

Chapter 12

Partial Differential Equations in Space

At last we have ascended to the ultimate rung of the dimensional ladder (at least for those of us living in a three-dimensional universe): partial differential equations in physical space. As in the one- and two-dimensional settings developed in the preceding chapters, the main protagonists are the Laplace and Poisson equations, modeling equilibrium configurations of solid bodies; the three-dimensional wave equation, governing vibrations of solids, liquids, and electromagnetic waves; and the three-dimensional heat equation, modeling spatial diffusion processes. To conclude this chapter — and the book — we will also analyze the particular three-dimensional Schrödinger equation that governs the hydrogen atom, and thereby characterizes atomic orbitals.

Fortunately, almost everything of importance has already appeared in the previous chapters, and appending a third dimension is, for the most part, simply a matter of appropriately adapting the constructions. We have already developed the principal solution techniques: separation of variables, Green's functions, and fundamental solutions. In three-dimensional problems, separation of variables is applicable in a variety of coordinate systems, including the usual rectangular, cylindrical, and spherical coordinates. The first two do not lead to anything fundamentally new, and are therefore relegated to the exercises. Separation in spherical coordinates requires spherical Bessel functions and spherical harmonics, which play essential roles in a wide variety of physical systems, both classical and quantum.

The Green's function for the three-dimensional Poisson equation in space can be identified as the classic Newton (Coulomb) $1/r$ gravitational (electrostatic) potential. The fundamental solution for the three-dimensional heat equation can be easily guessed from its one- and two-dimensional forms. The three-dimensional wave equation, surprisingly, has an explicit solution formula, named after Kirchhoff, of electrical fame, but originally due to Poisson. Counterintuitively, the best way to handle the two-dimensional wave equation is by “descending” from the simpler(!) three-dimensional Kirchhoff formula. Descent reveals a remarkable difference between waves in planar and spatial media. Huygens' Principle states that three-dimensional waves emanating from a localized initial disturbance remain localized as they propagate through space. In contrast, initially concentrated two-dimensional disturbances leave a slowly decaying remnant that never entirely disappears.

The final section is concerned with the Schrödinger equation for a hydrogen atom, that is, the quantum-dynamical system governing the spatial motion of a single electron around a positively charged nucleus. As we will see, the spherical harmonic eigensolutions account for the observed quantum energy levels of atoms that underly the periodic table and hence the foundations of molecular chemistry.

12.1 The Three-Dimensional Laplace and Poisson Equations

We begin our investigations, as usual, with systems in equilibrium, deferring dynamics until later. The prototypical equilibrium system is the three-dimensional Laplace equation

$$\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = 0, \quad (12.1)$$

in which $\mathbf{x} = (x, y, z)^T$ represents rectangular coordinates on \mathbb{R}^3 . The solutions $u(x, y, z)$ continue to be known as *harmonic functions*. The Laplace equation models unforced equilibria; *Poisson's equation* is the inhomogeneous version

$$-\Delta u = f(x, y, z), \quad (12.2)$$

whose right-hand side represents some form of external forcing.

The basic boundary value problem for the Laplace and Poisson equations seeks a solution inside a bounded domain $\Omega \subset \mathbb{R}^3$ subject to either *Dirichlet boundary conditions*, prescribing the function values on the domain's boundary:

$$u = h \quad \text{on} \quad \partial\Omega, \quad (12.3)$$

or *Neumann boundary conditions*, prescribing its normal derivative or flux through the boundary:

$$\frac{\partial u}{\partial \mathbf{n}} = k \quad \text{on} \quad \partial\Omega, \quad (12.4)$$

or *mixed boundary conditions*, in which one imposes Dirichlet conditions on part of the boundary and Neumann conditions on the remainder. Keep in mind that the boundary of the solid domain Ω consists of one or more piecewise smooth closed surfaces, which will be oriented by use of the outward — meaning exterior to the domain — unit normal \mathbf{n} .

The boundary value problems for the three-dimensional Laplace and Poisson equations govern a wide variety of physical systems, including:

- *Heat conduction*: The solution u represents the equilibrium temperature in a solid body. The inhomogeneity f represents some form of internal heat source or sink. Dirichlet conditions correspond to fixing the temperature on the bounding surface(s), whereas homogeneous Neumann conditions correspond to an insulated boundary, i.e., one that does not allow any heat flux.
- *Ideal fluid flow*: Here the solution u to the Laplace equation represents the velocity potential for an incompressible, irrotational steady-state fluid flow inside a container governed by the velocity vector field $\mathbf{v} = \nabla u$. Homogeneous Neumann boundary conditions correspond to a solid boundary that the fluid cannot penetrate.
- *Elasticity*: In certain restricted contexts, u represents an equilibrium deformation of a solid body, e.g., the radial deformation of an elastic ball.
- *Electrostatics*: In applications to electromagnetism, u is the electric potential in a conducting medium; its gradient ∇u prescribes the electromotive force on a charged particle. The inhomogeneity f represents an external electrostatic force field.
- *Gravitation*: The Newtonian gravitational potential in flat empty space is also prescribed by the Laplace equation. (In contrast, Einstein's theory of general relativity requires a vastly more complicated nonlinear system of partial differential equations, [75].)

Self-Adjoint Formulation and Minimum Principle

The Laplace and Poisson equations naturally fit into the general self-adjoint equilibrium framework summarized in Chapter 9. We introduce the L^2 inner products

$$\begin{aligned}\langle u, \tilde{u} \rangle &= \iiint_{\Omega} u(x, y, z) \tilde{u}(x, y, z) \, dx \, dy \, dz, \\ \langle \mathbf{v}, \tilde{\mathbf{v}} \rangle &= \iiint_{\Omega} \mathbf{v}(x, y, z) \cdot \tilde{\mathbf{v}}(x, y, z) \, dx \, dy \, dz,\end{aligned}\tag{12.5}$$

between, respectively, scalar fields u, \tilde{u} , and vector fields $\mathbf{v}, \tilde{\mathbf{v}}$, which are defined on the domain $\Omega \subset \mathbb{R}^3$. We assume that the functions in question are sufficiently nice in order that these inner products be well defined; if Ω is unbounded, this, in essence, requires that they decay reasonably rapidly to zero at large distances.

When subject to suitable homogeneous boundary conditions, the three-dimensional Laplace equation can be placed in our standard self-adjoint form

$$-\Delta u = -\nabla \cdot \nabla u = \nabla^* \circ \nabla u.\tag{12.6}$$

This relies on the fact that the adjoint of the gradient operator with respect to the L^2 inner products (12.5) is minus the divergence operator:

$$\nabla^* \mathbf{v} = -\nabla \cdot \mathbf{v}.\tag{12.7}$$

As usual, the determination of the adjoint rests on an integration by parts formula, which, in three-dimensional space, is a consequence of the Divergence Theorem from multivariable calculus, [8, 108]:

Theorem 12.1. *Let $\Omega \subset \mathbb{R}^3$ be a bounded domain whose boundary $\partial\Omega$ consists of one or more piecewise smooth simple closed surfaces. Let \mathbf{n} denote the unit outward normal to the boundary of Ω . Let \mathbf{v} be a C^1 vector field defined on Ω and continuous up to its boundary. Then the surface integral, with respect to surface area, of the normal component of \mathbf{v} over the boundary of the domain equals the triple integral of its divergence over the domain:*

$$\iint_{\partial\Omega} \mathbf{v} \cdot \mathbf{n} \, dS = \iiint_{\Omega} \nabla \cdot \mathbf{v} \, dx \, dy \, dz.\tag{12.8}$$

Replacing \mathbf{v} by the product $u\mathbf{v}$ of a scalar field u and a vector field \mathbf{v} yields

$$\iiint_{\Omega} (u \nabla \cdot \mathbf{v} + \nabla u \cdot \mathbf{v}) \, dx \, dy \, dz = \iiint_{\Omega} \nabla \cdot (u \mathbf{v}) \, dx \, dy \, dz = \iint_{\partial\Omega} u (\mathbf{v} \cdot \mathbf{n}) \, dS.\tag{12.9}$$

Rearranging the terms produces the desired *integration by parts formula* for triple integrals:

$$\iiint_{\Omega} (\nabla u \cdot \mathbf{v}) \, dx \, dy \, dz = \iint_{\partial\Omega} u (\mathbf{v} \cdot \mathbf{n}) \, dS - \iiint_{\Omega} u (\nabla \cdot \mathbf{v}) \, dx \, dy \, dz.\tag{12.10}$$

The boundary surface integral will vanish, provided either $u = 0$ or $\mathbf{v} \cdot \mathbf{n} = \mathbf{0}$ at each point on $\partial\Omega$. When $u = 0$ on all of $\partial\Omega$, we have homogeneous Dirichlet conditions. Setting $\mathbf{v} \cdot \mathbf{n} = \mathbf{0}$ everywhere on $\partial\Omega$ results in the homogeneous Neumann boundary value problem owing to the identification of $\mathbf{v} = \nabla u$. Finally, the mixed boundary value problem takes $u = 0$ on part of $\partial\Omega$ and $\mathbf{v} \cdot \mathbf{n} = \mathbf{0}$ on the rest. Thus, subject to one of these choices, the integration by parts formula (12.10) reduces to

$$\langle \nabla u, \mathbf{v} \rangle = \langle u, -\nabla \cdot \mathbf{v} \rangle,\tag{12.11}$$

which suffices to establish the adjoint formula (12.7).

Remark: Adopting more general weighted inner products results in a more general elliptic boundary value problem. See Exercise 12.1.9 for details.

According to Theorem 9.20, the self-adjoint formulation (12.6) automatically implies positive semi-definiteness of the boundary value problem, with positive definiteness if $\ker \nabla = \{0\}$. Since, on a connected domain, only constant functions are annihilated by the gradient operator — see Lemma 6.16, which also applies to three-dimensional domains — both the Dirichlet and mixed boundary value problems are positive definite, while the Neumann boundary value problem is only positive semi-definite.

Finally, in the positive definite cases, Theorem 9.26 implies that the solution can be characterized by the three-dimensional version of the Dirichlet minimization principle (9.82).

Theorem 12.2. *The solution $u(x, y, z)$ to the Poisson equation (12.2) subject to homogeneous Dirichlet or mixed boundary conditions (12.3) is the unique function that minimizes the Dirichlet integral*

$$\frac{1}{2} \|\| \nabla u \|\|^2 - \langle u, f \rangle = \iiint_{\Omega} \left[\frac{1}{2} (u_x^2 + u_y^2 + u_z^2) - fu \right] dx dy dz \quad (12.12)$$

among all C^2 functions that satisfy the prescribed boundary conditions.

As in the two-dimensional version discussed in Chapter 9, the Dirichlet minimization principle continues to hold in the case of the inhomogeneous Dirichlet boundary value problem. Modifications for the inhomogeneous mixed boundary value problem appear in Exercise 12.1.13.

Exercises

- 12.1.1. Find bases for the following: (a) the space of harmonic polynomials $u(x, y, z)$ of degree ≤ 2 ; (b) the space of homogeneous cubic harmonic polynomials $u(x, y, z)$.
- 12.1.2. *True or false:* (a) Every harmonic polynomial is homogeneous.
(b) Every homogeneous polynomial is harmonic.
- 12.1.3. Solve the Poisson boundary value problem $-\Delta u = 1$ on the unit ball $x^2 + y^2 + z^2 < 1$ with homogeneous Dirichlet boundary conditions. *Hint:* Look for a polynomial solution.
- ◇ 12.1.4. Prove that if $u(x, y, z)$ solves the Laplace equation, then so does the translated function $U(x, y, z) = u(x - a, y - b, z - c)$ for constants a, b, c .
- ◇ 12.1.5. (a) Prove that if $u(x, y, z)$ solves Laplace's equation, so does the rescaled function $U(x, y, z) = u(\lambda x, \lambda y, \lambda z)$ for any constant λ . (b) More generally, show that $U(x, y, z) = \mu u(\lambda x, \lambda y, \lambda z) + c$ solves Laplace's equation for any constants λ, μ, c .
- ◇ 12.1.6. Let A be a constant nonsingular 3×3 matrix, $u(\mathbf{x})$ a C^1 scalar field, and $\mathbf{v}(\mathbf{x})$ a C^1 vector field. Set $U(\mathbf{x}) = u(A\mathbf{x})$ and $\mathbf{V}(\mathbf{x}) = \mathbf{v}(A\mathbf{x})$. Prove that
(a) $\nabla U(\mathbf{x}) = A^T \nabla u(A\mathbf{x})$, (b) $\nabla \cdot \mathbf{V}(\mathbf{x}) = w(A\mathbf{x})$, where $w(\mathbf{x}) = \nabla \cdot (A\mathbf{v})(\mathbf{x})$.
- ◇ 12.1.7. Prove that every rotation and reflection is a symmetry of the Laplace equation. In other words, if Q is any 3×3 orthogonal matrix, so $Q^T Q = I$, and $u(\mathbf{x})$ is a harmonic function, then so is $U(\mathbf{x}) = u(Q\mathbf{x})$. *Hint:* Use Exercise 12.1.6.

- ◇ 12.1.8. *The Weak Maximum Principle:* Let $\Omega \subset \mathbb{R}^2$ be a bounded domain. Let $u(x, y, z)$ solve the Poisson equation $-\Delta u = f(x, y, z)$, where $f(x, y, z) < 0$ for all $(x, y, z) \in \Omega$.
- (a) Prove that the maximum value of u occurs on the boundary $\partial\Omega$.
Hint: Explain why u cannot have a local maximum at any interior point in Ω .
- (b) Generalize your result to the case $f(x, y, z) \leq 0$.
Hint: Look at $v_\varepsilon(x, y, z) = u(x, y, z) + \varepsilon(x^2 + y^2 + z^2)$ and let $\varepsilon \rightarrow 0^+$.

- ◇ 12.1.9. Find the equilibrium equations corresponding to minimizing $\|\nabla u\|^2$ subject to homogeneous Dirichlet boundary conditions, where the indicated norm is based on the weighted inner product

$$\langle\langle \mathbf{v}, \mathbf{w} \rangle\rangle = \iiint_{\Omega} \mathbf{v}(x, y, z) \cdot \mathbf{w}(x, y, z) \sigma(x, y, z) dx dy dz,$$

with $\sigma(x, y, z) > 0$ a positive scalar function.

- ◇ 12.1.10. Prove the following vector calculus identities:

$$(a) \nabla \cdot (u \mathbf{v}) = \nabla u \cdot \mathbf{v} + u \nabla \cdot \mathbf{v}, \quad (b) \nabla \times (u \mathbf{v}) = \nabla u \times \mathbf{v} + u \nabla \times \mathbf{v},$$

$$(c) \nabla \cdot (\mathbf{v} \times \mathbf{w}) = (\nabla \times \mathbf{v}) \cdot \mathbf{w} - \mathbf{v} \cdot (\nabla \times \mathbf{w}), \quad (d) \nabla \times (\nabla \times \mathbf{v}) = \nabla(\nabla \cdot \mathbf{v}) - \Delta \mathbf{v}.$$

(In the final term, the Laplacian Δ acts component-wise on the vector field \mathbf{v} .)

- ◇ 12.1.11. Let Ω be a bounded domain with piecewise smooth boundary $\partial\Omega$. Prove the following

identities: (a) $\iiint_{\Omega} \Delta u dx dy dz = \iint_{\partial\Omega} \frac{\partial u}{\partial \mathbf{n}} dS,$

(b) $\iiint_{\Omega} u \Delta u dx dy dz = \iint_{\partial\Omega} u \frac{\partial u}{\partial \mathbf{n}} dS - \iiint_{\Omega} \|\nabla u\|^2 dx dy dz.$

- 12.1.12. Suppose the inhomogeneous Neumann boundary value problem (12.1, 4) has a solution.

(a) Prove that $\iint_{\partial\Omega} k dS = 0$. (b) Is the solution unique? If not, what is the most general solution? (c) State and prove an analogous result for the inhomogeneous Poisson equation $-\Delta u = f(x, y, z)$. (d) Provide a physical explanation for your answers.

- ◇ 12.1.13. Find a minimization principle that characterizes the solution to the inhomogeneous mixed boundary value problem $-\Delta u = f$ on Ω , with $u = g$ on $D \subsetneq \partial\Omega$, and $\partial u / \partial \mathbf{n} = h$ on $N = \partial\Omega \setminus D$.

