Separation of Variables in 3D/2D Linear PDE

The method of separation of variables introduced for 1D problems is also applicable in higher dimensions—under some particular conditions that we will discuss below. The general idea is the same—to work with ONB's of eigenvectors of Hermitian operators. Once again the most important operator is the Laplace operator (for the sake of definiteness, we consider the 3D case)

$$\Delta \equiv \nabla^2 \equiv \partial_\alpha \partial_\alpha \, . \tag{1}$$

We use the notation $\partial_\alpha = \partial/\partial r_\alpha$, $(r_1 = x,\ r_2 = y,\ r_3 = z)$; here and in what follows, the summation over recurring subscripts is implied. Given a vector space ν of functions $u(\mathbf{r})$, $\mathbf{r} \in \Omega$, where Ω is a domain bounded by a surface S, we want to reveal the boundary conditions for the functions u on the surface S that (i) are consistent with the vector properties of ν and (ii) under which Laplace operator is Hermitian in ν. We assume that the inner product is defined by the integral with the weighting function equal to unity,

$$\langle\, f \,|\, g \,\rangle = \int_\Omega f^* g \, d^3 r \, , \tag{2}$$

and write

$$\begin{aligned} \langle\, f \,|\Delta|\, g \,\rangle &= \int_\Omega f^* \partial_\alpha \partial_\alpha g \, d^3 r = \int_\Omega [\partial_\alpha (f^* \partial_\alpha g) - (\partial_\alpha f^*) \partial_\alpha g)] \, d^3 r = \\ &= \int_\Omega [\partial_\alpha (f^* \partial_\alpha g) - \partial_\alpha (g \partial_\alpha f^*) + g \partial_\alpha \partial_\alpha f^*] \, d^3 r = \\ &= \int_\Omega \mathrm{div}(f^* \nabla g) \, d^3 r - \int_\Omega \mathrm{div}(g \nabla f^*) \, d^3 r + \langle\, \Delta f \,|\, g \,\rangle = \\ &= \int_S (f^* \nabla g) \, d\mathbf{S} - \int_S (g \nabla f^*) \, d\mathbf{S} + \langle\, \Delta f \,|\, g \,\rangle \, . \end{aligned} \tag{3}$$

We see that for the Laplace operator to be Hermitian the two surface integrals should be equal to zero. The two characteristic cases when this takes place are when $\forall f \in \nu$ either

$$f = 0 \,|_{\mathbf{r} \in S} \, , \tag{4}$$

or

$$\nabla f \perp \mathbf{n} \,|_{\mathbf{r} \in S} \, , \tag{5}$$

where vector $\mathbf{n}$ is normal to the surface at the given $\mathbf{r}$.

For definiteness, let us discuss the heat equation

$$u_t = \Delta u \, . \tag{6}$$

In terms of the heat equation, the condition (4) means that the temperature is kept fixed at one and the same value—equal to zero without loss of generality, as a constant can be always subtracted off—on the surface S, while the condition (5) is the condition of the absence of the heat flux through the surface—it takes place when the system is thermally isolated.

Introducing ONB of the eigenfunctions of the Laplace operator, $\{e_m(\mathbf{r})\}$ (we define the eigenvalues of Laplace operator with the sign minus as we expect that these will be non-positive),

$$\Delta e_m = -\lambda_m e_m \; , \tag{7}$$

we expand the solution in the Fourier series with respect to this basis—the same way we did it in 1D:

$$u(\mathbf{r}, t) \; = \; \sum_m q_m(t)\, e_m(\mathbf{r}) \; . \tag{8}$$

We then plug this into the heat equation, and get ordinary differential equations for q's,

$$\dot{q}_m = -\lambda_m q_m \; , \tag{9}$$

with the initial conditions

$$q_m(0) = \int d\mathbf{r}\, e_m^*(\mathbf{r})\, u(\mathbf{r}, t=0) \; . \tag{10}$$

The real problem, however, is to find $\{e_m(\mathbf{r})\}$ and λ's. In a general case of arbitrary shape of the surface S, Eq. (7)—the so-called Helmholtz equation—can be solved only numerically. The two simple cases when it is possible to obtain analytic solutions are: (i) the case of rectangular geometry and (ii) the case of rotationally-symmetric geometry. Also simple is the case of cylindrical symmetry in 3D, which corresponds to rotational symmetry in the xy-plane, and rectangular geometry along the z-axis.

