x). \end{aligned} \quad (\text{A.111})$$

With Eqs. (A.110), (A.106) and (A.108), the zeroth-order spherical Hankel function is  $h_0^{(2)}(x) = \frac{e^{-ix}}{-ix}$ .

**Alternative implementation by cylindrical functions.** We can transform the spherical Bessel differential equation by inserting  $y = x^\alpha u$  and obtain after division by  $x^\alpha$

$$\begin{aligned} x^\alpha u'' + 2\alpha x^{\alpha-1} u' + \alpha(\alpha-1)u + 2x^{\alpha-1} u' + 2\alpha x^{\alpha-2} u + [1 - n(n+1)x^{-2}]u &= 0 \\ u'' + 2\frac{\alpha+1}{x} u' + \left[ 1 + \frac{\alpha(\alpha+1) - n(n+1)}{x^2} \right] u &= 0. \end{aligned}$$

For  $\alpha = -\frac{1}{2}$ , the equation for  $u$  becomes the Bessel differential equation with  $\alpha(\alpha+1) - n(n+1) = -(n^2 + n + \frac{1}{4}) = -(n + \frac{1}{2})^2$

$$u'' + \frac{1}{x} u' + \left[ 1 - \frac{(n + \frac{1}{2})^2}{x^2} \right] u = 0. \quad (\text{A.112})$$

Consequently, the spherical Bessel functions and spherical Hankel functions of the second kind can be implemented using the Bessel and Hankel functions that can be found in any standard maths programming library. The specific relations are:

$$j_n(x) = \sqrt{\frac{\pi}{2}} \frac{1}{x} J_{n+\frac{1}{2}}(x), \quad h_n^{(2)}(x) = \sqrt{\frac{\pi}{2}} \frac{1}{x} H_{n+\frac{1}{2}}^{(2)}(x). \quad (\text{A.113})$$

### A.6.5 Green's Function in Spherical Solutions, Angular Distributions, Plane Waves

We can write the inhomogeneous Helmholtz equation  $(\Delta + k^2)G = -\delta$  to be excited by a source at the direction  $\theta_0$  at the radius  $r_0$ . We decompose the excitation into a Delta function in radius and direction  $-r_0^{-2}\delta(r - r_0)\delta(\theta_0^T\theta - 1)$ . The directional part needs not be restricted to the spherical Dirac delta function, so we can take a distribution of sources at  $r_0$ , weighted by the panning function  $g(\theta)$ ,

$$(\Delta + k^2) p = -r_0^{-2}\delta(r - r_0) g(\theta). \quad (\text{A.114})$$

From the spherical basis solutions, we know that at a radius other than  $r_0$ ,  $p$  can be expanded into spherical harmonics

$$p = \sum_{n=0}^{\infty} \sum_{m=-n}^n \psi_{nm} Y_n^m(\theta). \quad (\text{A.115})$$

Acting on the decomposition of  $p$ , the directional part of the Laplacian will yield the eigenvalue  $\Delta_{\varphi,\zeta} Y_n^m = -n(n+1) r^{-2} Y_n^m$  of the spherical harmonics, and its radial part  $r^2 \Delta_r = \frac{\partial^2}{\partial r^2} + 2r^{-1} \frac{\partial}{\partial r}$ , as around Eq. (6.11), hence

$$\begin{aligned} & (\Delta + k^2) \sum_{n=0}^{\infty} \sum_{m=-n}^n \psi_{nm} Y_n^m(\theta) = \\ & \sum_{n=0}^{\infty} \sum_{m=-n}^n \left[ \frac{\partial^2}{\partial r^2} + \frac{2\partial}{r\partial r} + k^2 - \frac{n(n+1)}{r^2} \right] \psi_{nm} Y_n^m(\theta) = -r_0^{-2}\delta(r - r_0) g(\theta). \end{aligned}$$