- ♡ 12.1.14. (a) Prove that, subject to suitable boundary conditions, the curl $\nabla \times$ defines a self-adjoint operator with respect to the L^2 inner product between vector fields. What kinds of boundary conditions do you need to impose for your integration by parts argument to be valid? *Hint:* Use the identity in Exercise 12.1.10(c). (b) What operator on vector fields is given by the self-adjoint composition $S = (\nabla \times)^* \circ (\nabla \times)$? (c) Choose a set of homogeneous boundary conditions that make S self-adjoint. Is the resulting boundary value problem $S[\mathbf{v}] = \mathbf{f}$ positive definite? If not, what does the Fredholm Alternative say about its solvability?

12.2 Separation of Variables for the Laplace Equation

In this section, we revisit the method of separation of variables in the context of the three-dimensional Laplace equation. As always, its applicability is unfortunately restricted to rather special, but important, geometric configurations, the simplest being rectangular, cylindrical, and spherical domains. Since the first two are straightforward extensions of their two-dimensional counterparts, we will discuss only spherically separable solutions in any detail.

The simplest domain to which the separation of variables method applies is a rectan-

gular box:

$$B = \{0 < x < a, 0 < y < b, 0 < z < c\}.$$

For functions of three variables, one begins the separation process by splitting off one of them, by setting $u(x, y, z) = v(x)w(y, z)$, say. The function $v(x)$ satisfies a simple second-order ordinary differential equation, while $w(y, z)$ solves the two-dimensional Helmholtz equation (11.21), which is further separated by writing $w(y, z) = p(y)q(z)$. The resulting fully separated solutions $u(x, y, z) = v(x)p(y)q(z)$ are (mostly) products of trigonometric and hyperbolic functions. Implementation of the technique and analysis of the resulting series solutions are relegated to Exercise 12.2.34.

In the case that the domain is a cylinder, one passes to *cylindrical coordinates* r, θ, z , where

$$x = r \cos \theta, \quad y = r \sin \theta, \quad z = z, \quad (12.13)$$

to effect the separation. Writing $u(r, \theta, z) = v(r, \theta)w(z)$, one finds that $w(z)$ satisfies a simple second-order ordinary differential equation, while $v(r, \theta)$ solves the two-dimensional polar Helmholtz equation (11.51) on a disk. Applying a further separation to $v(r, \theta)$, as in Chapter 11, produces fully separable solutions $u(r, \theta, z) = p(r)q(\theta)w(z)$ as products of Bessel functions of the cylindrical radius r , trigonometric functions of the polar angle θ , and hyperbolic functions of z ; see Exercise 12.2.40.

The most interesting case is that of spherical coordinates, which we proceed to analyze in detail in the following subsection.

Remark: These are just three of the many coordinate systems in which the three-dimensional Laplace equation separates. See [78, 79] for 37 additional exotic types, including ellipsoidal, toroidal, and parabolic spheroidal coordinates. The resulting separable solutions are written in terms of new classes of special functions that solve interesting second-order ordinary differential equations, all of Sturm–Liouville form (9.71).

Laplace's Equation in a Ball

Suppose a solid ball (e.g., the Earth) is subject to a specified steady temperature distribution on its spherical boundary. Our task is to determine the equilibrium temperature within the ball. We assume that the body is composed of an isotropic, uniform medium and, to slightly simplify the analysis, choose units in which its radius equals 1.

To find the equilibrium temperature within the ball, we must solve the Dirichlet boundary value problem

$$\begin{aligned} \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} &= 0, & x^2 + y^2 + z^2 &< 1, \\ u(x, y, z) &= h(x, y, z), & x^2 + y^2 + z^2 &= 1, \end{aligned} \quad (12.14)$$

where h is prescribed on the bounding unit sphere. Problems in spherical geometries are most naturally analyzed in *spherical coordinates* r, φ, θ . Our convention is to set

$$x = r \sin \varphi \cos \theta, \quad y = r \sin \varphi \sin \theta, \quad z = r \cos \varphi, \quad (12.15)$$

where $-\pi < \theta \leq \pi$ is the *azimuthal angle* or *longitude*, while $0 \leq \varphi \leq \pi$ is the *zenith angle* or *latitude* on the sphere of radius $r = \sqrt{x^2 + y^2 + z^2}$. In other words, φ measures

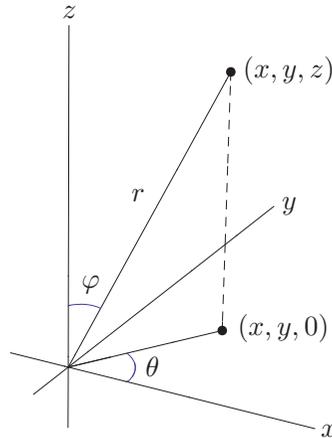


Figure 12.1. Spherical coordinates.

the angle between the vector $(x, y, z)^T$ and the positive z -axis, while θ measures the angle between its projection $(x, y, 0)^T$ on the (x, y) -plane and the positive x -axis; see [Figure 12.1](#). On Earth, longitude θ is measured from the Greenwich prime meridian, while latitude is measured from the equator, and so equals $\frac{1}{2}\pi - \varphi$ (although the everyday units are degrees, not radians), whereby φ is sometimes referred to as the “co-latitude”.

Warning: In many books, particularly those in physics, the roles of θ and φ are *reversed*, leading to much confusion when one is perusing the literature. We prefer the mathematical convention, since the azimuthal angle θ coincides with the cylindrical angle coordinate — as well as the polar coordinate on the (x, y) -plane — thus avoiding unnecessary confusion when going from one coordinate system to the other. You must be attentive to the convention being used when consulting any reference!

In spherical coordinates, the Laplace equation for $u(r, \varphi, \theta)$ takes the form

$$\Delta u = \frac{\partial^2 u}{\partial r^2} + \frac{2}{r} \frac{\partial u}{\partial r} + \frac{1}{r^2} \frac{\partial^2 u}{\partial \varphi^2} + \frac{\cos \varphi}{r^2 \sin \varphi} \frac{\partial u}{\partial \varphi} + \frac{1}{r^2 \sin^2 \varphi} \frac{\partial^2 u}{\partial \theta^2} = 0. \quad (12.16)$$

This important formula is the final result of a fairly nasty chain rule computation, whose details are left to the motivated reader. (Set aside lots of paper and keep an eraser handy!)

To construct separable solutions to the spherical coordinate form (12.16) of the Laplace equation, we begin by separating off the radial part of the solution, setting

$$u(r, \varphi, \theta) = v(r) w(\varphi, \theta). \quad (12.17)$$

Substituting this ansatz into (12.16), multiplying the resulting equation through by $\frac{r^2}{vw}$, and then placing all the terms involving r on one side yields

$$\frac{1}{v} \left(r^2 \frac{d^2 v}{dr^2} + 2r \frac{dv}{dr} \right) = -\frac{1}{w} \Delta_S[w], \quad (12.18)$$

where

$$\Delta_S[w] = \frac{\partial^2 w}{\partial \varphi^2} + \frac{\cos \varphi}{\sin \varphi} \frac{\partial w}{\partial \varphi} + \frac{1}{\sin^2 \varphi} \frac{\partial^2 w}{\partial \theta^2}. \quad (12.19)$$

The second-order differential operator Δ_S , which involves only the angular components of the full Laplacian operator Δ , is of particular significance. It is known as the *spherical Laplacian*, and governs the equilibrium and dynamics of thin spherical shells — see Example 12.15 below.

Returning to equation (12.18), our usual separation argument applies. The left-hand side depends only on r , while the right-hand side depends only on the angles φ, θ . This can occur only when both sides are equal to a common separation constant, which we denote by μ . As a consequence, the radial component $v(r)$ satisfies the ordinary differential equation

$$r^2 v'' + 2r v' - \mu v = 0, \quad (12.20)$$

which is of Euler type (11.89), and hence can be readily solved. However, let us put this equation aside for the time being, and concentrate our efforts on the more complicated angular components.

The second equation in (12.18) assumes the form

$$\Delta_S[w] + \mu w = \frac{\partial^2 w}{\partial \varphi^2} + \frac{\cos \varphi}{\sin \varphi} \frac{\partial w}{\partial \varphi} + \frac{1}{\sin^2 \varphi} \frac{\partial^2 w}{\partial \theta^2} + \mu w = 0. \quad (12.21)$$

This second-order partial differential equation can be regarded as the eigenvalue equation for the spherical Laplacian operator Δ_S and is known as the *spherical Helmholtz equation*. To find explicit solutions, we adopt a further separation of angular variables,

$$w(\varphi, \theta) = p(\varphi) q(\theta), \quad (12.22)$$

which we substitute into (12.21). Dividing the result by the product $w = pq$, multiplying by $\sin^2 \varphi$, and then rearranging terms, we are led to the separated system

$$\frac{1}{p} \left(\sin^2 \varphi \frac{d^2 p}{d\varphi^2} + \cos \varphi \sin \varphi \frac{dp}{d\varphi} \right) + \mu \sin^2 \varphi = -\frac{1}{q} \frac{d^2 q}{d\theta^2} = \nu,$$

where, by our usual argument, ν is another separation constant. The spherical Helmholtz equation thereby splits into a pair of ordinary differential equations

$$\sin^2 \varphi \frac{d^2 p}{d\varphi^2} + \cos \varphi \sin \varphi \frac{dp}{d\varphi} + (\mu \sin^2 \varphi - \nu) p = 0, \quad \frac{d^2 q}{d\theta^2} + \nu q = 0.$$

The equation for $q(\theta)$ is easy to solve. As one circumnavigates the sphere, the azimuthal angle θ increases from $-\pi$ to π , so $q(\theta)$ must be a 2π -periodic function. Thus, $q(\theta)$ solves the well-studied periodic boundary value problem treated, for instance, in (4.109). Up to a constant multiple, nonzero periodic solutions occur only when the separation constant assumes one of the values $\nu = m^2$, where $m = 0, 1, 2, \dots$ is an integer, with

$$q(\theta) = \cos m\theta \quad \text{or} \quad \sin m\theta, \quad m = 0, 1, 2, \dots \quad (12.23)$$

Each positive $\nu = m^2 > 0$ admits two linearly independent 2π -periodic solutions, while when $\nu = 0$, only the constant solutions are periodic.

The Legendre Equation and Ferrers Functions

With this information, we endeavor to solve the zenith differential equation

$$\sin^2 \varphi \frac{d^2 p}{d\varphi^2} + \cos \varphi \sin \varphi \frac{dp}{d\varphi} + (\mu \sin^2 \varphi - m^2) p = 0. \quad (12.24)$$

This is not so easy, and constructing analytic formulas for its solutions requires some ingenuity. The motivation behind the following steps may not be so apparent; indeed, they are the culmination of a long, detailed study of this important differential equation by mathematicians over the last 200 years.

As an initial simplification, let us get rid of the trigonometric functions, by invoking the change of variables

$$t = \cos \varphi, \quad \text{with} \quad p(\varphi) = P(\cos \varphi) = P(t). \quad (12.25)$$

Since

$$0 \leq \varphi \leq \pi, \quad \text{we have} \quad 0 \leq \sqrt{1-t^2} = \sin \varphi \leq 1.$$

According to the chain rule,

$$\begin{aligned} \frac{dp}{d\varphi} &= \frac{dP}{dt} \frac{dt}{d\varphi} = -\sin \varphi \frac{dP}{dt} = -\sqrt{1-t^2} \frac{dP}{dt}, \\ \frac{d^2p}{d\varphi^2} &= -\sin \varphi \frac{d}{dt} \left(-\sqrt{1-t^2} \frac{dP}{dt} \right) = (1-t^2) \frac{d^2P}{dt^2} - t \frac{dP}{dt}. \end{aligned}$$

Substituting these expressions into (12.24), we conclude that $P(t)$ must satisfy

$$(1-t^2)^2 \frac{d^2P}{dt^2} - 2t(1-t^2) \frac{dP}{dt} + [\mu(1-t^2) - m^2] P = 0. \quad (12.26)$$

Unfortunately, the resulting differential equation is still not elementary, but at least its coefficients are polynomials. It is known as the *Legendre differential equation* of order m , having first been employed by Adrien-Marie Legendre to study the gravitational attraction of *ellipsoidal* bodies. In the cases of interest to us, the order parameter m is an integer, while the separation constant μ plays the role of an eigenvalue.

Power series solutions to the Legendre equation can be constructed by the standard techniques presented in Section 11.3. The most general solution is a new type of special function, called a *Legendre function*, [86]. However, it turns out that the solutions we are actually interested in can all be written in terms of elementary algebraic functions. First of all, since $t = \cos \varphi$, the solution only needs to be defined on the interval $-1 \leq t \leq 1$, the so-called *cut locus*. The endpoints of the cut locus, $t = 1$ and $t = -1$, correspond to the sphere's north pole, $\varphi = 0$, and south pole, $\varphi = \pi$, respectively. Both endpoints are singular points for the Legendre equation, since the coefficient $(1-t^2)^2$ of the leading-order derivative vanishes when $t = \pm 1$. In fact, both are regular singular points, as you are asked to show in Exercise 12.2.11. Since ultimately we need the separable solution (12.17) to be a well-defined function of x, y, z (even at points where the spherical coordinates degenerate, i.e., on the z -axis), we need $p(\varphi)$ to be well defined at $\varphi = 0$ and π , and this requires $P(t)$ to be bounded at the singular points:

$$|P(-1)| < \infty, \quad |P(+1)| < \infty. \quad (12.27)$$

Let us begin our analysis with the Legendre equation of order $m = 0$

$$(1-t^2) \frac{d^2P}{dt^2} - 2t \frac{dP}{dt} + \mu P = 0. \quad (12.28)$$

In this case, the eigenfunctions, i.e., solutions to the Legendre boundary value problem (12.27–28), are the *Legendre polynomials*

$$P_n(t) = \frac{(-1)^n}{2^n n!} \frac{d^n}{dt^n} (1-t^2)^n, \quad (12.29)$$

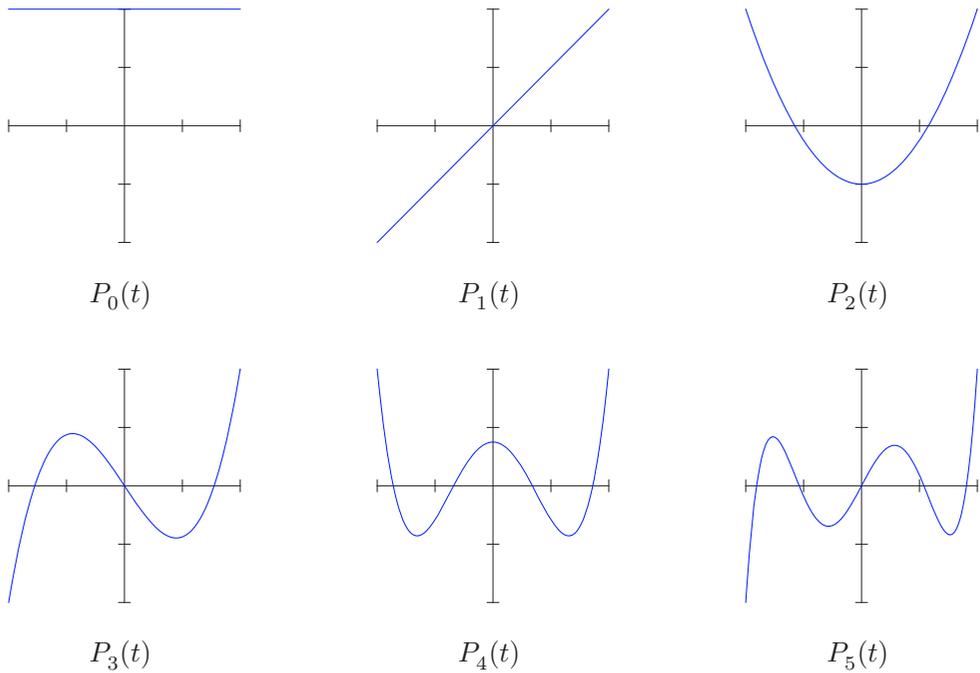


Figure 12.2. Legendre polynomials.

with corresponding eigenvalue parameter $\mu = n(n+1)$. (The initial factor is by common convention, [86]; see (12.64) for the explicit formula.) The first few are

$$\begin{aligned}
 P_0(t) &= 1, & P_1(t) &= t, & P_2(t) &= \frac{3}{2}t^2 - \frac{1}{2}, & P_3(t) &= \frac{5}{2}t^3 - \frac{3}{2}t, \\
 P_4(t) &= \frac{35}{8}t^4 - \frac{15}{4}t^2 + \frac{3}{8}, & P_5(t) &= \frac{63}{8}t^5 - \frac{35}{4}t^3 + \frac{15}{8}t,
 \end{aligned}$$

and are graphed in [Figure 12.2](#).