Helmholtz and Laplace Equations in Rectangular Geometry

Suppose the domain Ω is a rectangle: $x \in [0, L_x]$, $y \in [0, L_y]$, and $z \in [0, L_z]$. We want to solve Helmholtz equation (7) with canonical boundary conditions at the faces $x = 0$, $x = L_x$, $y = 0$, and $y = L_y$. As we will see later, it is not important whether the boundary conditions at the faces $z = 0$ and $z = L_z$ are canonical or not. For example,

$$e \mid_{x=0} = e \mid_{x=L_x} = 0 \; , \tag{11}$$

$$e_y \,|_{y=0} = e_y \,|_{y=L_y} = 0 \; . \tag{12}$$

We start by noticing that 3D Laplace operator

$$\Delta \;=\; \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \; , \tag{13}$$

contains a 1D Laplace operator $\partial^2/\partial x^2$, which is Hermitian for in the vector space of the functions of x satisfying (11). We thus can introduce corresponding ONB, $\{X_{m_x}(x)\}$,

$$X''_{m_x}(x) \;=\; -\lambda^{(x)}_{m_x} \, X_{m_x}(x) \; , \tag{14}$$

and expand the solution in the Fourier series:

$$e(\mathbf{r}) \;=\; \sum_{m_x} Q_{m_x}(y,z) \, X_{m_x}(x) \; . \tag{15}$$

The idea is precisely the same as when solving 1D time-dependent equations. Now instead of variable t we have a pair of variables (y, z). Correspondingly, we plug (15) into (7), take advantage of (14) and of the orthogonality of $|\, X \,\rangle$'s. This yields

$$\left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) Q_{m_x} = -\tilde{\lambda} Q_{m_x} \; , \tag{16}$$

with

$$\tilde{\lambda} = \lambda - \lambda^{(x)}_{m_x} \; . \tag{17}$$

From (16) we see that the function Q_{m_x} actually does not depend on m_x, since $\tilde{\lambda}$ is just one of the eigenvalues of this equation and Eq. (17) is just a relation between this number and the global eigenvalue λ. Remarkably, after separating out the variable x we arrive at the problem similar to the original one, but in lower dimensions. Hence, we can use the trick once again—now with the variable y:

$$Y''_{m_y}(y) \;=\; -\lambda^{(y)}_{m_y} \, Y_{m_y}(y) \; , \tag{18}$$

$$Q(y,z) \;=\; \sum_{m_y} Z_{m_y}(z) \, Y_{m_y}(y) \; , \tag{19}$$

$$Z''_{m_y}(z) \;=\; -\tilde{\tilde{\lambda}} \, Z_{m_y}(z) \; , \tag{20}$$

with

$$\tilde{\tilde{\lambda}} \;=\; \tilde{\lambda} - \lambda^{(x)}_{m_x} \;=\; \lambda - \lambda^{(x)}_{m_x} - \lambda^{(y)}_{m_y} \; . \tag{21}$$

From (20) we conclude that Z_{m_y} does not depend on m_y.

The final step depends on the type of the problem being solved in terms of the boundary conditions at $z = 0$ and $z = L_z$. If these are the canonical conditions and we are looking for all eigenfunctions and eigenvalues, then (20) has the same meaning as (14) and (18):

$$Z''_{m_z}(z) \;=\; -\lambda^{(z)}_{m_z}\, Z_{m_z}(z) \;, \tag{22}$$

and we arrive at the following final answers for the 3D basis:

$$e_{m_x\, m_y\, m_z}(\mathbf{r}) \;=\; X_{m_x}(x)\, Y_{m_y}(y)\, Z_{m_z}(z) \;, \tag{23}$$

and for the eigenvalues:

$$\lambda_{m_x\, m_y\, m_z} \;=\; \lambda^{(x)}_{m_x} \;+\; \lambda^{(y)}_{m_y} \;+\; \lambda^{(z)}_{m_z} \;. \tag{24}$$