Obviously,  $\psi_{nm}$  must depend on  $k$  and  $r$ , so we may pull the factor  $k$  into the differentials  $\frac{d}{dr} = k \frac{d}{dkr}$  to get the differential operator  $k^2 \left[ \frac{d^2}{d(kr)^2} + \frac{2}{kr} \frac{d}{d(kr)} + 1 - \frac{n(n+1)}{(kr)^2} \right]$  and observe  $kr$  as its variable on the left, and we replace  $kr$  by  $x$  for brevity. Applying the factor  $k^{-2}$  and the spherical harmonics transform  $\int_{\mathbb{S}^2} Y_n^{m'}(\theta) d\theta$  on the equation removes the double sum on the left (orthogonality) and decomposes the panning function  $g(\theta)$  on the right into  $\gamma_{nm}$

$$\left[ \frac{d^2}{dx^2} + \frac{2}{x} \frac{d}{dx} + 1 - \frac{n(n+1)}{x^2} \right] \psi_{nm} = -(kr_0)^{-2} \delta(r - r_0) \gamma_{nm}.$$

We collect the  $x$ -independent term  $\gamma_{nm}$  as factors of the solution  $\psi_{nm} = y \gamma_{nm}$  and get

$$y'' + \frac{2}{x} y' + \left[ 1 - \frac{n(n+1)}{x^2} \right] y = -x_0^{-2} \delta(r - r_0), \quad (\text{A.116})$$

the inhomogeneous spherical Bessel differential equation. As described, e.g., in [16, 17], the inhomogeneous differential equation can be solved by the Lagrangian *variation of the parameters* for equations of the type  $y'' + py' + qy = r$ , knowing its independent homogeneous solutions  $y_1 = h_n^{(2)}(x)$  and  $y_2 = j_n(x)$ .

It uses a solution  $y = uy_1 + vy_2$  with variable parameters  $u$  and  $v$ , which upon first and second-order differentiation becomes

$$\begin{aligned} y &= uy_1 + vy_2, & y' &= uy_1' + u'y_1 + vy_2' + v'y_2 \\ y'' &= uy_1'' + 2u'y_1' + u''y_1 + vy_2'' + 2v'y_2' + v''y_2. \end{aligned}$$

Inserted into the equation  $y'' + py' + qy = r$ , this yields

$$\begin{aligned} &\underbrace{u(y_1'' + py_1' + qy_1)}_{=0} + \underbrace{v(y_2'' + py_2' + qy_2)}_{=0} + u''y_1 + 2u'y_1' + v''y_2 + 2v'y_2' \\ &\quad + p(u'y_1 + v'y_2) = \\ &(u'y_1 + v'y_2)' + u'y_1' + v'y_2' + p(u'y_1 + v'y_2) = u'y_1' + v'y_2' + \left(\frac{d}{dx} + p\right)(u'y_1 + v'y_2) = r. \end{aligned}$$

Now two functions  $u$  and  $v$  are to be determined from only one equation, so we may pose an additional constraint. The above equation would simplify if the term  $(u'y_1 + v'y_2)$  vanished. By this and the simplified equation, we get two conditions

$$\begin{aligned} \text{I :} & \quad u'y_1 + v'y_2 = 0 \\ \text{II :} & \quad u'y_1' + v'y_2' = r \end{aligned}$$

and obtain by elimination with either  $A = \text{I } y_1' - \text{II } y_1$  or  $B = \text{I } y_2' - \text{II } y_2$

$$\begin{aligned} \text{A :} & \quad \underbrace{v'(y_1'y_2 - y_1y_2')}_{-W} = -r y_1 \\ \text{B :} & \quad \underbrace{u'(y_1'y_2 - y_1y_2')}_{-W} = -r y_2. \end{aligned}$$

So that the solution  $y = uy_1 + vy_2$  uses  $u = \int \frac{r y_2}{W} dx$  and  $v = \int \frac{r y_1}{W} dx$ . In our case, we have  $y_1 = h_n^{(2)}(x)$ ,  $y_2 = j_n(x)$ ,  $r = -x_0^{-2}\delta(r - r_0)$ , and the Wronskian  $W = (ix^2)^{-1}$  from Eq. (A.97), hence with integration constants enforcing the physical solutions:

$$y = -h_n^{(2)}(x) \int_0^x ix^2 j_n(x) x_0^{-2} \delta(r - r_0) dx - j_n(x) \int_x^\infty ix^2 h_n^{(2)}(x) x_0^{-2} \delta(r - r_0) dx.$$