Each Legendre polynomial clearly satisfies the boundary conditions (12.27). To verify that they are indeed solutions to the differential equation (12.28), we set

$$Q_n(t) = (1 - t^2)^n.$$

By the chain rule, the derivative of $Q_n(t)$ is

$$Q'_n = -2nt(1 - t^2)^{n-1}, \quad \text{and hence} \quad (1 - t^2)Q'_n = -2nt(1 - t^2)^n = -2ntQ_n.$$

Differentiating the latter formula yields

$$(1 - t^2)Q''_n - 2tQ'_n = -2ntQ'_n - 2nQ_n, \quad \text{or} \quad (1 - t^2)Q''_n = -2(n-1)tQ'_n - 2nQ_n.$$

A simple induction proves that the k^{th} order derivative $Q_n^{(k)}(t) = \frac{d^k Q_n}{dt^k}$ satisfies

$$\begin{aligned}
 (1 - t^2)Q_n^{(k+2)} &= -2(n-k-1)tQ_n^{(k+1)} - 2[n + (n-1) + \cdots + (n-k)]Q_n^{(k)} \\
 &= -2(n-k-1)tQ_n^{(k+1)} - (k+1)(2n-k)Q_n^{(k)}.
 \end{aligned} \tag{12.30}$$

In particular, when $k = n$, this reduces to

$$(1 - t^2)Q_n^{(n+2)} = 2tQ_n^{(n+1)} - n(n + 1)Q_n^{(n)} = 0,$$

and so $\widehat{P}_n(t) = Q_n^{(n)}(t)$ satisfies

$$(1 - t^2)\widehat{P}_n'' - 2t\widehat{P}_n' + n(n + 1)\widehat{P}_n = 0,$$

which is precisely the order 0 Legendre equation (12.28) with $\mu = n(n + 1)$. The Legendre polynomial P_n is a constant multiple of \widehat{P}_n , and hence it too satisfies the order 0 Legendre equation. According to Theorem 12.3 below, the Legendre polynomials form a complete system of eigenfunctions for the order 0 Legendre boundary value problem.

When the order $m > 0$, the eigenfunctions of the Legendre boundary value problem (12.26–27) are not always polynomials. They are known as the *Ferrers functions*, named after the nineteenth-century British mathematician Norman Ferrers, or, more generally, as *associated Legendre functions*. They have the explicit formula[†]

$$\begin{aligned} P_n^m(t) &= (1 - t^2)^{m/2} \frac{d^m}{dt^m} P_n(t) \\ &= (-1)^n \frac{(1 - t^2)^{m/2}}{2^n n!} \frac{d^{n+m}}{dt^{n+m}} (1 - t^2)^n, \end{aligned} \quad n = m, m + 1, \dots, \quad (12.31)$$

which generalizes the formula (12.29) for the Legendre polynomials. The eigenvalue parameter for $P_n^m(t)$ is also $\mu = n(n + 1)$. In particular $P_n^0(t) = P_n(t)$. Here is a list of the first few Ferrers functions, which, for completeness, includes Legendre polynomials:

$$\begin{aligned} P_0^0(t) &= 1, & P_1^0(t) &= t, & P_1^1(t) &= \sqrt{1 - t^2}, \\ P_2^0(t) &= -\frac{1}{2} + \frac{3}{2}t^2, & P_2^1(t) &= 3t\sqrt{1 - t^2}, & P_2^2(t) &= 3(1 - t^2), \\ P_3^0(t) &= -\frac{3}{2}t + \frac{5}{2}t^3, & P_3^1(t) &= \left(-\frac{3}{2} + \frac{15}{2}t^2\right)\sqrt{1 - t^2}, \\ P_3^2(t) &= 15t(1 - t^2), & P_3^3(t) &= 15(1 - t^2)^{3/2}, \\ P_4^0(t) &= \frac{3}{8} - \frac{15}{4}t^2 + \frac{35}{8}t^4, & P_4^1(t) &= \left(-\frac{15}{2}t + \frac{35}{2}t^3\right)\sqrt{1 - t^2}, \\ P_4^2(t) &= \left(-\frac{15}{2} + \frac{105}{2}t^2\right)(1 - t^2), & P_4^3(t) &= 105t(1 - t^2)^{3/2}, & P_4^4(t) &= 105(1 - t^2)^2. \end{aligned} \quad (12.32)$$

When $m = 2k \leq n$ is an even integer, $P_n^m(t)$ is a polynomial function, while when $m = 2k + 1 \leq n$ is odd, there is an extra factor of $\sqrt{1 - t^2}$. Keep in mind that the square root is real and positive, since we are restricting our attention to the interval $-1 \leq t \leq 1$. If $m > n$, formula (12.31) reduces to the zero function and so is not included in the final tally.

Warning: Even though half of the Ferrers functions are polynomials, only those with $m = 0$, i.e., $P_n(t) = P_n^0(t)$, are called *Legendre polynomials*.

[†] *Warning:* Some authors include a $(-1)^m$ factor in the formula, resulting in the opposite sign when m is odd. Another source of confusion is that many tables define the associated Legendre functions using the alternative initial factor $(t^2 - 1)^{m/2}$. But this is unsuitable, since we are solely interested in values of t lying in the interval $-1 \leq t \leq 1$, and this convention would result in a complex-valued function when m is odd. Following [86], we use the term “Ferrers function” to refer to the restriction of the associated Legendre function to the cut locus $-1 \leq t \leq 1$.

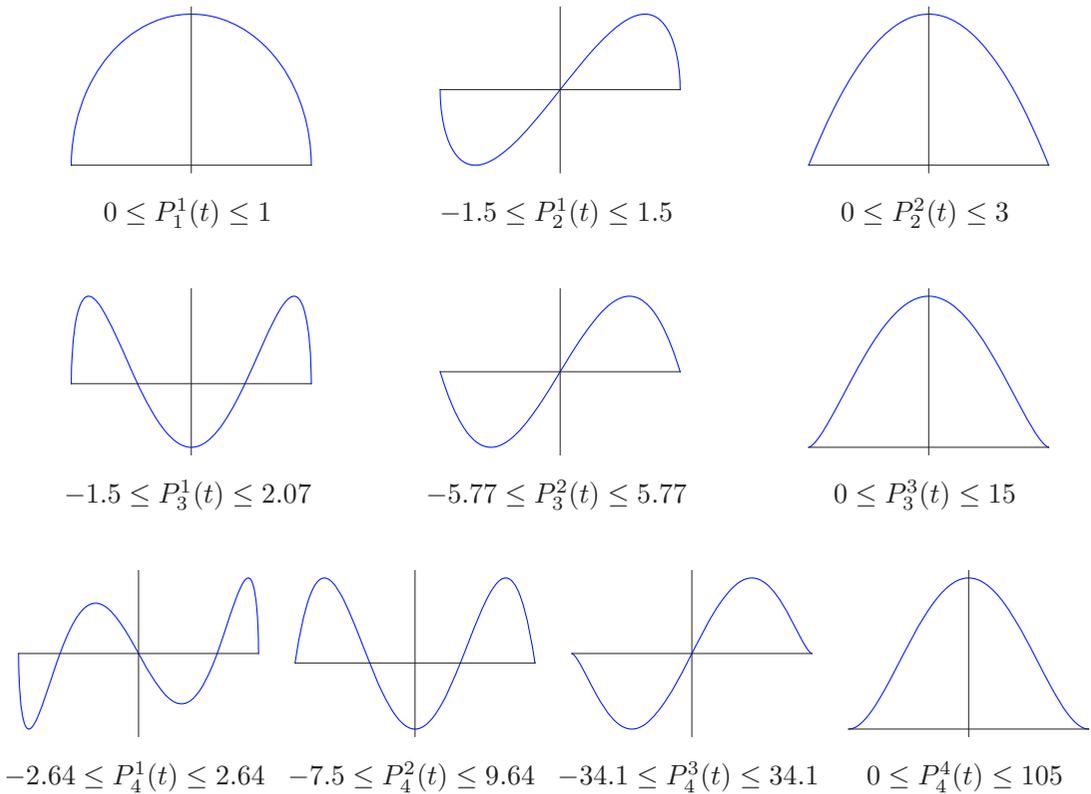


Figure 12.3. Ferrers functions.

Figure 12.3 displays graphs of the Ferrers functions $P_n^m(t)$ for $1 \leq m \leq n \leq 4$. Pay particular attention to the fact that, owing to the choice of normalization factor, the graphs have very different vertical scales, as indicated by their minimum and maximum values (rounded to two decimal places) written below each — although one always has the freedom to rescale the eigenfunctions as desired, e.g., so as to be orthonormal.

To show that the Ferrers functions $P_n^m(t)$ satisfy the Legendre differential equation (12.26) of order m , we substitute $k = m + n$ in (12.30):

$$(1 - t^2) \frac{d^2 R_n^m}{dt^2} - 2(m + 1)t \frac{dR_n^m}{dt} + (m + n + 1)(n - m) R_n^m = 0, \quad (12.33)$$

where

$$R_n^m(t) = Q_n^{(m+n)}(t).$$

This is *not* the order m Legendre equation, but it can be converted into it by setting

$$R_n^m(t) = (1 - t^2)^{-m/2} S_n^m(t).$$

Differentiating, we obtain

$$\begin{aligned}\frac{dR_n^m}{dt} &= (1-t^2)^{-m/2} \frac{dS_n^m}{dt} - mt(1-t^2)^{-m/2-1} S_n^m, \\ \frac{d^2 R_n^m}{dt^2} &= (1-t^2)^{-m/2} \frac{d^2 S_n^m}{dt^2} - 2mt(1-t^2)^{-m/2-1} \frac{dS_n^m}{dt} \\ &\quad + [m + m(m+1)t^2] (1-t^2)^{-m/2-2} S_n^m.\end{aligned}$$

Therefore, after a little algebra, equation (12.33) takes the alternative form

$$\begin{aligned}(1-t^2)^{-m/2+1} \frac{d^2 S_n^m}{dt^2} - 2t(1-t^2)^{-m/2} \frac{dS_n^m}{dt} \\ + [n(n+1)(1-t^2) - m^2] (1-t^2)^{-m/2-1} S_n^m = 0,\end{aligned}$$

which, when multiplied by $(1-t^2)^{m/2+1}$, is precisely the order m Legendre equation (12.26) with $\mu = n(n+1)$. Thus,

$$S_n^m(t) = (1-t^2)^{m/2} R_n^m(t) = (1-t^2)^{m/2} \frac{d^{n+m}}{dt^{n+m}} (1-t^2)^n,$$

which is a constant multiple of the Ferrers function $P_n^m(t)$, is a solution to the order m Legendre equation. Moreover, we note that

$$P_n^m(1) = P_n^m(-1) = 0, \quad \text{when } m > 0, \quad (12.34)$$

and we conclude that $P_n^m(t)$ is an eigenfunction for the order m Legendre boundary value problem.

The following result states that the Ferrers functions provide a complete list of solutions to the Legendre boundary value problem (12.26–27).

Theorem 12.3. *Let $m \geq 0$ be a nonnegative integer. Then the order m Legendre boundary value problem prescribed by (12.26–27) has eigenvalues $\mu_n = n(n+1)$ for $n = 0, 1, 2, \dots$, and associated eigenfunctions $P_n^m(t)$, where $m = 0, \dots, n$. Moreover, the Ferrers eigenfunctions form a complete orthogonal system relative to the L^2 inner product on the cut locus $[-1, 1]$.*

Returning to the zenith variable φ via (12.25), Theorem 12.3 implies that our original boundary value problem

$$\sin^2 \varphi \frac{d^2 p}{d\varphi^2} + \cos \varphi \sin \varphi \frac{dp}{d\varphi} + (\mu \sin^2 \varphi - m^2) p = 0, \quad |p(0)|, |p(\pi)| < \infty, \quad (12.35)$$

has its eigenvalues and eigenfunctions expressed in terms of the Ferrers functions:

$$\mu_n = n(n+1), \quad p_n^m(\varphi) = P_n^m(\cos \varphi), \quad \text{for } 0 \leq m \leq n. \quad (12.36)$$

Since $P_n^m(t)$ is either a polynomial or a polynomial multiplied by a power of $\sqrt{1-t^2}$, the eigenfunction $p_n^m(\varphi)$ is a trigonometric polynomial of degree n , which we call a *trigono-*

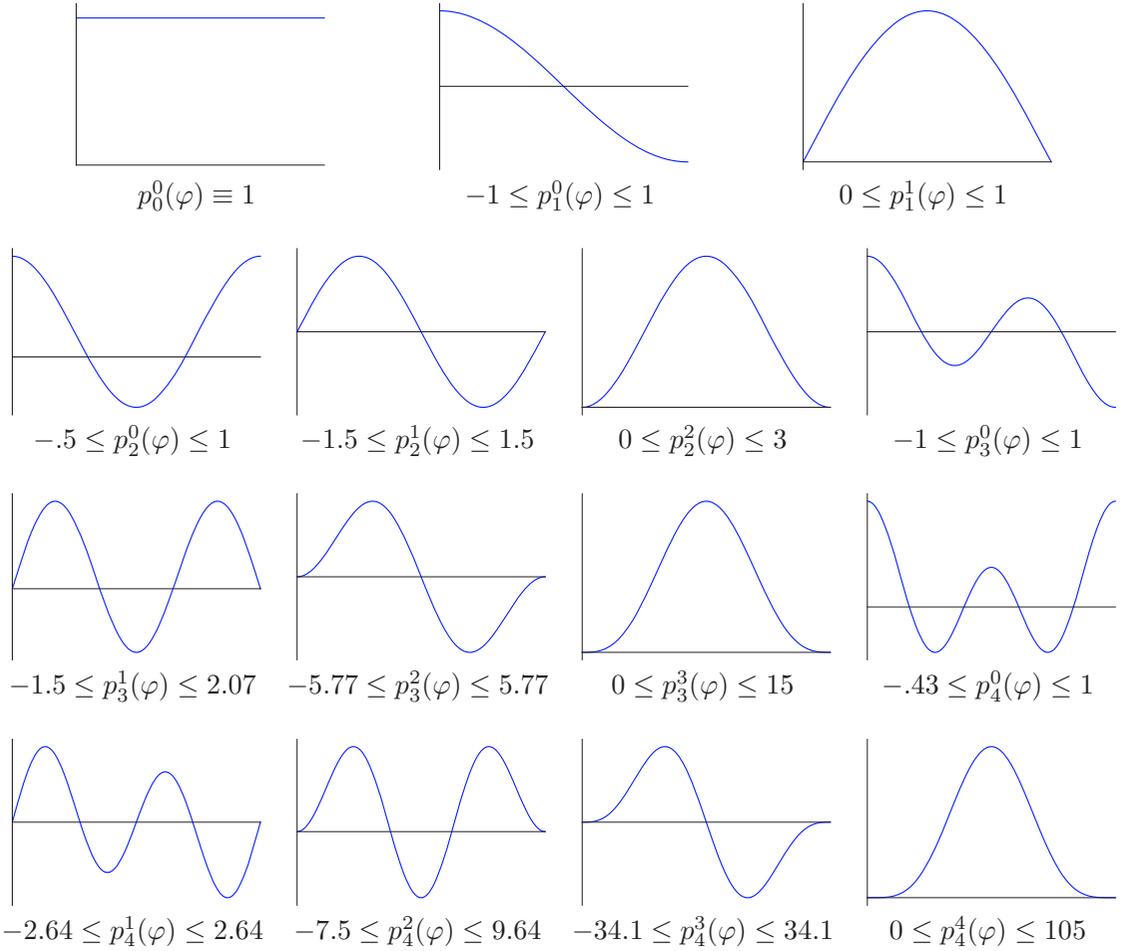


Figure 12.4. Trigonometric Ferrers functions.

metric Ferrers function. Here are the first few, written in Fourier form, as in (3.38):

$$\begin{aligned}
 p_0^0(\varphi) &= 1, & p_1^0(\varphi) &= \cos \varphi, & p_1^1(\varphi) &= \sin \varphi, \\
 p_2^0(\varphi) &= \frac{1}{4} + \frac{3}{4} \cos 2\varphi, & p_2^1(\varphi) &= \frac{3}{2} \sin 2\varphi, & p_2^2(\varphi) &= \frac{3}{2} - \frac{3}{2} \cos 2\varphi, \\
 p_3^0(\varphi) &= \frac{3}{8} \cos \varphi + \frac{5}{8} \cos 3\varphi, & p_3^1(\varphi) &= \frac{3}{8} \sin \varphi + \frac{15}{8} \sin 3\varphi, \\
 p_3^2(\varphi) &= \frac{15}{4} \cos \varphi - \frac{15}{4} \cos 3\varphi, & p_3^3(\varphi) &= \frac{45}{4} \sin \varphi - \frac{15}{4} \sin 3\varphi, & & (12.37) \\
 p_4^0(\varphi) &= \frac{9}{64} + \frac{5}{16} \cos 2\varphi + \frac{35}{64} \cos 4\varphi, & p_4^1(\varphi) &= \frac{5}{8} \sin 2\varphi + \frac{35}{16} \sin 4\varphi, \\
 p_4^2(\varphi) &= \frac{45}{16} + \frac{15}{4} \cos 2\varphi - \frac{105}{16} \cos 4\varphi, & p_4^3(\varphi) &= \frac{105}{4} \sin 2\varphi - \frac{105}{8} \sin 4\varphi, \\
 p_4^4(\varphi) &= \frac{315}{8} - \frac{105}{2} \cos 2\varphi + \frac{105}{8} \cos 4\varphi.
 \end{aligned}$$

It is also instructive to plot the eigenfunctions in terms of the zenith angle φ ; see Figure 12.4. As in Figure 12.3, the vertical scales are not the same, as indicated by the listed minimum and maximum values.