In the case when we need to find the solution of the Helmholtz equation

$$\Delta u + \lambda u = 0 \tag{25}$$

with some *given* λ and non-canonical boundary conditions for the variable z, Eq. (20) together with these conditions simply fixes the coefficients $Z_{m_x\, m_y}(z)$ in the Fourier expansion

$$u(x,y,z) \;=\; \sum_{m_x\, m_y} Z_{m_x\, m_y}(z)\, X_{m_x}(x)\, Y_{m_y}(y) \;. \tag{26}$$

Note that in the case of $\lambda = 0$ Eq. (25) becomes Laplace equation

Problem 30. Find the lowest eigen frequency of the rectangular 3D resonator described by the wave equation (c is the sound velocity)

$$u_{tt} = c^2 \Delta u \;, \qquad\quad x \in [0, L_x], \quad y \in [0, L_y], \quad z \in [0, L_z] \;, \tag{27}$$

with the boundary conditions

$$u\,|_{x=0} \;=\; u\,|_{x=L_x} \;=\; 0 \;, \tag{28}$$

$$u_y\,|_{y=0} \;=\; u_y\,|_{y=L_y} \;=\; 0 \;, \tag{29}$$

$$u\,|_{z=0} \;=\; 0 \;, \qquad\quad u_z\,|_{z=L_z} \;=\; 0 \;. \tag{30}$$

Comment. An eigen frequency is a frequency corresponding to a normal mode. And the normal mode is the solution which is an eigenfunction of the Laplace operator and thus does not change its shape—up to the time-varying amplitude—during the evolution.

2D Helmholtz and Laplace Equations in Polar Coordinates

Consider Helmholtz equation (25) in two dimensions with the function u defined in 2D plane in the region between two circles, the smaller one of the radius r_1, and the lager one of the radius r_2 (see Fig. 1). The limiting cases $r_1 \to 0$ and $r_2 \to \infty$ are also included. The function $u \equiv u(\rho, \varphi)$—we use polar coordinates—is subject to certain boundary conditions at the boundaries of its domain of definition. For example,

$$u(\rho = r_1,\, \varphi) = f_1(\varphi)\;, \qquad u(\rho = r_2,\, \varphi) = f_2(\varphi)\;. \tag{31}$$

If $f_1 = f_2 = 0$, these conditions are canonical and we are dealing with an eigenvalue problem.—The solution exists only for some special λ's. We face such a problem when constructing ONB of Laplace operator. Alternatively, the value of λ can be fixed—say, $\lambda = 0$, in which case (25) becomes Laplace equation, and the boundary conditions may be arbitrary.

Such a geometry allows one to separate the variables. Analyzing the structure of 2D Laplace operator in polar coordinates,

$$\Delta \;=\; \frac{1}{\rho}\,\frac{\partial}{\partial\rho}\,\rho\,\frac{\partial}{\partial\rho} \;+\; \frac{1}{\rho^2}\,\frac{\partial^2}{\partial\varphi^2}\;, \tag{32}$$

we see that the variable φ enters the expression in the form of 1D Laplace operator $\partial^2/\partial\varphi^2$. This operator is Hermitian in the space of single-valued functions of the angle φ, because single-valuedness is equivalent to the 2π-periodicity, and Laplace operator is Hermitian in the space of periodic functions. Hence, we can utilize ONB of the eigenfunctions of the operator $\partial^2/\partial\varphi^2$:

$$\Phi_m(\varphi) = \mathrm{e}^{im\varphi}/\sqrt{2\pi}\;, \qquad m = 0, \pm 1, \pm 2, \dots\;, \tag{33}$$

$$\frac{\partial^2 \Phi_m}{\partial\varphi^2} \;=\; -m^2\,\Phi_m\;, \tag{34}$$

$$\int_0^{2\pi} \Phi_m(\varphi)^*\,\Phi_n(\varphi)\,d\varphi \;=\; \delta_{mn}\;. \tag{35}$$

We expand the function $u(\rho, \varphi)$ in the Fourier series

$$u(\rho, \varphi) = \sum_{m=-\infty}^{\infty} R_m(\rho)\,\Phi_m(\varphi) \tag{36}$$

and plug this expansion in (25). Taking into account (34) and constructing inner products with the functions $\Phi_m(\varphi)$ we obtain an independent equation