To convert  $\delta(r - r_0)$  into  $\delta(x - x_0)$  with  $x = kr$ , we use  $\int \delta(x) dx = \int \delta(r) dr = 1$  with the integration constant replaced,  $\frac{dx}{dr} = k$ , hence  $dx = k dr$  and obviously by  $\int \delta(x) k dr = \int \delta(r) dr$  we find  $\delta(r) = k \delta(x)$ ,

$$\begin{aligned}
y &= -h_n^{(2)}(x) \int_0^x i x^2 j_n(x) k x_0^{-2} \delta(x - x_0) dx - j_n(x) \int_x^\infty i x^2 h_n^{(2)}(x) k x_0^{-2} \delta(x - x_0) dx \\
&= -i k \begin{cases} h_n^{(2)}(x) j_n(x_0), & \text{for } x \geq x_0, \\ j_n(x) h_n^{(2)}(x_0) & \text{for } x \leq x_0. \end{cases}
\end{aligned}$$

The solution becomes after re-substituting  $x = kr$  and expanding  $\psi_{nm} = y \gamma_{nm}$  over the spherical harmonics  $p = \sum_{n=0}^\infty \sum_{m=-n}^n \psi_{nm} Y_n^m(\theta)$ :

$$p = -i k \sum_{n=0}^\infty \sum_{m=-n}^n \gamma_{nm} Y_n^m(\theta) \begin{cases} h_n^{(2)}(kr) j_n(kr_0), & \text{for } r \geq r_0, \\ j_n(kr) h_n^{(2)}(kr_0) & \text{for } r \leq r_0. \end{cases} \quad (\text{A.117})$$

**Green's function.** For the Green's function at the direction  $\theta_0$ , the angular panning function is expanded as  $\phi_{nm} = Y_n^m(\theta_0)$ , and we get the formulation of the Green's function in terms of spherical basis functions:

$$G = -i k \sum_{n=0}^\infty \sum_{m=-n}^n Y_n^m(\theta_0) Y_n^m(\theta) \begin{cases} h_n^{(2)}(kr) j_n(kr_0) & \text{for } r \geq r_0, \\ j_n(kr) h_n^{(2)}(kr_0) & \text{for } r \leq r_0. \end{cases} \quad (\text{A.118})$$

**Plane waves/far field approximation.** Equation (6.7) in Sect. 6.3.1 formulates plane waves  $p = e^{ik\theta_0^T r}$  as far-field limit  $p = 4\pi \lim_{r_0 \rightarrow \infty} \frac{r_0}{e^{-ikr_0}} G = \lim_{r_0 \rightarrow \infty} \frac{1}{-ik h_0^{(2)}(kr_0)} G$ . Using Eq. (A.117), a distribution of plane waves driven by the gains  $g(\theta) = \sum_n \sum_m \gamma_{nm} Y_n^m$  consequently yields with  $\lim_{r_0 \rightarrow \infty} h_n^{(2)}(kr_0) = i^n h_0^{(2)}(kr_0)$ ,

$$\begin{aligned}
p &= 4\pi \sum_{n=0}^\infty \sum_{m=-n}^n j_n(kr) \left[ \lim_{r_0 \rightarrow \infty} \frac{h_n^{(2)}(kr_0)}{h_0^{(2)}(kr_0)} \right] Y_n^m(\theta) \gamma_{nm} \\
&= 4\pi \sum_{n=0}^\infty \sum_{m=-n}^n i^n j_n(kr) Y_n^m(\theta) \gamma_{nm}.
\end{aligned} \quad (\text{A.119})$$

or for a single plane-wave direction  $\gamma_{nm} = Y_n^m(\theta_0)$

$$p = 4\pi \sum_{n=0}^\infty \sum_{m=-n}^n i^n j_n(kr) Y_n^m(\theta) Y_n^m(\theta_0). \quad (\text{A.120})$$

## A.7 Sine and Tangent Law

The sine and tangent law [18] observes the sound pressure of plane waves at to locations  $x = 0$ ,  $y = \pm d$  at ear distance in order to simulate the ear signals. A plane wave from the left half of the room from the angle  $\varphi > 0$  first arrives at the left ear

$p_{\text{left}} = e^{i kd \sin \varphi}$  and later on the right one  $p_{\text{right}} = e^{-i kd \sin \varphi}$ . The phase difference is  $\Phi_{\varphi} = 2 kd \sin \varphi$ .