Spherical Harmonics

At this stage, we have determined both angular components of our separable solutions (12.22). Multiplying the two parts together results in the spherical angle functions

$$\begin{aligned} Y_n^m(\varphi, \theta) &= p_n^m(\varphi) \cos m\theta, & n &= 0, 1, 2, \dots, \\ \tilde{Y}_n^m(\varphi, \theta) &= p_n^m(\varphi) \sin m\theta, & m &= 0, 1, \dots, n, \end{aligned} \quad (12.38)$$

known as *spherical harmonics*. They satisfy the *spherical Helmholtz equation*

$$\Delta_S Y_n^m + n(n+1)Y_n^m = 0 = \Delta_S \tilde{Y}_n^m + n(n+1)\tilde{Y}_n^m, \quad (12.39)$$

and so are eigenfunctions for the spherical Laplacian operator, (12.19), with associated eigenvalues $\mu_n = n(n+1)$ for $n = 0, 1, 2, \dots$. The n^{th} eigenvalue μ_n admits a $(2n+1)$ -dimensional eigenspace, spanned by the spherical harmonics

$$Y_n^0(\varphi, \theta), Y_n^1(\varphi, \theta), \dots, Y_n^n(\varphi, \theta), \tilde{Y}_n^1(\varphi, \theta), \dots, \tilde{Y}_n^n(\varphi, \theta).$$

(The omitted function $\tilde{Y}_n^0(\varphi, \theta) \equiv 0$ is trivial, and so does not contribute.) In [Figure 12.5](#) we plot the first few spherical harmonic surfaces $r = Y_n^m(\varphi, \theta)$. In these graphs, in view of the spherical coordinate formulae (12.15), points with a negative r coordinate appear on the opposite side of the origin from their positive r counterparts. Incidentally, the graphs of the other spherical harmonic surfaces $r = \tilde{Y}_n^m(\varphi, \theta)$, when $m > 0$, are obtained by rotation around the z -axis by 90° ; see [Exercise 12.2.20](#). On the other hand, the graphs of Y_n^0 are cylindrically symmetric (why?), and hence unaffected by such a rotation.

Self-adjointness of the spherical Laplacian, as per [Exercise 12.2.21](#), implies that the spherical harmonics are orthogonal with respect to the L^2 inner product

$$\langle f, g \rangle = \iint_{S_1} f g \, dS = \int_{-\pi}^{\pi} \int_0^{\pi} f(\varphi, \theta) g(\varphi, \theta) \sin \varphi \, d\varphi \, d\theta \quad (12.40)$$

given by integrating the product of the functions with respect to the surface area element $dS = \sin \varphi \, d\varphi \, d\theta$ on the unit sphere $S_1 = \{\|\mathbf{x}\| = 1\}$. More correctly, self-adjointness only guarantees orthogonality of the harmonics corresponding to distinct eigenvalues: $\mu_n \neq \mu_l$. However, the orthogonality relations

$$\begin{aligned} \langle Y_n^m, Y_l^k \rangle &= \iint_{S_1} Y_n^m Y_l^k \, dS = 0, & \text{for } & (m, n) \neq (k, l), \\ \langle Y_n^m, \tilde{Y}_l^k \rangle &= \iint_{S_1} Y_n^m \tilde{Y}_l^k \, dS = 0, & \text{for all } & (m, n), (k, l), \\ \langle \tilde{Y}_n^m, \tilde{Y}_l^k \rangle &= \iint_{S_1} \tilde{Y}_n^m \tilde{Y}_l^k \, dS = 0, & \text{for } & (m, n) \neq (k, l), \end{aligned} \quad (12.41)$$

do, in fact, hold in full generality; [Exercise 12.2.22](#) asks you to supply the details. Moreover, their norms can be explicitly computed:

$$\|Y_n^0\|^2 = \frac{4\pi}{2n+1}, \quad \|Y_n^m\|^2 = \|\tilde{Y}_n^m\|^2 = \frac{2\pi(n+m)!}{(2n+1)(n-m)!}, \quad m = 1, \dots, n. \quad (12.42)$$

Proofs of the latter formulae are outlined in [Exercise 12.2.24](#).

With some further work, it can be shown that the spherical harmonics form a complete orthogonal system of functions on the unit sphere. This means that any reasonable (e.g.,

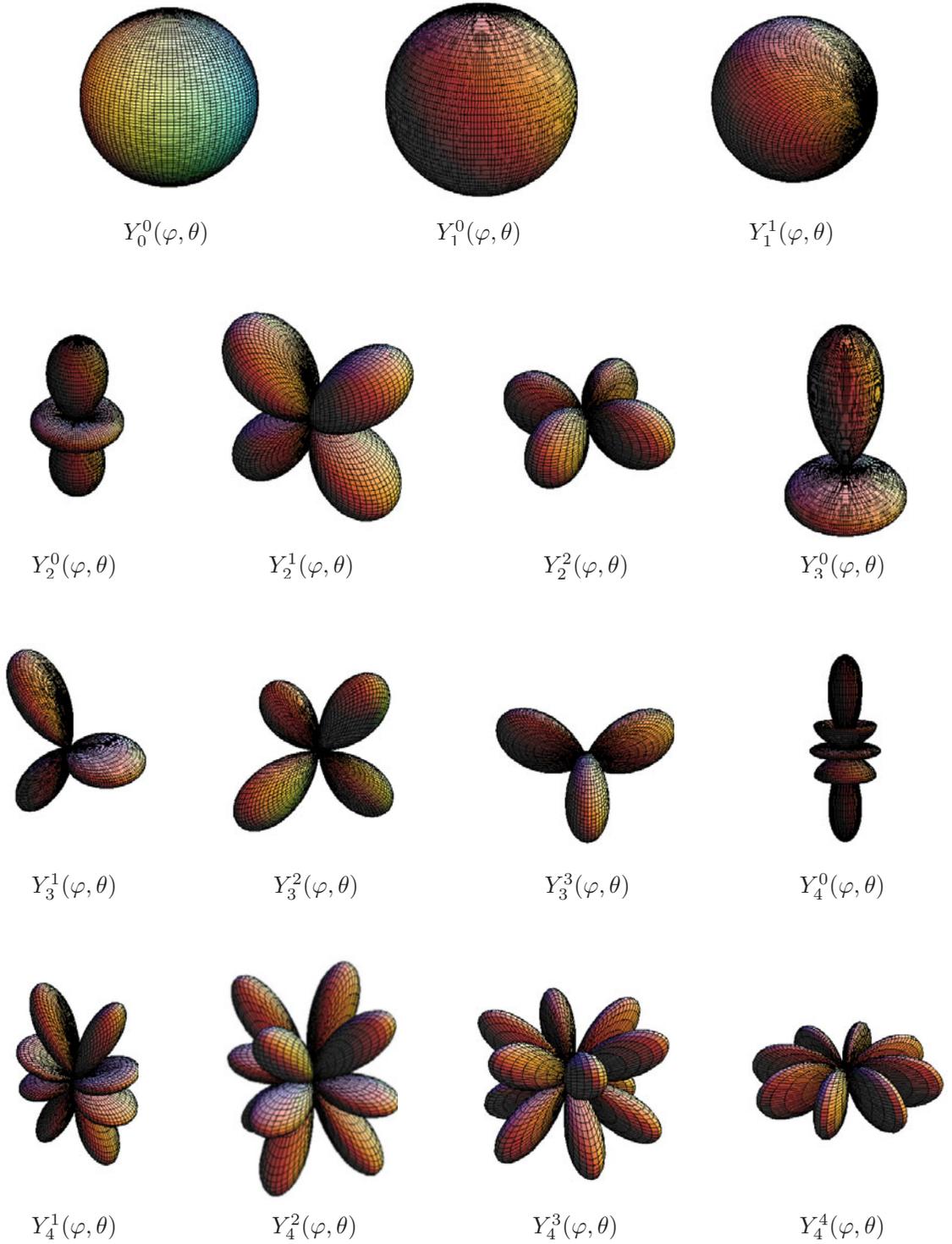


Figure 12.5. Spherical harmonics.

piecewise C^1 or even L^2) function $h: S_1 \rightarrow \mathbb{R}$, can be expanded into a convergent *spherical harmonic series*

$$h(\varphi, \theta) = \frac{c_{0,0}}{2} + \sum_{n=1}^{\infty} \left(\frac{c_{0,n}}{2} Y_n^0(\varphi) + \sum_{m=1}^n \left[c_{m,n} Y_n^m(\varphi, \theta) + \tilde{c}_{m,n} \tilde{Y}_n^m(\varphi, \theta) \right] \right). \quad (12.43)$$

Applying the orthogonality relations (12.41), we find that the spherical harmonic coefficients are given by the inner products

$$c_{0,n} = \frac{2 \langle h, Y_n^0 \rangle}{\|Y_n^0\|^2}, \quad c_{m,n} = \frac{\langle h, Y_n^m \rangle}{\|Y_n^m\|^2}, \quad \tilde{c}_{m,n} = \frac{\langle h, \tilde{Y}_n^m \rangle}{\|\tilde{Y}_n^m\|^2}, \quad \begin{array}{l} 0 \leq n, \\ 1 \leq m \leq n, \end{array}$$

or, explicitly, using (12.40) and the formulae (12.42) for the norms,

$$\begin{aligned} c_{m,n} &= \frac{(2n+1)(n-m)!}{2\pi(n+m)!} \int_{-\pi}^{\pi} \int_0^{\pi} h(\varphi, \theta) p_n^m(\varphi) \cos m\theta \sin \varphi \, d\varphi \, d\theta, \\ \tilde{c}_{m,n} &= \frac{(2n+1)(n-m)!}{2\pi(n+m)!} \int_{-\pi}^{\pi} \int_0^{\pi} h(\varphi, \theta) p_n^m(\varphi) \sin m\theta \sin \varphi \, d\varphi \, d\theta. \end{aligned} \quad (12.44)$$

As with an ordinary Fourier series, the extra $\frac{1}{2}$ was appended to the $c_{0,n}$ terms in (12.43) so that equations (12.44) remain valid for all values of m, n . In particular, the constant term in the spherical harmonic series is the mean of the function h over the unit sphere:

$$\frac{c_{0,0}}{2} = \frac{1}{4\pi} \iint_{S_1} h \, dS = \frac{1}{4\pi} \int_{-\pi}^{\pi} \int_0^{\pi} h(\varphi, \theta) \sin \varphi \, d\varphi \, d\theta. \quad (12.45)$$

Remark: Establishing uniform convergence of a spherical harmonic series (12.43) is more challenging than in the Fourier series case, because, unlike the trigonometric functions, the orthonormal spherical harmonics are not uniformly bounded. A recent survey of what is known in this regard can be found in [10].

Remark: An alternative approach is to replace the real trigonometric functions by complex exponentials, and work with the *complex spherical harmonics*[†]

$$\mathcal{Y}_n^m(\varphi, \theta) = Y_n^m(\varphi, \theta) + i \tilde{Y}_n^m(\varphi, \theta) = p_n^m(\varphi) e^{im\theta}, \quad \begin{array}{l} n = 0, 1, 2, \dots, \\ m = -n, -n+1, \dots, n. \end{array} \quad (12.46)$$

The associated orthogonality and expansion formulas are relegated to the exercises.

Harmonic Polynomials

To complete our solution to the Laplace equation on the solid ball, we still need to solve the ordinary differential equation (12.20) for the radial component $v(r)$. In view of our analysis of the spherical Helmholtz equation, the original separation constant is $\mu = n(n+1)$ for some nonnegative integer $n \geq 0$, and so the radial equation takes the form

$$r^2 v'' + 2r v' - n(n+1)v = 0. \quad (12.47)$$

[†] Here we use the convention that $Y_n^m = Y_n^{-m}$, $\tilde{Y}_n^m = -\tilde{Y}_n^{-m}$, and $\tilde{Y}_n^0 \equiv 0$, which is compatible with their defining formulas (12.38).

To solve this Euler equation, we substitute the power ansatz $v(r) = r^\alpha$, and find that the exponent α must satisfy the quadratic indicial equation

$$\alpha^2 + \alpha - n(n + 1) = 0, \quad \text{and hence} \quad \alpha = n \quad \text{or} \quad \alpha = -(n + 1).$$

Therefore, the two linearly independent solutions are

$$v_1(r) = r^n \quad \text{and} \quad v_2(r) = r^{-n-1}. \tag{12.48}$$

Since we are currently interested only in solutions that remain bounded at $r = 0$ — the center of the ball — we will retain just the first solution $v(r) = r^n$ for our subsequent analysis.

At this stage, we have solved all three ordinary differential equations for the separable solutions. We combine (12.23, 38, 48) to produce the following spherically separable solutions to the Laplace equation:

$$\begin{aligned} H_n^m &= r^n Y_n^m(\varphi, \theta) = r^n p_n^m(\varphi) \cos m\theta, & n &= 0, 1, 2, \dots, \\ \tilde{H}_n^m &= r^n \tilde{Y}_n^m(\varphi, \theta) = r^n p_n^m(\varphi) \sin m\theta, & m &= 0, 1, \dots, n. \end{aligned} \tag{12.49}$$

Although apparently complicated, these solutions are, perhaps surprisingly, elementary polynomial functions of the rectangular coordinates x, y, z , and hence are *harmonic polynomials*. The first few are

$$\begin{aligned} H_0^0 &= 1, & H_1^0 &= z, & H_2^0 &= z^2 - \frac{1}{2}x^2 - \frac{1}{2}y^2, & H_3^0 &= z^3 - \frac{3}{2}x^2z - \frac{3}{2}y^2z, \\ H_1^1 &= x, & H_2^1 &= 3xz, & & & H_3^1 &= 6xz^2 - \frac{3}{2}x^3 - \frac{3}{2}xy^2, \\ \tilde{H}_1^1 &= y, & \tilde{H}_2^1 &= 3yz, & & & \tilde{H}_3^1 &= 6yz^2 - \frac{3}{2}x^2y - \frac{3}{2}y^3, \\ & & H_2^2 &= 3x^2 - 3y^2, & H_3^2 &= 15x^2z - 15y^2z, & & \\ & & \tilde{H}_2^2 &= 6xy, & \tilde{H}_3^2 &= 30xyz, & & \\ & & & & H_3^3 &= 15x^3 - 45xy^2, & & \\ & & & & \tilde{H}_3^3 &= 45x^2y - 15y^3. & & \end{aligned} \tag{12.50}$$

The polynomials

$$H_n^0, H_n^1, \dots, H_n^n, \tilde{H}_n^1, \dots, \tilde{H}_n^n$$

are homogeneous of degree n . Orthogonality of the spherical harmonics implies that they form a basis for the vector space comprised of all homogeneous harmonic polynomials of degree n , which hence has dimension $2n + 1$.