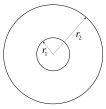

Figure 1: Domain of definition of the function u.

for each R_m:

$$\left(\frac{1}{\rho}\frac{d}{d\rho}\,\rho\,\frac{d}{d\rho} - \frac{m^2}{\rho^2} + \lambda\right) R_m(\rho) = 0 \;, \tag{37}$$

which can be rewritten as

$$\rho^2 R_m'' + \rho R_m' + (\lambda\rho^2 - m^2) R_m = 0 \;. \tag{38}$$

Eq. (38) is called Bessel equation. [And its solutions are Bessel functions.] Bessel equation is a second-order ordinary differential equation, which implies that each R_m is defined up to two unknown constants to be fixed by the boundary conditions:

$$\sum_{m=-\infty}^{\infty} R_m(r_1)\,\Phi_m(\varphi) = f_1(\varphi) \;, \tag{39}$$

$$\sum_{m=-\infty}^{\infty} R_m(r_2)\,\Phi_m(\varphi) = f_2(\varphi) \;, \tag{40}$$

from which we get

$$R_m(r_1) = \int_0^{2\pi} \mathrm{e}^{-im\varphi} f_1(\varphi)\,d\varphi/\sqrt{2\pi} \;, \tag{41}$$

$$R_m(r_2) = \int_0^{2\pi} \mathrm{e}^{-im\varphi} f_2(\varphi)\,d\varphi/\sqrt{2\pi} \;. \tag{42}$$

In the case $r_1 \to 0$ (or $r_2 \to \infty$) the corresponding boundary condition is replaced with the requirement that the function R_m be finite. This requirement works as a boundary condition for the following reason. A generic solution to the Bessel equation is divergent in both limits, $\rho \to 0$ and $\rho \to \infty$. The requirement that the function $R_m(\rho)$ be finite, say, at $\rho \to 0$ is equivalent to the requirement that the amplitude of the divergent at $\rho \to 0$ term be zero. Hence, the requirement just fixes one of the two unknown parameters of the generic solution. In the case of the eigenvalue problem and, correspondingly, canonical boundary conditions, it is impossible to fix both parameters from the boundary conditions. Indeed, by definition, the canonical boundary conditions are consistent with the vector properties of corresponding set of functions, which means that they should be insensitive to multiplying a function by any constant. [And that is why the solution in this case exists only at some special λ's—the eigenvalues.] Typical canonical boundary conditions in polar coordinates are $R(\rho = r_b) = 0$ or $R'(\rho = r_b) = 0$, where r_b is the boundary radius. Note that the above-discussed requirements that $R(\rho = 0)$ or $R(\rho = \infty)$ be finite are also canonical.—They are consistent with vector properties.

Eigenfunctions of Laplace operator. The structure of the eigenfunctions of Laplace operator in the 2D polar geometry is as follows.

$$e_{mn}(\mathbf{r}) \;=\; R_{mn}(\rho)\, \Phi_m(\varphi)\;, \tag{43}$$

$$\Delta e_{mn}(\mathbf{r}) \;=\; -\lambda_{mn}\, e_{mn}(\mathbf{r})\;, \tag{44}$$

where the subscript n enumerates the eigenvalues and corresponding solutions $R_{mn}(\rho)$ of the Bessel equation Eq. (38). Since this equation is different for different m's, both the eigenvalue and the solution depend on m. As is expected for a Hermitian operator, the eigenfunctions are orthogonal:

$$\langle\, e_{m_1 n_1} \,|\, e_{m_2 n_2} \,\rangle \;\equiv\; \int_{r_1}^{r_2} d\rho\, \rho \int_0^{2\pi} d\varphi\, e^*_{m_1 n_1}(\mathbf{r})\, e_{m_2 n_2}(\mathbf{r}) \;=\; \delta_{m_1 m_2}\, \delta_{n_1 n_2} \tag{45}$$

in view of the following two *separate* orthogonality relations:

$$\langle\, \Phi_{m_1} \,|\, \Phi_{m_2} \,\rangle \;\equiv\; \int_0^{2\pi} d\varphi\, \Phi^*_{m_1}(\varphi)\, \Phi_{m_2}(\varphi) \;=\; \delta_{m_1 m_2}\;, \tag{46}$$

$$\langle\, R_{m n_1} \,|\, R_{m n_2} \,\rangle \;\equiv\; \int_{r_1}^{r_2} d\rho\, \rho\, R^*_{m n_1}(\rho)\, R_{m n_2}(\rho) \;=\; \delta_{n_1 n_2}\;. \tag{47}$$

Note that two functions R are orthogonal only when they correspond to one and the same m, because only in this case they are eigenfunctions of one and the same Hermitian operator. Note also that the proper weighting function ρ unambiguously follows from the form of the Sturm-Liouville operator in Eq. (37).