A superimposed pair of plane waves from the directions  $\pm\alpha$  arrives at the left ear as  $p_{\text{left}} = g_1 e^{i kd \sin \alpha} + g_2 e^{-i kd \sin \alpha}$ , right as  $p_{\text{right}} = g_1 e^{-i kd \sin \alpha} + g_2 e^{i kd \sin \alpha} = p_{\text{left}}^*$ . The phase difference  $\Phi_{\pm\alpha} = 2\angle p_{\text{left}} = 2 \arctan \frac{(g_1 - g_2) \sin(kd \sin \alpha)}{(g_1 + g_2) \cos(kd \sin \alpha)}$  can be linearized for long wave lengths  $kd \rightarrow 0$  to  $\Phi_{\pm\alpha} \approx 2 \arctan \left( kd \frac{g_1 - g_2}{g_1 + g_2} \sin \alpha \right) \approx 2 \frac{g_1 - g_2}{g_1 + g_2} kd \sin \alpha$ .

Comparing the phase difference of the single plane wave with the one of the superimposed pair,  $2 kd \sin \varphi = 2 kd \frac{g_1 - g_2}{g_1 + g_2} \sin \alpha$ , one arrives at the sine law

$$\sin \varphi = \frac{g_1 - g_2}{g_1 + g_2} \sin \alpha.$$

If we claim our hearing to possess the ability to not only estimate the interaural phase difference  $\Phi$  but also its derivative with regard to head rotation  $\frac{\partial \Phi}{\partial \delta}$ , we arrive at a value pair of binaural features  $(\Phi_{\varphi}, \frac{\partial \Phi_{\varphi}}{\partial \delta}) = 2 kd (\sin \varphi, \cos \varphi)$  than should match the one of the stereophonic plane-wave pair. For stereo, the phase difference derived with regard to head rotation is  $2 kd \frac{\partial}{\partial \delta} \Phi_{\pm\alpha} \approx 2 kd \frac{\frac{g_1}{\partial \delta} \sin(\alpha + \delta)|_{\delta=0} + g_2 \frac{\partial}{\partial \delta} \sin(-\alpha + \delta)|_{\delta=0}}{g_1 + g_2} = 2 kd \frac{g_1 + g_2}{g_1 + g_2} \cos \alpha = 2 kd \cos \alpha$ , and yields  $(\Phi_{\pm\alpha}, \frac{\partial \Phi_{\pm\alpha}}{\partial \delta}) = 2 kd (\frac{g_1 - g_2}{g_1 + g_2} \sin \alpha, \cos \alpha)$ . In polar coordinates, the radius of both value pairs differs. While the plane wave yields a value pair at the radius  $2 kd$  in the binaural feature space, the stereophonic waves is of the radius  $2 kd$  only at  $\pm\alpha$ , at which one of the two gains must vanish, and amplitude panning can be used to connect these two points  $2 kd (\pm \sin \alpha, \cos \alpha)$  by a straight line. The plane wave with the most similar feature pair must lie on the same polar angle. We may equate the tangents of both points  $\frac{\Phi_{\varphi}}{\frac{\partial \Phi_{\varphi}}{\partial \delta}} = \frac{\Phi_{\pm\alpha}}{\frac{\partial \Phi_{\pm\alpha}}{\partial \delta}}$  and obtain the tangent law:

$$\tan \varphi = \frac{g_1 - g_2}{g_1 + g_2} \tan \alpha.$$

If instead of the angle of a plane wave with the closest features to those of a given amplitude difference is searched, but the closest features of an amplitude difference matching those of a given plane wave, then the sine law is the best match, even in the two-dimensional feature space.

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