The harmonic polynomials (12.49) form a complete system, and therefore the general solution to the Laplace equation inside the unit ball can be written as a harmonic polynomial series:

$$u(x, y, z) = \frac{c_{0,0}}{2} + \sum_{n=1}^{\infty} \left(\frac{c_{0,n}}{2} H_n^0(x, y, z) + \sum_{m=1}^n [c_{m,n} H_n^m(x, y, z) + \tilde{c}_{m,n} \tilde{H}_n^m(x, y, z)] \right), \tag{12.51}$$

or equivalently, in spherical coordinates,

$$u(r, \varphi, \theta) = \frac{c_{0,0}}{2} + \sum_{n=1}^{\infty} \left(\frac{c_{0,n}}{2} r^n Y_n^0(\varphi) + \sum_{m=1}^n [c_{m,n} r^n Y_n^m(\varphi, \theta) + \tilde{c}_{m,n} r^n \tilde{Y}_n^m(\varphi, \theta)] \right). \tag{12.52}$$

The coefficients $c_{m,n}, \tilde{c}_{m,n}$ are uniquely prescribed by the boundary conditions. Indeed, substituting (12.52) into the Dirichlet boundary conditions on the unit sphere $r = 1$ yields

$$u(1, \varphi, \theta) = \frac{c_{0,0}}{2} + \sum_{n=1}^{\infty} \left(\frac{c_{0,n}}{2} Y_n^0(\varphi) + \sum_{m=1}^n [c_{m,n} Y_n^m(\varphi, \theta) + \tilde{c}_{m,n} \tilde{Y}_n^m(\varphi, \theta)] \right) = h(\varphi, \theta). \tag{12.53}$$

Thus, the coefficients $c_{m,n}, \tilde{c}_{m,n}$ are given by the inner product formulae (12.44). If the terms in the resulting series are uniformly bounded — which occurs for all piecewise continuous functions h , as well as all L^2 functions and many generalized functions such as the delta function — then the harmonic polynomial series (12.52) converges everywhere, and, in fact, uniformly on any smaller ball $\|\mathbf{x}\| = r \leq r_0 < 1$.

Averaging, the Maximum Principle, and Analyticity

In rectangular coordinates, the n^{th} summand of the series (12.51) is a homogeneous polynomial of degree n . Therefore, repeating the argument used in the two-dimensional situation (4.115), we conclude that the harmonic polynomial series is, in fact, a power series, and hence provides the *Taylor expansion for the harmonic function $u(x, y, z)$ at the origin!* In particular, its convergence for all $r < 1$ implies that the harmonic function $u(x, y, z)$ is analytic at $x = y = z = 0$.

The constant term in such a Taylor series can be identified with the value of the function at the origin: $u(0, 0, 0) = \frac{1}{2} c_{0,0}$. On the other hand, since $u = h$ on $S_1 = \partial\Omega$, the coefficient formula (12.45) tells us that

$$u(0, 0, 0) = \frac{c_{0,0}}{2} = \frac{1}{4\pi} \iint_{S_1} u \, dS. \tag{12.54}$$

Therefore, we have established the three-dimensional counterpart of Theorem 4.8: the value of a harmonic function u at the center of the sphere is equal to the average of its values on the sphere’s surface. Moreover, each partial derivative $\frac{\partial^{i+j+k} u}{\partial x^i \partial y^j \partial z^k}(0, 0, 0)$ appears, up to a factor, as the coefficient of the terms $x^i y^j z^k$ in the Taylor series, and hence can be expressed as a certain linear combination of the coefficients $c_{m,n}, \tilde{c}_{m,n}$, which are in turn given by the integral formulae (12.44).

More generally, the value of a harmonic function at the center of any ball contained within its domain equals the average of its values over the bounding sphere. As with the planar version in Theorem 4.8, it is preferable to give a direct proof that doesn’t rely on the series expansion (12.51).

Theorem 12.4. *If $u(\mathbf{x})$ is a harmonic function defined on a domain $\Omega \subset \mathbb{R}^3$, then u is analytic inside Ω . Moreover, its value at any $\mathbf{x}_0 \in \Omega$ is obtained by averaging its values on any sphere $S_a = \{\|\mathbf{x} - \mathbf{x}_0\| = a\}$ centered at \mathbf{x}_0 :*

$$u(\mathbf{x}_0) = \frac{1}{4\pi a^2} \iint_{S_a} u \, dS, \tag{12.55}$$

provided the enclosed ball lies within its domain of analyticity: $B_a = \{\|\mathbf{x} - \mathbf{x}_0\| \leq a\} \subset \Omega$.

Proof: Let us denote the average of u over the sphere of radius a by

$$\begin{aligned} g(a) &= \frac{1}{4\pi a^2} \iint_{S_a} u \, dS \\ &= \frac{1}{4\pi} \int_{-\pi}^{\pi} \int_0^{\pi} u(x_0 + a \sin \varphi \cos \theta, y_0 + a \sin \varphi \sin \theta, z_0 + a \cos \varphi) \sin \varphi \, d\varphi \, d\theta. \end{aligned}$$

By continuity, as the radius $a \rightarrow 0$, the average of u on the sphere S_a tends to its value at the center: $g(a) \rightarrow u(\mathbf{x}_0)$.

On the other hand, since $u \in C^2$ and harmonic in $B_a \subset \Omega$, the derivative

$$\begin{aligned} g'(a) &= \frac{1}{4\pi} \int_{-\pi}^{\pi} \int_0^{\pi} \left(\sin \varphi \cos \theta \frac{\partial u}{\partial x} + \sin \varphi \sin \theta \frac{\partial u}{\partial y} + \cos \varphi \frac{\partial u}{\partial z} \right) \sin \varphi \, d\varphi \, d\theta \\ &= \frac{1}{4\pi a^2} \iint_{S_a} \frac{\partial u}{\partial \mathbf{n}} \, dS = \frac{1}{4\pi a^2} \iiint_{B_a} \Delta u \, dx \, dy \, dz = 0, \end{aligned}$$

where \mathbf{n} denotes the unit outwards normal to $S_a = \partial B_a$, and we used the divergence identity in Exercise 12.1.11(a). We conclude that $g(a)$ is constant, and hence $g(a) = u(\mathbf{x}_0)$ for any $a > 0$ provided $B_a \subset \Omega$. *Q.E.D.*

Arguing as in the planar case of Theorem 4.9, we readily establish the corresponding *Strong Maximum Principle* for harmonic functions of three variables.

Theorem 12.5. *A nonconstant harmonic function cannot have a local maximum or minimum at any interior point of its domain of definition. Moreover, its global maximum or minimum (if any) is located on the boundary of the domain.*

For instance, the Maximum Principle implies that the maximum and minimum temperatures in a solid body in thermal equilibrium are to be found only on its boundary. In physical terms, since heat energy must flow away from an internal maximum and towards an internal minimum, any local temperature extremum inside the body would preclude it from being in thermal equilibrium. The Maximum Principle immediately implies a Uniqueness Theorem for both the Laplace and Poisson equations, cf. Theorem 4.10, which in turn establishes the solution formula (12.51) and hence analyticity of every harmonic function.

Example 12.6. In this example, we shall determine the electrostatic potential inside a hollow sphere when the upper and lower hemispheres are held at different constant potentials. This device is called a *spherical capacitor* and is realized experimentally by separating the two charged conducting hemispherical shells by a thin insulating ring at the equator. A straightforward scaling argument allows us to choose our units so that the sphere has unit radius, while the potential is set equal to 1 on the upper hemisphere and equal to 0, i.e., grounded, on the lower hemisphere. The resulting electrostatic potential satisfies the Laplace equation

$$\Delta u = 0 \quad \text{inside a solid ball} \quad \|\mathbf{x}\| < 1, \quad (12.56)$$

and is subject to Dirichlet boundary conditions

$$u(x, y, z) = h(x, y, z) \equiv \begin{cases} 1, & z > 0, \\ 0, & z < 0, \end{cases} \quad \text{on the unit sphere} \quad \|\mathbf{x}\| = 1. \quad (12.57)$$

The solution will be prescribed by a harmonic polynomial series (12.51) whose coefficients are fixed by the boundary values (12.57). Before tackling the required computation,

let us first note that since the boundary data does not depend upon the azimuthal angle θ , the solution $u = u(r, \varphi)$ will also be independent of θ . Therefore, we need only consider the θ -independent spherical harmonic polynomials (12.38), which are those with $m = 0$. Thus,

$$u(x, y, z) = \frac{1}{2} \sum_{n=0}^{\infty} c_n H_n^0(x, y, z) = \frac{1}{2} \sum_{n=0}^{\infty} c_n r^n P_n(\cos \varphi), \tag{12.58}$$

where we abbreviate $c_n = c_{0,n}$. The boundary conditions (12.57) require

$$u|_{r=1} = \frac{1}{2} \sum_{n=0}^{\infty} c_n P_n(\cos \varphi) = h(\varphi) = \begin{cases} 1, & 0 \leq \varphi < \frac{1}{2}\pi, \\ 0, & \frac{1}{2}\pi < \varphi \leq \pi. \end{cases}$$

The coefficients are given by (12.44), which, in the case $m = 0$, reduce to

$$c_n = \frac{2n+1}{2\pi} \iint_{S_1} h Y_n^0 dS = (2n+1) \int_0^{\pi/2} P_n(\cos \varphi) \sin \varphi d\varphi = (2n+1) \int_0^1 P_n(t) dt, \tag{12.59}$$

since $h = 0$ when $\frac{1}{2}\pi < \varphi \leq \pi$. The first few are $c_0 = 1$, $c_1 = \frac{3}{2}$, $c_2 = 0$, $c_3 = -\frac{7}{8}$, $c_4 = 0$. Therefore, the solution has the explicit Taylor expansion

$$\begin{aligned} u(x, y, z) &= \frac{1}{2} + \frac{3}{4} r \cos \varphi - \frac{21}{128} r^3 \cos \varphi - \frac{35}{128} r^3 \cos 3\varphi + \dots \\ &= \frac{1}{2} + \frac{3}{4} z + \frac{21}{32} (x^2 + y^2) z - \frac{7}{16} z^3 + \dots \end{aligned} \tag{12.60}$$

Note in particular that the value $u(0, 0, 0) = \frac{1}{2}$ at the center of the sphere is the average of its boundary values, in accordance with Theorem 12.4. The solution depends only on the cylindrical coordinates r, z , which is a consequence of the invariance of the Laplace equation under general rotations, coupled with the invariance of the boundary data under rotations around the z -axis.

Remark: The same solution $u(x, y, z)$ describes the thermal equilibrium in a solid sphere whose upper hemisphere is held at temperature 1° and lower hemisphere at 0° .

Example 12.7. A closely related problem is to determine the electrostatic potential *outside* a spherical capacitor. As in the preceding example, we take our capacitor of radius 1, with electrostatic charge of 1 on the upper hemisphere and 0 on the lower hemisphere. Here, we need to solve the Laplace equation $\Delta u = 0$ in the unbounded domain $\Omega = \{\|\mathbf{x}\| > 1\}$ — the exterior of the unit sphere — subject to the same Dirichlet boundary conditions (12.57). We anticipate that the potential will be vanishingly small at large distances away from the capacitor: $r = \|\mathbf{x}\| \gg 1$. Therefore, the harmonic polynomial solutions (12.49) will not help us solve this problem, since (except for the constant case) they become unboundedly large far away from the origin.

However, revisiting our original separation of variables argument will produce a different class of solutions having the desired decay properties. When we solved the radial equation (12.47), we discarded the solution $v_2(r) = r^{-n-1}$ because it had a singularity at the origin. In the present situation, the behavior of the function at $r = 0$ is irrelevant; our requirement is that the solution decay as $r \rightarrow \infty$, and $v_2(r)$ has this property. Therefore, we will utilize the *complementary harmonic functions*

$$\begin{aligned} K_n^m(x, y, z) &= r^{-2n-1} H_n^m(x, y, z) = r^{-n-1} Y_n^m(\varphi, \theta) = r^{-n-1} p_n^m(\varphi) \cos m\theta, \\ \tilde{K}_n^m(x, y, z) &= r^{-2n-1} \tilde{H}_n^m(x, y, z) = r^{-n-1} \tilde{Y}_n^m(\varphi, \theta) = r^{-n-1} p_n^m(\varphi) \sin m\theta, \end{aligned} \tag{12.61}$$

for solving such exterior problems. For the capacitor problem, we need only those that are independent of θ , whereby $m = 0$. We write the resulting solution as a series

$$u(x, y, z) = \frac{1}{2} \sum_{n=0}^{\infty} c_n K_n^0(x, y, z) = \frac{1}{2} \sum_{n=0}^{\infty} c_n r^{-n-1} P_n(\cos \varphi). \quad (12.62)$$

The boundary conditions

$$u|_{r=1} = \frac{1}{2} \sum_{n=0}^{\infty} c_n P_n(\cos \varphi) = h(\varphi) \equiv \begin{cases} 1, & 0 \leq \varphi < \frac{1}{2}\pi, \\ 0, & \frac{1}{2}\pi < \varphi \leq \pi, \end{cases}$$

are identical to those in the previous example. Therefore, the coefficients are given by (12.59), leading to the series expansion

$$\begin{aligned} u(x, y, z) &= \frac{1}{2r} + \frac{3 \cos \varphi}{4r^2} - \frac{21 \cos \varphi + 35 \cos 3\varphi}{128r^4} + \dots \\ &= \frac{1}{2\sqrt{x^2 + y^2 + z^2}} + \frac{3z}{4(x^2 + y^2 + z^2)^{3/2}} + \frac{21(x^2 + y^2)z - 14z^3}{32(x^2 + y^2 + z^2)^{7/2}} + \dots \end{aligned} \quad (12.63)$$

Observe that the higher-order terms become negligible at large distances, and hence the potential is asymptotic to that associated with a point charge concentrated at the origin of magnitude $\frac{1}{2}$, which is the average of the boundary potential over the sphere. This is indicative of a general fact, to be explored in Exercise 12.2.32.

Exercises

- 12.2.1. A solid ball of radius R has its upper hemispherical surface held at temperature T_1 and its lower hemispherical surface held at temperature T_0 . Find the resulting equilibrium temperature.
- 12.2.2. A solid ball has its top hemispherical surface insulated and its bottom hemispherical surface held at a fixed temperature of 10° . Find its equilibrium temperature.
- 12.2.3. Find the potential inside a spherical capacitor of radius R when the upper hemisphere is at potential α and the lower is at β .
- 12.2.4. Find the potential $u(x, y, z)$ inside a unit spherical capacitor that has the indicated boundary values on the unit sphere $x^2 + y^2 + z^2 = 1$: (a) x , (b) $x^2 + y^2$, (c) x^3 .
Hint: The potential is a polynomial.
- 12.2.5. Each point on the spherical boundary of a solid ball of radius 1 has temperature equal to its zenith angle φ . (i) Find the value of the equilibrium temperature at the center of the ball. (ii) Find the Taylor polynomial of degree 3, based at the origin, for the equilibrium temperature distribution.
- 12.2.6. Solve Exercise 12.2.5 when the boundary temperature equals (a) $\cos \varphi$, (b) $\cos \theta$, (c) θ .
- 12.2.7. A solid spherical container of radius 3 cm contains a hollow spherical cavity of radius 1 cm in its center. The inner cavity is filled with boiling water at 100° , while the entire container is immersed in an ice water bath at 0° . Assume that the container is in thermal equilibrium. *True or false:* The temperature at a point half-way between the container's inner and outer boundaries is 50° . If true, explain. If false, what is the temperature at such a point?
- 12.2.8. Find the electrostatic potential between two concentric spherical metal shells of respective radii 1 and 1.2, given that the inner shell is grounded, while the outer shell has potential equal to 1.