Laplace equation. This case, $\lambda = 0$, is especially simple, because R_m's now are just polynomials (A's and B's are constants):

$$R_m(\rho) = A_m \rho^m + B_m \rho^{-m} \ , \qquad m \neq 0 \ , \qquad (\lambda = 0) \ , \tag{48}$$

$$R_0(\rho) = A_0 + B_0 \ln \rho \ , \qquad (\lambda = 0) \ . \tag{49}$$

Example. Suppose we are looking for the function $u(\rho, \varphi)$ that satisfies the Laplace equation

$$\Delta u = 0 \tag{50}$$

everywhere in 2D plane, except for the two circles (Fig. 1), where it is subject to the boundary conditions

$$u(\rho = r_1, \, \varphi) = \sin \varphi \ , \tag{51}$$

$$u(\rho = r_2, \, \varphi) = \cos \varphi \ , \tag{52}$$

and tends to zero at $\rho \to \infty$.

Solution. First we note that there are 3 independent regions:

(a) $\rho \in [0, r_1]$,
(b) $\rho \in [r_1, r_2]$,
(c) $\rho \in [r_2, \infty)$.

We thus have to separately solve the problem in each of the regions.
(a) Here we have the boundary condition (62) and the requirement that u be finite at $\rho = 0$. The latter means that we exclude the singular terms from the solution (36), (48)-(49), and write

$$u = \sum_{m=-\infty}^{\infty} A_m \rho^{|m|} \, \Phi_m(\varphi) \equiv A_0 + \sum_{m=1}^{\infty} \rho^m (C_m \sin m\varphi + D_m \cos m\varphi) \ . \tag{53}$$

The representation in terms of sines and cosines is convenient here, because of the particular form of the boundary conditions.—We immediately see that only one term of the series is non-zero. Namely, the one with $\sin \varphi$; and the answer is

$$u = (\rho / r_1) \sin \varphi \equiv y / r_1 \ . \tag{54}$$

(c) This case is similar to the previous one. Now we exclude the terms divergent in the limit of $\rho \to \infty$ and write

$$u = \sum_{m=1}^{\infty} \rho^{-m}(C_m \sin m\varphi + D_m \cos m\varphi) \ . \tag{55}$$

The relevant boundary condition is Eq. (52), from which we see that the only non-zero term is that with $\cos\varphi$, and find

$$u = (r_2/\rho)\cos\varphi \ . \tag{56}$$

(b) Once again we use the sine-cosine representation:

$$u = A_0 + B_0 \ln\rho + \sum_{m=1}^{\infty} \left\{ \left[C_m\rho^m + \frac{\tilde{C}_m}{\rho^m} \right] \sin m\varphi + \left[D_m\rho^m + \frac{\tilde{D}_m}{\rho^m} \right] \cos m\varphi \right\} . \tag{57}$$

We have two terms that are non-orthogonal to the boundary conditions, the term with $\sin\varphi$ and the term with $\cos\varphi$. Corresponding coefficients are easily found from the boundary conditions:

$$C_1 r_1 + \tilde{C}_1/r_1 = 1 \ , \qquad C_1 r_2 + \tilde{C}_1/r_2 = 0 \ , \tag{58}$$

$$D_1 r_1 + \tilde{D}_1/r_1 = 0 \ , \qquad D_1 r_2 + \tilde{D}_1/r_2 = 1 \ . \tag{59}$$

The final answer is:

$$u = \frac{r_1\,(r_2^2/\rho - \rho)\sin\varphi}{r_2^2 - r_1^2} + \frac{r_2\,(\rho - r_1^2/\rho)\cos\varphi}{r_2^2 - r_1^2} \ . \tag{60}$$