- ◇ 12.2.9. Use the chain rule to establish the formula (12.16) for the Laplacian in spherical coordinates.
- ◇ 12.2.10. (a) Prove that $t = \pm 1$ are both regular singular points for the order 0 Legendre differential equation (12.28). (b) Prove that the Legendre eigenvalue problem (12.27–28) is defined by a self-adjoint operator with respect to the L^2 inner product on the cut locus $[-1, 1]$. (c) Discuss the orthogonality of the Legendre polynomials.
- ◇ 12.2.11. Solve Exercise 12.2.10 for the Legendre eigenvalue problem (12.26–27) of order m along with the relevant Ferrers eigenfunctions.
- ◇ 12.2.12. Suppose $m > 0$. (a) Find the Green's function for the boundary value problem

$$(1 - t^2) \frac{d^2 P}{dt^2} - 2t \frac{dP}{dt} - \frac{m^2}{1 - t^2} P = f(t), \quad |P(-1)|, |P(1)| < \infty.$$

Hint: The homogeneous differential equation has solutions $\left(\frac{1+t}{1-t}\right)^{\frac{m}{2}}$ and $\left(\frac{1-t}{1+t}\right)^{\frac{m}{2}}$.

- (b) Use part (a) to prove completeness of the Ferrers functions of order $m > 0$ on $[-1, 1]$.
- (c) Explain why there is no Green's function in the order $m = 0$ case.

Remark: When $m = 0$, one can use the trick of Example 9.49 to prove completeness. Although the Green's function for the modified operator does not have an explicit elementary formula, one can prove that it has logarithmic singularities at the endpoints, and hence finite double L^2 norm. See [120; §43] for details.

12.2.13. What happens when $n < m$ in formula (12.31)?

- ◇ 12.2.14. Prove that the Legendre polynomial (12.29) has the explicit formula

$$P_n(t) = \sum_{0 \leq 2m \leq n} (-1)^m \frac{(2n - 2m)!}{2^n (n - m)! m! (n - 2m)!} t^{n-2m}. \quad (12.64)$$

- ◇ 12.2.15. Prove the following recurrence relation for the Ferrers functions:

$$P_n^{m+1}(t) = \sqrt{1 - t^2} \frac{dP_n^m}{dt} + \frac{mt}{\sqrt{1 - t^2}} P_n^m(t). \quad (12.65)$$

- ♡ 12.2.16. In this exercise, we determine the L^2 norms of the Ferrers functions. (a) First, prove that $\int_{-1}^1 (1 - t^2)^n dt = \frac{2^{2n+1} (n!)^2}{(2n + 1)!}$. *Hint:* Set $t = \cos \theta$ and then integrate by parts repeatedly. (b) Prove that $\|P_n\|^2 = \frac{2}{2n + 1}$. *Hint:* Integrate by parts repeatedly and then use part (a). (c) Prove that $\|P_n^{m+1}\|^2 = (n - m)(n + m + 1) \|P_n^m\|^2$. *Hint:* Use (12.65) and an integration by parts. (d) Finally, prove that $\|P_n^m\|^2 = \frac{2}{2n + 1} \frac{(n + m)!}{(n - m)!}$.

12.2.17. (a) Prove that $P_n^m(t)$ is an even or odd function according to whether $m + n$ is an even or odd integer. (b) Prove that its Fourier form, $p_n^m(\varphi)$, depends only on $\cos n \varphi, \cos(n - 2) \varphi, \cos(n - 4) \varphi, \dots$ if m is even, and only on $\sin n \varphi, \sin(n - 2) \varphi, \sin(n - 4) \varphi, \dots$ if m is odd.

12.2.18. Let m be fixed. Are the functions $p_n^m(\varphi)$ for $n = 0, 1, 2, \dots$ mutually orthogonal with respect to the standard L^2 inner product on $[0, \pi]$? If not, is there an inner product that makes them orthogonal functions?

12.2.19. Prove that the surfaces defined by the first three spherical harmonics Y_0^0, Y_1^0 , and Y_1^1 , as in Figure 12.5, are all spheres. Find their centers and radii.

- ◇ 12.2.20. Explain why the surface defined by $r = \tilde{Y}_n^m(\varphi, \theta)$ is obtained by rotating that defined by $r = Y_n^m(\varphi, \theta)$ around the z -axis by 90° .

◇ 12.2.21. Prove directly that the spherical Laplacian Δ_S is a self-adjoint linear operator with respect to the inner product (12.40).

◇ 12.2.22. (a) In view of Exercise 12.2.21, which orthogonality relations in (12.41) follow from their status as eigenfunctions of the spherical Laplacian?
 (b) Prove the general orthogonality formulae by direct computation.

◇ 12.2.23. State and prove the orthogonality of the complex spherical harmonics (12.46). Then establish the following formula for their norms:

$$\|\mathcal{Y}_n^m\|^2 = \iint_{S_1} |\mathcal{Y}_n^m|^2 dS = \frac{4\pi(n+m)!}{(2n+1)(n-m)!} \quad \begin{array}{l} n = 0, 1, 2, \dots, \\ m = -n, -n+1, \dots, n. \end{array} \quad (12.66)$$

◇ 12.2.24. Prove the formulae (12.42) for the norms of the spherical harmonics.

Hint: Use Exercise 12.2.16.

◇ 12.2.25. Justify the formulas in (12.50) for (a) H_1^0 , (b) H_2^0 , (c) \widetilde{H}_2^1 .

12.2.26. Find formulas for the following harmonic polynomials (i) in spherical coordinates; (ii) in rectangular coordinates: (a) H_4^0 , (b) H_4^4 , (c) \widetilde{H}_4^4 .

12.2.27. Explain why every polynomial solution of the Laplace equation is a linear combination of the harmonic polynomials (12.49). *Hint:* Look at its Taylor series.

12.2.28. (a) Prove that if $u(x, y, z)$ is any harmonic polynomial, then so are $u(y, x, z)$, $u(z, x, y)$, and all other functions obtained by permuting the variables x, y, z . (b) Discuss the effect of such permutations on the basis harmonic polynomials $H_n^m(x, y, z)$ appearing in (12.50).

12.2.29. Find the formulas in rectangular coordinates for the following complementary harmonic functions: (a) K_0^0 , (b) K_1^1 , (c) K_2^0 , (d) \widetilde{K}_2^1 .

◇ 12.2.30. Let $u(x, y, z)$ be a harmonic function defined on the unit ball $r \leq 1$. Prove that its gradient at the center, $\nabla u(\mathbf{0})$, equals the average of the vector field $\mathbf{v}(\mathbf{x}) = \mathbf{x}u(\mathbf{x})$ over the unit sphere $r = 1$.

◇ 12.2.31. (a) Suppose $u(x, y, z)$ is a solution to the Laplace equation. Prove that the function $U(x, y, z) = r^{-1}u(x/r^2, y/r^2, z/r^2)$ obtained by *inversion* is also a solution. (b) Explain how inversion can be used to solve boundary value problems on the exterior of a sphere. (c) Use inversion to relate the solutions to Examples 12.6 and 12.7.

◇ 12.2.32. Suppose $u(r, \varphi, \theta)$ is the potential exterior to a spherical capacitor of unit radius.
 (a) Prove that $\lim_{r \rightarrow \infty} r u(r, \varphi, \theta)$ equals the average value of u on the sphere.
 (b) Use Exercise 12.2.31 to deduce this result as a consequence of Theorem 12.4.

12.2.33. (a) Write out, using spherical coordinates, formulas for the L^2 inner product and norm for scalar fields $f(r, \varphi, \theta)$ and $g(r, \varphi, \theta)$ on a solid ball of unit radius centered at the origin.
 (b) Let $f(x, y, z) = z$ and $g(x, y, z) = x^2 + y^2$. Find $\|f\|$, $\|g\|$ and $\langle f, g \rangle$.
 (c) Verify the Cauchy-Schwarz and triangle inequalities for these two functions.

◇ 12.2.34. Use separation of variables to construct a Fourier series solution to the Laplace equation on a rectangular box, $B = \{0 < x < a, 0 < y < b, 0 < z < c\}$, subject to the

$$\text{Dirichlet boundary conditions } u(x, y, z) = \begin{cases} h(x, y), & z = 0, \quad 0 < x < a, \quad 0 < y < b, \\ 0, & \text{at all other points in } \partial B. \end{cases}$$

12.2.35. Find the equilibrium temperature distribution inside a unit cube that has 100° temperature on its top face, 0° on its bottom face, while all four side faces are insulated.

12.2.36. Solve Exercise 12.2.35 when the top face of the cube has temperature

$$u(x, y, 1) = \cos \pi x \cos \pi y.$$

♣ 12.2.37. A solid unit cube is in thermal equilibrium when subject to 100° temperature on its top face and 0° on all other faces. *True or false:* The temperature at the center equals the average temperature over the surface of the cube.

12.2.38. Solve the boundary value problem

$$-\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} - \frac{\partial^2 u}{\partial z^2} + u = \cos x \cos y, \quad 0 < x, y, z < \pi,$$

$$u(x, y, 0) = 1, \quad \frac{\partial u}{\partial z}(x, y, \pi) = \frac{\partial u}{\partial y}(x, 0, z) = \frac{\partial u}{\partial y}(x, \pi, z) = \frac{\partial u}{\partial z}(0, y, z) = \frac{\partial u}{\partial x}(\pi, y, z) = 0.$$

12.2.39. Let C be the cylinder of height 1 and diameter 1 that sits on the (x, y) -plane centered on the z -axis. (a) Write out, in cylindrical coordinates, the explicit formula for the L^2 inner product and norm on C .

(b) Let $f(x, y, z) = z$ and $g(x, y, z) = x^2 + y^2$. Find $\|f\|, \|g\|$ and $\langle f, g \rangle$.

(c) Verify the Cauchy-Schwarz and triangle inequalities for these two functions.

◇ 12.2.40. (a) Write out the Laplace equation in cylindrical coordinates.

(b) Use separation of variables to construct a series solution to the Laplace equation on the cylinder $C = \{x^2 + y^2 < 1, 0 < z < 1\}$, subject to the Dirichlet boundary conditions

$$u(x, y, z) = \begin{cases} h(x, y), & z = 0, \quad x^2 + y^2 < 1, \\ 0, & \text{at all other points in } \partial C. \end{cases}$$

12.2.41. A cylinder of radius 1 and height 2 has 100° temperature on its top face, 0° on its bottom face, while its curved side is fully insulated. Find its equilibrium temperature distribution.

12.2.42. Solve Exercise 12.2.41 if the curved sides are kept at 0° instead.

12.3 Green's Functions for the Poisson Equation

We now turn to the inhomogeneous form of the three-dimensional Laplace equation: the *Poisson equation*

$$-\Delta u = f, \tag{12.67}$$

on a solid domain $\Omega \subset \mathbb{R}^3$. In order to uniquely specify the solution, we must impose appropriate boundary conditions: Dirichlet or mixed. (As in the planar version, Neumann boundary value problems have either infinitely many solutions or no solutions, depending upon whether the Fredholm conditions are satisfied or not.) We only need to discuss the case of homogeneous boundary conditions, since, by linear superposition, an inhomogeneous boundary value problem can be split into a homogeneous boundary value problem for the inhomogeneous Poisson equation along with an inhomogeneous boundary value problem for the homogeneous Laplace equation.

As in Chapter 6, we begin by analyzing the case of a delta function inhomogeneity that is concentrated at a single point in the domain. Thus, for each $\boldsymbol{\xi} = (\xi, \eta, \zeta) \in \Omega$, the *Green's function* $G(\mathbf{x}; \boldsymbol{\xi}) = G(x, y, z; \xi, \eta, \zeta)$ is the unique solution to the Poisson equation

$$-\Delta u = \delta(\mathbf{x} - \boldsymbol{\xi}) = \delta(x - \xi) \delta(y - \eta) \delta(z - \zeta) \quad \text{for all } \mathbf{x} \in \Omega, \tag{12.68}$$

subject to the chosen homogeneous boundary conditions. The solution to the general Poisson equation (12.67) is then obtained by superposition: We write the forcing function

$$f(x, y, z) = \iiint_{\Omega} f(\xi, \eta, \zeta) \delta(x - \xi) \delta(y - \eta) \delta(z - \zeta) d\xi d\eta d\zeta \tag{12.69}$$

as a linear superposition of delta functions. By linearity, the solution

$$u(x, y, z) = \iiint_{\Omega} f(\xi, \eta, \zeta) G(x, y, z; \xi, \eta, \zeta) d\xi d\eta d\zeta \tag{12.70}$$

to the homogeneous boundary value problem for the Poisson equation (12.67) is then given as the corresponding superposition of the Green's function solutions.

The Green's function can also be used to solve the inhomogeneous Dirichlet boundary value problem

$$-\Delta u = 0, \quad \mathbf{x} \in \Omega, \quad u = h, \quad \mathbf{x} \in \partial\Omega. \quad (12.71)$$

The same argument that was used in the two-dimensional situation produces the solution

$$u(\mathbf{x}) = - \iint_{\partial\Omega} \frac{\partial G}{\partial \mathbf{n}}(\mathbf{x}; \boldsymbol{\xi}) h(\boldsymbol{\xi}) dS, \quad (12.72)$$

where the normal derivative is taken with respect to the variable $\boldsymbol{\xi} \in \partial\Omega$. In the case that Ω is a solid ball, this integral formula effectively sums the spherical harmonic series (12.51); see Theorem 12.12 below.

The Free-Space Green's Function

Only in a few specific instances is an explicit formula for the Green's function known. Nevertheless, certain general guiding features can be readily established. The starting point is to investigate the Poisson equation (12.68) when the domain $\Omega = \mathbb{R}^3$ is all of three-dimensional space. We impose boundary constraints by seeking a solution that goes to zero, $u(\mathbf{x}) \rightarrow 0$, at large distances, $\|\mathbf{x}\| \rightarrow \infty$. Since the Laplacian operator is invariant under translations, we can, without loss of generality, place our delta impulse at the origin, and concentrate on solving the particular case

$$-\Delta u = \delta(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3.$$

Since $\delta(\mathbf{x}) = 0$ for all $\mathbf{x} \neq \mathbf{0}$, the desired solution will, in fact, be a solution to the homogeneous Laplace equation

$$\Delta u = 0, \quad \mathbf{x} \neq \mathbf{0},$$

save, possibly, for a singularity at the origin.

The Laplace equation models the equilibria of a uniform isotropic medium, and so, as noted in Exercise 12.1.7, is also invariant under three-dimensional rotations. This suggests that, in any radially symmetric configuration, the solution should depend only on the distance $r = \|\mathbf{x}\|$ from the origin. Referring to the spherical coordinate form (12.16) of the Laplacian operator, if u is a function of r only, then its derivatives with respect to the angular coordinates φ, θ are zero, and so $u(r)$ solves the ordinary differential equation

$$\frac{d^2 u}{dr^2} + \frac{2}{r} \frac{du}{dr} = 0. \quad (12.73)$$

This equation is, in effect, a first-order linear ordinary differential equation for $v = du/dr$ and hence is particularly easy to solve:

$$\frac{du}{dr} = v(r) = -\frac{b}{r^2}, \quad \text{and hence} \quad u(r) = a + \frac{b}{r},$$

where a, b are arbitrary constants. The constant solution $u(r) = a$ does not die away at large distances, nor does it have a singularity at the origin. Therefore, if our intuition is valid, the desired solution should be of the form

$$u = \frac{b}{r} = \frac{b}{\|\mathbf{x}\|} = \frac{b}{\sqrt{x^2 + y^2 + z^2}}. \quad (12.74)$$

Indeed, this function is harmonic — solves Laplace's equation — everywhere away from the origin and has a singularity at $\mathbf{x} = \mathbf{0}$.