Problem 31. Find the function $u(\rho,\varphi)$ defined in the region $\rho \in [r_1, r_2]$—here ρ and φ are the polar coordinates—and satisfying the Laplace equation,

$$\Delta u = 0 \ , \tag{61}$$

with the boundary conditions

$$u(r_1,\,\varphi) = 1 \ , \qquad u(r_2,\,\varphi) = \sin\varphi \ . \tag{62}$$

Helmholtz/Laplace Equation in 3D: Spherical Coordinates

Let us generalize the two-dimensional consideration of the previous section to the 3D case. We have 3D Helmholtz (Laplace, if $\lambda = 0$) equation:

$$\Delta u + \lambda u = 0 \,, \tag{63}$$

where the function u is defined in 3D space in the region between two spheres, the smaller one with the radius r_1, and the lager one, with the radius r_2 (Fig. 1). In this geometry, it is convenient to use spherical coordinates r, θ, φ:

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

For the boundary conditions for the function $u \equiv u(r,\,\theta,\,\varphi)$ we take—for the sake of definiteness—the 3D analog of (31):

$$u(r=r_1,\,\theta,\,\varphi) = f_1(\theta,\,\varphi) \,, \qquad u(r=r_2,\,\theta,\,\varphi) = f_2(\theta,\,\varphi) \,. \tag{64}$$

The problem (63)-(64) is solved by separating the variable r from the angular variables. The 3D Laplace operator in the spherical coordinates is:

$$\Delta \;=\; \frac{1}{r^2}\,\frac{\partial}{\partial r}\,r^2\,\frac{\partial}{\partial r} \;-\; \frac{1}{r^2}\,\hat{\mathbf{l}}^2 \,, \tag{65}$$

where

$$\hat{\mathbf{l}}^2 \;=\; -\left[\frac{1}{\sin\theta}\,\frac{\partial}{\partial\theta}\,\sin\theta\,\frac{\partial}{\partial\theta} \;+\; \frac{1}{\sin^2\theta}\,\frac{\partial^2}{\partial\varphi^2}\right] \,. \tag{66}$$

It is worth noting that the operator $\mathbf{l}^2$ is the square of a Hermitian vector operator

$$\hat{\mathbf{l}} = -i\mathbf{r}\times\nabla \,, \tag{67}$$

playing a very important role in Quantum Mechanics.—The operator $\hbar\hat{\mathbf{l}}$ is the operator of angular momentum of a quantum particle. Note also that while the sign minus in (67) is a matter of definition, the number i is crucial; without it the operator would be *anti*-Hermitian (an operator L is anti-Hermitian if $L^\dagger = -L$).

The operator $\hat{\mathbf{l}}^2$ is a Hermitian operator in the space of single-valued functions of the angular variables $(\theta,\,\varphi)$. Hence, it features ONB of eigenfunctions, $Y \equiv Y(\theta,\varphi)$,

$$\hat{\mathbf{l}}^2\,Y \;=\; \tilde{\lambda}\,Y \,. \tag{68}$$

These functions are called *spherical harmonics*. Analyzing the structure of Eq. (66), we see that the φ-dependent part of the operator $\hat{\mathbf{l}}^2$ is nothing else than the Hermitian operator $\partial^2/\partial\varphi^2$, which is already known to us from the 2D case. This means that one can solve (68) by separating φ from θ in terms of the eigenfunctions $\Phi_m(\varphi)$—see (33)-(35):

$$Y(\theta, \varphi) \; = \sum_{m=-\infty}^{\infty} \Theta_m(\theta)\, \Phi_m(\varphi) \; . \tag{69}$$

We plug this into (68), take into account (66) and (34), and the orthogonality of $|\Phi_m\rangle$'s. This results in the following Sturm-Liouville problem

$$\left[\frac{1}{\sin\theta} \frac{d}{d\theta} \sin\theta \, \frac{d}{d\theta} \; - \; \frac{m^2}{\sin^2\theta} \right] \Theta_m \; = -\tilde{\lambda}\Theta_m \; , \tag{70}$$

in which the number m plays a role of an external parameter. By definition of spherical coordinates, $\theta \in [0, \pi]$, and the boundary conditions for our problem are just the requirements that $\Theta(\theta)$ be finite at $\theta = 0$ and $\theta = \pi$. For any given m, there is an infinite number of the eigenfunctions and eigenvalues. The theory of Eq. (70) says that the eigenvalues are

$$\tilde{\lambda}_{ml} = l(l+1), \qquad\qquad l = |m|, \; |m|+1, \; |m|+2, \; \ldots \; . \tag{71}$$

Note that while the eigenvalues do not depend on m explicitly, the smallest possible number l is equal to $|m|$. Corresponding solution Θ_{ml} is given—up to a normalization factor C_{lm}—by the so-called *associated Legendre polynomials*, $P_{lm}(\cos\theta)$.

$$\Theta_{ml}(\theta) \; = C_{lm} P_{lm}(\cos\theta) \; . \tag{72}$$

There exists an explicit expression for the associated Legendre polynomials (which are, strictly speaking, polynomials only up to a certain non-polynomial pre-factor):

$$P_{lm}(\chi) \; = \; \frac{1}{2^l l!} \, (1-\chi^2)^{m/2} \, \frac{d^{l+m}}{(d\chi)^{l+m}} \, (\chi^2 - 1)^l \; . \tag{73}$$

For $P_{lm}(\cos\theta)$ it can be also written as

$$P_{lm}(\cos\theta) \; = \; \frac{1}{2^l l!} \, \sin^m\theta \, \frac{d^{l+m}}{(d\cos\theta)^{l+m}} \, (\cos^2\theta - 1)^l \; . \tag{74}$$

For example,

$$
\begin{aligned}
P_{0,0}(\cos\theta) &= 1 \ , \\
P_{1,0}(\cos\theta) &= \cos\theta \ , \\
P_{1,1}(\cos\theta) &= \sin\theta \ , \\
P_{1,-1}(\cos\theta) &= -\sin\theta \ .
\end{aligned}
$$

The orthonormalization relation for the functions Θ_{ml} is [the weighting function follows from the form of the Sturm-Liouville operator in Eq. (70)]

$$\int_0^\pi d\theta \, \sin\theta \, \Theta_{ml_1} \Theta_{ml_2} \ = \ \delta_{l_1 l_2} \ . \tag{75}$$

It implies that

$$\int_0^\pi d\theta \, \sin\theta \, (\Theta_{ml})^2 \ = \ 1 \ . \tag{76}$$

Eq. (76) is satisfied when

$$C_{lm} \ = \ \sqrt{\frac{(2l+1)(l-m)!}{2(l+m)!}} \ . \tag{77}$$

We have constructed the ONB of spherical harmonics,

$$Y_{lm}(\theta,\varphi) \ = \ C_{lm} \, P_{lm}(\cos\theta) \, \Phi_m(\varphi) \tag{78}$$

featuring the following properties

$$\hat{\mathbf{l}}^2 \, Y_{lm}(\theta,\, \varphi) \ = \ -l(l+1) \, Y_{lm}(\theta,\, \varphi) \ , \tag{79}$$

$$\langle Y_{l_1 m_1} | Y_{l_2 m_2} \rangle \equiv \int_0^{2\pi} d\varphi \int_0^\pi d\theta \, \sin\theta \, Y^*_{l_1 m_1}(\theta,\varphi) \, Y_{l_2 m_2}(\theta,\varphi) = \delta_{l_1 l_2} \, \delta_{m_1 m_2} \ . \tag{80}$$

Now we expand the solution $u(r,\, \theta,\, \varphi)$ in the Fourier series with respect to this ONB:

$$u(r,\, \theta\,, \varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} R_{lm}(r) \, Y_{lm}(\theta,\, \varphi) \ . \tag{81}$$

Plugging this into (63) and taking into account (65)-(66) and (79), we get

$$\sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{lm}(\theta,\, \varphi) \left[\frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} \ - \ \frac{l(l+1)}{r^2} + \lambda \right] R_{lm}(r) = 0 \ . \tag{82}$$