The solution (12.74) is, up to a constant multiple, the three-dimensional Newtonian gravitational potential due to a point mass at the origin. Its gradient,

$$\mathbf{f}(\mathbf{x}) = \nabla \left(\frac{b}{\|\mathbf{x}\|} \right) = - \frac{b \mathbf{x}}{\|\mathbf{x}\|^3}, \quad (12.75)$$

defines the gravitational force vector at the point \mathbf{x} . When $b > 0$, the force $\mathbf{f}(\mathbf{x})$ points toward the mass at the origin. Its magnitude

$$\|\mathbf{f}\| = \frac{b}{\|\mathbf{x}\|^2} = \frac{b}{r^2}$$

is proportional to the reciprocal of the squared distance, which is the well-known inverse square law of three-dimensional Newtonian gravity. Formula (12.75) can also be interpreted as the electrostatic force due to a concentrated electric charge at the origin, with (12.74) giving the corresponding Coulomb potential. The constant b is positive when the charges are of opposite signs, leading to an attractive force, and negative in the repulsive case of like charges.

Returning to our problem, the remaining task is to fix the multiple b such that the Laplacian of our candidate solution (12.74) has a delta function singularity at the origin; equivalently, we must determine $a = 1/b$ such that

$$-\Delta(r^{-1}) = a \delta(\mathbf{x}). \quad (12.76)$$

This equation is certainly valid away from the origin, since $\delta(\mathbf{x}) = 0$ when $\mathbf{x} \neq \mathbf{0}$. To investigate near the singularity, we integrate both sides of (12.76) over a small solid ball $B_\varepsilon = \{\|\mathbf{x}\| \leq \varepsilon\}$ of radius ε :

$$-\iint\int_{B_\varepsilon} \Delta(r^{-1}) \, dx \, dy \, dz = \iint\int_{B_\varepsilon} a \delta(\mathbf{x}) \, dx \, dy \, dz = a, \quad (12.77)$$

where we used the definition of the delta function to evaluate the right-hand side. On the other hand, since $\Delta r^{-1} = \nabla \cdot \nabla r^{-1}$, we can use the divergence theorem (12.8) to evaluate the left-hand integral, whence

$$\iint\int_{B_\varepsilon} \Delta(r^{-1}) \, dx \, dy \, dz = \iint\int_{B_\varepsilon} \nabla \cdot \nabla(r^{-1}) \, dx \, dy \, dz = \iint_{S_\varepsilon} \frac{\partial}{\partial \mathbf{n}} \left(\frac{1}{r} \right) \, dS,$$

where the surface integral is over the bounding sphere $S_\varepsilon = \partial B_\varepsilon = \{\|\mathbf{x}\| = \varepsilon\}$. The sphere's unit normal \mathbf{n} points in the radial direction, and hence the normal derivative coincides with differentiation with respect to r ; in particular,

$$\frac{\partial}{\partial \mathbf{n}} \left(\frac{1}{r} \right) = \frac{\partial}{\partial r} \left(\frac{1}{r} \right) = - \frac{1}{r^2}.$$

The surface integral can now be explicitly evaluated:

$$\iint_{S_\varepsilon} \frac{\partial}{\partial \mathbf{n}} \left(\frac{1}{r} \right) \, dS = - \iint_{S_\varepsilon} \frac{1}{r^2} \, dS = - \iint_{S_\varepsilon} \frac{1}{\varepsilon^2} \, dS = -4\pi,$$

since S_ε has surface area $4\pi\varepsilon^2$. Substituting this result back into (12.77), we conclude that

$$a = 4\pi, \quad \text{and hence} \quad -\Delta r^{-1} = 4\pi \delta(\mathbf{x}). \quad (12.78)$$

This is our desired formula! We conclude that a solution to the Poisson equation with a delta function impulse at the origin is

$$G(x, y, z) = \frac{1}{4\pi r} = \frac{1}{4\pi \|\mathbf{x}\|} = \frac{1}{4\pi \sqrt{x^2 + y^2 + z^2}}, \tag{12.79}$$

which is the three-dimensional Newtonian potential due to a unit point mass situated at the origin.

If the singularity is concentrated at some other point $\boldsymbol{\xi} = (\xi, \eta, \zeta)$, then we merely translate the preceding solution. This leads immediately to the *free-space Green's function*

$$G(\mathbf{x}; \boldsymbol{\xi}) = G(\mathbf{x} - \boldsymbol{\xi}) = \frac{1}{4\pi \|\mathbf{x} - \boldsymbol{\xi}\|} = \frac{1}{4\pi \sqrt{(x - \xi)^2 + (y - \eta)^2 + (z - \zeta)^2}}. \tag{12.80}$$

The superposition principle (12.70) implies the following integral formula for the solutions to the Poisson equation on all of three-dimensional space.

Theorem 12.8. *Assuming that $f(\mathbf{x}) \rightarrow 0$ sufficiently rapidly as $\|\mathbf{x}\| \rightarrow \infty$, a particular solution to the Poisson equation*

$$-\Delta u = f, \quad \text{for } \mathbf{x} \in \mathbb{R}^3, \tag{12.81}$$

is given by

$$u_\star(\mathbf{x}) = \frac{1}{4\pi} \iiint_{\mathbb{R}^3} \frac{f(\boldsymbol{\xi})}{\|\mathbf{x} - \boldsymbol{\xi}\|} d\boldsymbol{\xi} = \frac{1}{4\pi} \iiint_{\mathbb{R}^3} \frac{f(\xi, \eta, \zeta) d\xi d\eta d\zeta}{\sqrt{(x - \xi)^2 + (y - \eta)^2 + (z - \zeta)^2}}. \tag{12.82}$$

The general solution is $u(x, y, z) = u_\star(x, y, z) + w(x, y, z)$, where $w(x, y, z)$ is an arbitrary harmonic function.

Example 12.9. In this example, we compute the gravitational (or electrostatic) potential in three-dimensional space due to a uniform solid ball, e.g., a spherical planet such as the Earth. By rescaling, it suffices to consider the case in which the forcing function is equal to 1 inside a ball of radius 1 and zero outside:

$$f(\mathbf{x}) = \begin{cases} 1, & \|\mathbf{x}\| < 1, \\ 0, & \|\mathbf{x}\| > 1. \end{cases}$$

The particular solution to the resulting Poisson equation (12.81) is given by the integral

$$u(\mathbf{x}) = \frac{1}{4\pi} \iiint_{\|\boldsymbol{\xi}\| < 1} \frac{1}{\|\mathbf{x} - \boldsymbol{\xi}\|} d\xi d\eta d\zeta. \tag{12.83}$$

Clearly, since the forcing function is radially symmetric, the solution $u = u(r)$ is also radially symmetric. To evaluate the integral, then, we can take $\mathbf{x} = (0, 0, z)$ to lie on the z -axis, so that $r = \|\mathbf{x}\| = |z|$. We use cylindrical coordinates $\boldsymbol{\xi} = (\rho \cos \theta, \rho \sin \theta, \zeta)$, so that

$$\|\mathbf{x} - \boldsymbol{\xi}\| = \sqrt{\rho^2 + (z - \zeta)^2}.$$

The integral in (12.83) can then be explicitly computed:

$$\begin{aligned} \frac{1}{4\pi} \int_{-1}^1 \int_0^{\sqrt{1-\zeta^2}} \int_0^{2\pi} \frac{\rho d\theta d\rho d\zeta}{\sqrt{\rho^2 + (z - \zeta)^2}} \\ = \frac{1}{2} \int_{-1}^1 \left(\sqrt{1 + z^2 - 2z\zeta} - |z - \zeta| \right) d\zeta = \begin{cases} \frac{1}{3|z|}, & |z| \geq 1, \\ \frac{1}{2} - \frac{z^2}{6}, & |z| \leq 1. \end{cases} \end{aligned}$$

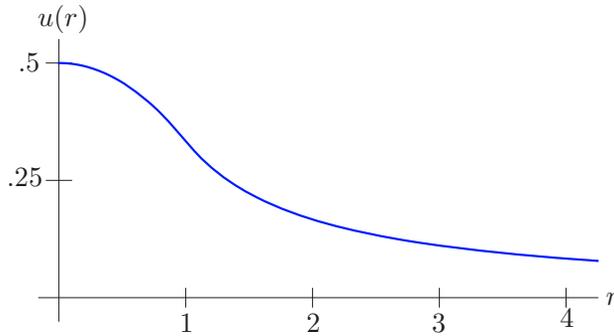


Figure 12.6. Solution to Poisson's equation in a solid ball.

Therefore, by radial symmetry, the solution is

$$u(\mathbf{x}) = \begin{cases} \frac{1}{3r}, & r = \|\mathbf{x}\| \geq 1, \\ \frac{1}{2} - \frac{r^2}{6}, & r = \|\mathbf{x}\| \leq 1, \end{cases} \quad (12.84)$$

plotted, as a function of $r = \|\mathbf{x}\|$, in [Figure 12.6](#). Note that, outside the solid ball, the solution is a Newtonian potential corresponding to a concentrated point mass of magnitude $\frac{4}{3}\pi$ — the total mass of the planet. We have thus demonstrated a well-known result in gravitation and electrostatics: the exterior potential due to a spherically symmetric mass (or electrically charged body) is the same as if all the mass (charge) were concentrated at its center. In the darkness of outer space, if you cannot see a spherical planet, you can determine only its mass, not its size, by measuring its external gravitational force.

Bounded Domains and the Method of Images

Suppose we now wish to solve the inhomogeneous Poisson equation (12.67) on a bounded domain $\Omega \subset \mathbb{R}^3$. To construct the desired Green's function, we proceed as follows. The Newtonian potential (12.80) is a particular solution to the underlying inhomogeneous equation

$$-\Delta u = \delta(\mathbf{x} - \boldsymbol{\xi}), \quad \mathbf{x} \in \Omega, \quad (12.85)$$

but it almost surely does not have the proper boundary values on $\partial\Omega$. By linearity, the general solution to such an inhomogeneous linear equation must take the form

$$u(\mathbf{x}) = \frac{1}{4\pi\|\mathbf{x} - \boldsymbol{\xi}\|} - v(\mathbf{x}), \quad (12.86)$$

where the first term is a particular solution, while $v(\mathbf{x})$ is an arbitrary solution to the homogeneous equation $\Delta v = 0$, i.e., an arbitrary harmonic function. The solution (12.86) satisfies the homogeneous boundary conditions, provided the boundary values of $v(\mathbf{x})$ match those of the Green's function. Let us explicitly state the result in the Dirichlet case.

Theorem 12.10. *The Green's function for the homogeneous Dirichlet boundary value problem*

$$-\Delta u = f \quad \text{for} \quad \mathbf{x} \in \Omega, \quad u = 0 \quad \text{for} \quad \|\mathbf{x}\| \in \partial\Omega,$$

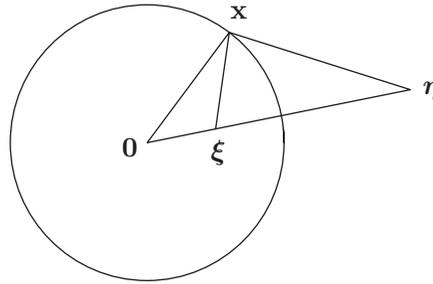


Figure 12.7. Method of Images for the unit ball.

for the Poisson equation in a domain $\Omega \subset \mathbb{R}^3$ has the form

$$G(\mathbf{x}; \boldsymbol{\xi}) = \frac{1}{4\pi \|\mathbf{x} - \boldsymbol{\xi}\|} - v(\mathbf{x}; \boldsymbol{\xi}), \quad \mathbf{x}, \boldsymbol{\xi} \in \Omega, \tag{12.87}$$

where $v(\mathbf{x}; \boldsymbol{\xi})$ is the harmonic function of $\mathbf{x} \in \Omega$ that satisfies

$$v(\mathbf{x}; \boldsymbol{\xi}) = \frac{1}{4\pi \|\mathbf{x} - \boldsymbol{\xi}\|} \quad \text{for all} \quad \mathbf{x} \in \partial\Omega. \tag{12.88}$$

In this manner, we have reduced the determination of the Green’s function to the solution to a particular family of Laplace boundary value problems, which are parametrized by the point $\boldsymbol{\xi} \in \Omega$. In certain domains with simple geometry, the Method of Images can be used to produce an explicit formula for the Green’s function. As in Section 6.3, the idea is to match the boundary values of the free-space Green’s function due to a delta impulse at a point inside the domain with one or more additional Green’s functions corresponding to impulses at points outside the domain — the “image points”.

The case of a solid ball of radius 1 with Dirichlet boundary conditions is the easiest to handle. Indeed, the *same* geometric construction that we used for a planar disk, redrawn in Figure 12.7, applies here. Although identical to Figure 6.13, we are re-interpreting it as a three-dimensional diagram, with the circle representing the unit sphere, while the lines remain lines. The required image point is given by *inversion*:

$$\boldsymbol{\eta} = \frac{\boldsymbol{\xi}}{\|\boldsymbol{\xi}\|^2}, \quad \text{whereby} \quad \|\boldsymbol{\xi}\| = \frac{1}{\|\boldsymbol{\eta}\|}.$$

By the similar triangles argument used before, we have

$$\frac{\|\boldsymbol{\xi}\|}{\|\mathbf{x}\|} = \frac{\|\mathbf{x}\|}{\|\boldsymbol{\eta}\|} = \frac{\|\mathbf{x} - \boldsymbol{\xi}\|}{\|\mathbf{x} - \boldsymbol{\eta}\|}, \quad \text{and therefore} \quad \|\mathbf{x}\| = 1.$$

As a result, the function

$$v(\mathbf{x}, \boldsymbol{\xi}) = \frac{1}{4\pi} \frac{\|\boldsymbol{\eta}\|}{\|\mathbf{x} - \boldsymbol{\eta}\|} = \frac{1}{4\pi} \frac{\|\boldsymbol{\xi}\|}{\|\boldsymbol{\xi} - \|\boldsymbol{\xi}\|^2 \mathbf{x}\|}$$

has the same boundary values on the unit sphere as the Newtonian potential:

$$\frac{1}{4\pi} \frac{\|\boldsymbol{\eta}\|}{\|\mathbf{x} - \boldsymbol{\eta}\|} = \frac{1}{4\pi \|\mathbf{x} - \boldsymbol{\xi}\|} \quad \text{whenever} \quad \|\mathbf{x}\| = 1.$$

We conclude that their difference

$$G(\mathbf{x}; \boldsymbol{\xi}) = \frac{1}{4\pi} \left(\frac{1}{\|\mathbf{x} - \boldsymbol{\xi}\|} - \frac{\|\boldsymbol{\xi}\|}{\|\boldsymbol{\xi} - \|\boldsymbol{\xi}\|^2 \mathbf{x}\|} \right) \tag{12.89}$$

has the required properties of the Green's function: it satisfies the Laplace equation inside the unit ball except at the delta function singularity $\mathbf{x} = \boldsymbol{\xi}$, and, moreover, $G(\mathbf{x}; \boldsymbol{\xi}) = 0$ has homogeneous Dirichlet conditions on the spherical boundary $\|\mathbf{x}\| = 1$.

With the Green's function in hand, we can apply the general superposition formula (12.70) to arrive at a solution to the Dirichlet boundary value problem for the Poisson equation in the unit ball.

Theorem 12.11. *The solution to the Dirichlet boundary value problem*

$$-\Delta u = f \quad \text{for} \quad \|\mathbf{x}\| < 1, \quad u = 0 \quad \text{for} \quad \|\mathbf{x}\| = 1,$$

on the unit ball is given by the integral

$$u(\mathbf{x}) = \frac{1}{4\pi} \iiint_{\|\boldsymbol{\xi}\| \leq 1} \left(\frac{1}{\|\mathbf{x} - \boldsymbol{\xi}\|} - \frac{\|\boldsymbol{\xi}\|}{\|\boldsymbol{\xi} - \|\boldsymbol{\xi}\|^2 \mathbf{x}\|} \right) f(\boldsymbol{\xi}) \, d\xi \, d\eta \, d\zeta. \tag{12.90}$$

By the same token, formula (12.72) provides a solution to the inhomogeneous Dirichlet boundary value problem for the Laplace equation on a ball.