In view of (80), this implies

$$\left[\frac{1}{r^2}\,\frac{d}{dr}\,r^2\,\frac{d}{dr}\;-\;\frac{l(l+1)}{r^2}+\lambda\right]R_{lm}(r)=0\;, \tag{83}$$

or, equivalently,

$$r^2R''_{lm}+2rR'_{lm}+[\lambda r^2-l(l+1)]R_{lm}=0\;. \tag{84}$$

The boundary conditions follow from

$$u(r_1,\,\theta\,,\varphi)=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}R_{lm}(r_1)\,Y_{lm}(\theta,\,\varphi)\;, \tag{85}$$

$$u(r_2,\,\theta\,,\varphi)=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}R_{lm}(r_2)\,Y_{lm}(\theta,\,\varphi)\;. \tag{86}$$

That is

$$R_{lm}(r_1)=\langle Y_{lm}|f_1\rangle\equiv\int_0^{2\pi}\!d\varphi\int_0^{\pi}\!d\theta\,\sin\theta\,Y^*_{lm}(\theta,\,\varphi)f_1(\theta,\,\varphi)\;, \tag{87}$$

$$R_{lm}(r_2)=\langle Y_{lm}|f_2\rangle\equiv\int_0^{2\pi}\!d\varphi\int_0^{\pi}\!d\theta\,\sin\theta\,Y^*_{lm}(\theta,\,\varphi)f_2(\theta,\,\varphi)\;. \tag{88}$$

The problem of finding functions R_{lm} in 3D is analogous to its 2D counterpart, considered previously. Moreover, introducing the new variable

$$Q_{lm}=\sqrt{r}\,R_{lm}\;, \tag{89}$$

we reduce Eq. (84) to the Bessel equation

$$r^2Q''_{lm}\;+\;rQ'_{lm}\;+\;[\,\lambda r^2-(l+1/2)^2\,]\,Q_{lm}=0\;. \tag{90}$$

As in 2D, the solution is especially simple in the case of Laplace equation ($\lambda=0$):

$$R_{lm}(r)=A_{lm}\,r^l+B_{lm}\,r^{-(l+1)}\qquad(\lambda=0)\;. \tag{91}$$

Here A's and B's are constants.

Problem 32. Find the solution $u(r,\theta,\varphi)$ of the stationary heat equation

$$\Delta u=0 \tag{92}$$

within a ball of the radius R; the boundary condition on the surface is

$$u\,|_{r=R}\;=\;\cos\theta. \tag{93}$$

Eigenfunctions of Laplace operator. The structure of the eigenfunctions of Laplace operator in the 3D spherical geometry is as follows.

$$e_{lmn}(\mathbf{r}) \;=\; R_{ln}(r)\, Y_{lm}(\theta,\varphi)\ , \tag{94}$$

$$\Delta e_{lmn}(\mathbf{r}) \;=\; -\lambda_{ln}\, e_{lmn}(\mathbf{r})\ , \tag{95}$$

where the subscript n enumerates the eigenvalues and corresponding solutions $R_{ln}(r)$ of Eq. (83). Since neither (83) nor canonical boundary conditions depend on m, both R and λ are m-independent. As is expected for a Hermitian operator, the eigenfunctions are orthogonal:

$$\begin{aligned}\langle\, e_{l_1m_1n_1} \,|\, e_{l_1m_2n_2} \,\rangle \;\equiv\; \int_{r_1}^{r_2} dr\, r^2 \int_0^{\pi} d\theta\, \sin\theta \int_0^{2\pi} d\varphi\, e^*_{l_1m_1n_1}(\mathbf{r})\, e_{l_2m_2n_2}(\mathbf{r}) = \\ = \; \delta_{l_1l_2}\, \delta_{m_1m_2}\, \delta_{n_1n_2}\end{aligned} \tag{96}$$

in view of Eq. (80) and

$$\langle\, R_{ln_1} \,|\, R_{ln_2} \,\rangle \;\equiv\; \int_{r_1}^{r_2} dr\, r^2 R^*_{ln_1}(r)\, R_{ln_2}(r) \;=\; \delta_{n_1n_2}\ . \tag{97}$$

Note that two functions R are orthogonal only when they correspond to one and the same l, because only in this case they are eigenfunctions of one and the same Hermitian operator. The proper weighting function r^2 follows from the form of the Sturm-Liouville operators in Eq. (83).