Theorem 12.12. *The solution to the Dirichlet boundary value problem*

$$-\Delta u = 0 \quad \text{for} \quad \|\mathbf{x}\| < 1, \quad u = h \quad \text{for} \quad \|\mathbf{x}\| = 1,$$

on the unit ball is given by the following surface integral:

$$u(\mathbf{x}) = \frac{1}{4\pi} \iint_{\|\boldsymbol{\xi}\|=1} \frac{1 - \|\mathbf{x}\|^2}{\|\boldsymbol{\xi} - \mathbf{x}\|^3} h(\boldsymbol{\xi}) \, dS. \tag{12.91}$$

Proof: We start with the explicit formula (12.89) for the Green's function on the unit ball. Since the normal derivative on the unit sphere $\|\boldsymbol{\xi}\| = 1$ can be written as $\partial/\partial \mathbf{n} = \boldsymbol{\xi} \cdot \nabla_{\boldsymbol{\xi}}$, a short computation demonstrates that

$$\frac{\partial G}{\partial \mathbf{n}}(\mathbf{x}; \boldsymbol{\xi}) = \frac{1}{4\pi} \left(\frac{\mathbf{x} \cdot \boldsymbol{\xi} - \|\boldsymbol{\xi}\|^2}{\|\mathbf{x} - \boldsymbol{\xi}\|^3} - \frac{\|\boldsymbol{\xi}\|^3 (\mathbf{x} \cdot \boldsymbol{\xi} - \|\boldsymbol{\xi}\|^2 \|\mathbf{x}\|^2)}{\|\boldsymbol{\xi} - \|\boldsymbol{\xi}\|^2 \mathbf{x}\|^3} \right) = \frac{1}{4\pi} \frac{\|\mathbf{x}\|^2 - 1}{\|\boldsymbol{\xi} - \mathbf{x}\|^3}.$$

The solution formula (12.91) thus immediately follows from (12.72). *Q.E.D.*

For example, the series solution (12.60) to the spherical capacitor problem of Example 12.6 can thus be re-expressed as a surface integral:

$$\begin{aligned} u(x, y, z) &= \frac{1}{4\pi} \iint_{\{\xi^2 + \eta^2 + \zeta^2 = 1, \zeta > 0\}} \frac{(1 - x^2 - y^2 - z^2) \, dS}{[(\xi - x)^2 + (\eta - y)^2 + (\zeta - z)^2]^{3/2}} \\ &= \int_{-\pi}^{\pi} \int_0^{\pi/2} \frac{(1 - x^2 - y^2 - z^2) \sin \varphi \, d\varphi \, d\theta}{[(\cos \theta \sin \varphi - x)^2 + (\sin \theta \sin \varphi - y)^2 + (\cos \varphi - z)^2]^{3/2}}. \end{aligned}$$

Exercises

- 12.3.1. Find the equilibrium temperature of a sphere of radius 1 whose boundary is held at 0° while a concentrated unit heat source is applied at (a) the center; (b) a point half-way between the center and the boundary.
- 12.3.2. A hot soldering iron is continually applied to the north pole of a solid spherical ball of radius 1. Find the equilibrium temperature.
- 12.3.3. Write down the gravitational potential — both external and internal — due to a spherical planet of radius R composed out of a uniform material with density ρ .
- 12.3.4. (a) Find the gravitational potential due to a spherical shell of unit density obtained by carving out a spherical cavity of radius a from a solid ball of radius $b > a$. *Hint:* Use the solution to Exercise 12.3.3. (b) What is the gravitational force inside the cavity? (c) Show that outside the shell, the gravitational potential is as if the entire mass were concentrated at the origin.
- ♣ 12.3.5. (a) Write down an integral formula for the gravitational potential and gravitational force field due to a mass of unit density in the shape of a solid unit cube that is centered at the origin. (b) Use numerical integration to determine the gravitational force vector at the points $(3, 0, 0)$ and $(\sqrt{3}, \sqrt{3}, \sqrt{3})$. Before doing the calculation, see whether you can predict which experiences a stronger force, and then check your prediction numerically. (c) Suppose the mass is re-formed into a sphere. How does this affect the gravitational force at the two points? First predict whether it will increase, decrease, or stay the same. Then test your prediction by computing the values and comparing with those you computed in part (b).
- 12.3.6. A thin hollow metal sphere of unit radius is grounded. Find the electrostatic potential inside the sphere due to a small solid metal ball of radius $\rho < 1$ placed at its center, assuming unit charge density throughout the ball.
- 12.3.7. A thin straight rod of unit density and length 2ℓ is fixed on the z -axis centered at the origin. Find the induced (a) gravitational potential and (b) gravitational force experienced by a point (x, y, z) not on the rod.
- ♡ 12.3.8. (a) Find the gravitational force due to a thin, uniform straight rod of unit density and infinite length by letting $\ell \rightarrow \infty$ in your solution to Exercise 12.3.7(b). (b) Show that the force field of part (a) has a potential function that can be identified with the two-dimensional logarithmic gravitational potential due to a point mass at the origin. Thus, two-dimensional gravitation can be regarded as a cross-section of three-dimensional gravitation due to infinitely long vertical line masses. (c) Is your potential function the limit, as $\ell \rightarrow \infty$, of the potential function you found in Exercise 12.3.7(a)? Discuss.
- 12.3.9. Which well-known solutions to the Laplace equation comes from setting $m = n = 0$ in (12.61)?
- 12.3.10. Use the Fredholm Alternative to analyze the existence and uniqueness of solutions to the homogeneous Neumann boundary value problem for the Poisson equation on a bounded domain $\Omega \subset \mathbb{R}^3$.
- ◇ 12.3.11. Mimic the proof of Theorem 6.19 to establish the solution formula (12.72).
- 12.3.12. Use the Method of Images to find the Green's function for a solid hemisphere of unit radius subject to homogeneous Dirichlet boundary conditions.

12.4 The Heat Equation for Three-Dimensional Media

Thermal diffusion in a uniform isotropic solid body $\Omega \subset \mathbb{R}^3$ is modeled by the three-dimensional *heat equation*

$$\frac{\partial u}{\partial t} = \gamma \Delta u = \gamma \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right), \quad (x, y, z) \in \Omega. \quad (12.92)$$

The positivity of the body's thermal diffusivity, $\gamma > 0$, is required on both physical and mathematical grounds. The physical derivation is exactly the same as that for the two-dimensional version (11.1), and does not need to be repeated in detail. Briefly, Fourier's law expresses the heat flux vector as a multiple of the temperature gradient, $\mathbf{w} = -\kappa \nabla u$, while energy conservation implies that its divergence is proportional to the rate of change of temperature: $\nabla \cdot \mathbf{w} = -\sigma u_t$. Combining these two physical laws and assuming uniformity, whereby κ and σ are constant, produces (12.92) with $\gamma = \kappa/\sigma$.

As always, we must impose suitable boundary conditions: either Dirichlet conditions $u = h$ that specify the boundary temperature; (homogeneous) Neumann conditions $\partial u/\partial \mathbf{n} = 0$ corresponding to an insulated boundary; or a mixture of the two. Given the body's temperature

$$u(t_0, x, y, z) = f(x, y, z) \quad (12.93)$$

at an initial time t_0 , it can be proved, [38, 61, 99], that the resulting initial-boundary value problem is well-posed, which means that there is a unique classical solution $u(t, x, y, z)$, defined at all subsequent times $t > t_0$, that depends continuously on the initial data.

As in the one- and two-dimensional versions, we begin by restricting our attention to homogeneous boundary conditions. Separation of variables works as usual, and we quickly review the basic ideas. One begins by imposing an exponential solution ansatz

$$u(t, \mathbf{x}) = e^{-\lambda t} v(\mathbf{x}).$$

Substituting into the differential equation and canceling the exponentials, it follows that v satisfies the Helmholtz eigenvalue problem

$$\gamma \Delta v + \lambda v = 0,$$

subject to the relevant boundary conditions. For Dirichlet and mixed boundary conditions, the Laplacian is a positive definite operator, and hence the eigenvalues are all strictly positive,

$$0 < \lambda_1 \leq \lambda_2 \leq \cdots, \quad \text{with} \quad \lambda_n \longrightarrow \infty, \quad \text{as} \quad n \rightarrow \infty.$$

Moreover, on a bounded domain, the Helmholtz eigenfunctions are complete, and so linear superposition implies that the solution can be written as an eigenfunction series

$$u(t, \mathbf{x}) = \sum_{n=1}^{\infty} c_n e^{-\lambda_n t} v_n(\mathbf{x}). \quad (12.94)$$

The coefficients c_n are uniquely prescribed by the initial condition (12.93):

$$u(t_0, \mathbf{x}) = \sum_{n=1}^{\infty} c_n e^{-\lambda_n t_0} v_n(\mathbf{x}) = f(\mathbf{x}). \quad (12.95)$$

Self-adjointness of the boundary value problem implies orthogonality of the eigenfunctions, and hence the coefficients are obtained via the usual inner product formulae:

$$c_n = e^{\lambda_n t_0} \frac{\langle f, v_n \rangle}{\|v_n\|^2} = e^{\lambda_n t_0} \frac{\iiint_{\Omega} f(\mathbf{x}) v_n(\mathbf{x}) dx dy dz}{\iiint_{\Omega} v_n(\mathbf{x})^2 dx dy dz}. \quad (12.96)$$

The resulting solution decays exponentially fast to thermal equilibrium, $u(t, \mathbf{x}) \rightarrow 0$ as $t \rightarrow \infty$, typically at a rate equal to the smallest positive eigenvalue $\lambda_1 > 0$, although special solutions, whose initial series coefficients vanish, will decay at a faster rate governed by a higher eigenvalue. Since the higher modes — the terms with $n \gg 0$ — go to zero extremely rapidly with increasing t , the solution can be well approximated by the first few terms in its eigenfunction expansion. As a consequence, the heat equation rapidly smooths out discontinuities and eliminates high-frequency noise in the initial data.

Unfortunately, explicit formulas for the eigenfunctions and eigenvalues are rare. Most explicit eigensolutions of the Helmholtz boundary value problem require a further separation of variables. In a rectangular box, one separates the solution into a product of functions depending upon the individual Cartesian coordinates, and the eigenfunctions are written as products of trigonometric functions; see Exercise 12.4.1 for details. In a cylindrical domain, the separation is effected in cylindrical coordinates, which leads to eigensolutions involving trigonometric and Bessel functions, as outlined in Exercise 12.4.5. The most interesting and enlightening case is a spherical domain, and we treat this particular problem in complete detail in the ensuing subsection.

Exercises

- ◇ 12.4.1. Let $B = \{0 < x < a, 0 < y < b, 0 < z < c\}$ be a solid box of size $a \times b \times c$.
- (a) Write down an initial-boundary value problem for the thermodynamics of the box when all its sides are all held at 0° and its initial temperature is $f(x, y, z)$. (b) Use separation of variables to construct the normal mode solutions. (c) Write down a series representing the general solution to the initial-boundary value problem. What are the formulas for the coefficients in your series? (d) What is the equilibrium temperature? How fast does the temperature in the box decay to equilibrium?
- 12.4.2. *True or false:* In the context of Exercise 12.4.1, among all boxes of a given volume V , a cube decays slowest to thermal equilibrium. What is the cube's decay rate?
- 12.4.3. Answer Exercises 12.4.1 and 12.4.2 when the top of the box, where $z = c$, is insulated.
- 12.4.4. A rectangular brick of size 1 cm \times 2 cm \times 3 cm made out of material with diffusion coefficient $\gamma = 6$ is insulated on five sides, while one of its small ends is held at temperature $u(x, y, 0) = \cos \pi x \cos 2\pi y$. (a) Find the eventual equilibrium temperature distribution. (b) If the brick is initially heated in an oven, how fast does it return to equilibrium?
- ◇ 12.4.5. Let $C = \{0 \leq \sqrt{x^2 + y^2} < a, 0 < z < h\}$ be a solid cylinder of radius a and height h .
- (a) Write down an initial-boundary value problem in cylindrical coordinates for the thermodynamics of the cylinder when its sides, top, and bottom are all held at 0° .
- (b) Use separation of variables to write down a series representing the general solution to the initial-boundary value problem. What are the formulas for the coefficients in your series?

- (c) What is the eventual equilibrium temperature?
 (d) How fast does the temperature in the cylinder go to equilibrium?

- 12.4.6. Find the solution to the initial-boundary value problem in Exercise 12.4.5 when the initial temperature of the cylinder is uniformly 30° . *Hint:* Use (11.112) to evaluate the coefficients.
- ♡ 12.4.7. A cylindrical can that contains 355 ml of soda is removed from the refrigerator. Find the optimal cylindrical shape for such a can in order to keep the soda cold the longest. Is this the manufactured shape of a standard soda can in your country?
- ♡ 12.4.8. *True or false:* Among all solid cylinders of a given volume, the one that reaches thermal equilibrium the slowest, when subject to homogeneous Dirichlet boundary conditions, is the one that has the least surface area. Justify your answer.
- ♡ 12.4.9. Among all fully insulated solid cylinders of unit volume, which cools down
 (i) the slowest? (ii) the fastest?
- ◇ 12.4.10. Write down a series for the solution to the homogeneous Neumann boundary value problem for the heat equation on a bounded domain $\Omega \subset \mathbb{R}^3$, corresponding to the thermodynamics of a completely insulated solid body. What is the equilibrium temperature of the body? Does the solution decay to equilibrium? If so, how fast?
- ◇ 12.4.11. Suppose $u(t, x, y, z)$ is a solution to the heat equation on a fully insulated bounded domain $\Omega \subset \mathbb{R}^3$. Use the identities in Exercise 12.1.11 to prove the following:
 (a) The total heat $H(t) = \iiint_{\Omega} u(t, x, y, z) dx dy dz$ is conserved, i.e., is constant. Explain how this can be used to determine the equilibrium temperature of the body.
 (b) If u is a non-equilibrium solution, its squared L^2 norm $E(t) = \iiint_{\Omega} u(t, x, y, z)^2 dx dy dz$ is a strictly decreasing function of t .
 (c) Use part (b) to prove uniqueness of solutions to the initial value problem.
- ◇ 12.4.12. State and prove a Maximum Principle for the three-dimensional heat equation.

Heating of a Ball

Our goal is to study heat propagation in a solid spherical body, e.g., the Earth.[†] For simplicity, we take the diffusivity $\gamma = 1$, and consider the heat equation on a solid spherical ball of unit radius, $B_1 = \{\|\mathbf{x}\| < 1\}$, that is subject to homogeneous Dirichlet boundary conditions. Once we know how to solve this particular case, an easy scaling argument, as outlined in Exercise 12.4.16, will allow us to find the solution for a ball of arbitrary radius and general diffusivity.

As usual, when dealing with a spherical geometry, we adopt spherical coordinates r, φ, θ , as in (12.15), in terms of which the heat equation takes the form

$$\frac{\partial u}{\partial t} = \Delta u = \frac{\partial^2 u}{\partial r^2} + \frac{2}{r} \frac{\partial u}{\partial r} + \frac{1}{r^2} \frac{\partial^2 u}{\partial \varphi^2} + \frac{\cos \varphi}{r^2 \sin \varphi} \frac{\partial u}{\partial \varphi} + \frac{1}{r^2 \sin^2 \varphi} \frac{\partial^2 u}{\partial \theta^2}, \quad (12.97)$$

where we have used our handy spherical coordinate formula (12.16) for the Laplacian. The

[†] In this admittedly simplistic model, we are assuming that the Earth is composed of a completely uniform and isotropic solid material.

standard diffusive separation of variables ansatz

$$u(t, r, \varphi, \theta) = e^{-\lambda t} v(r, \varphi, \theta)$$

requires us to analyze the spherical coordinate form of the Helmholtz equation

$$\Delta v + \lambda v = \frac{\partial^2 v}{\partial r^2} + \frac{2}{r} \frac{\partial v}{\partial r} + \frac{1}{r^2} \frac{\partial^2 v}{\partial \varphi^2} + \frac{\cos \varphi}{r^2 \sin \varphi} \frac{\partial v}{\partial \varphi} + \frac{1}{r^2 \sin^2 \varphi} \frac{\partial^2 v}{\partial \theta^2} + \lambda v = 0 \quad (12.98)$$

on the unit ball $\Omega = \{r < 1\}$ under homogeneous Dirichlet boundary conditions. To make further progress, we invoke a second variable separation, splitting off the radial coordinate by setting

$$v(r, \varphi, \theta) = p(r) w(\varphi, \theta).$$

The function w must be 2π -periodic in θ and well defined on the z -axis, i.e., when $\varphi = 0, \pi$. Substituting this ansatz into (12.98), and separating all the r -dependent terms from those terms depending on the angular variables φ, θ leads to a pair of differential equations involving a separation constant, denoted by μ . The first is an ordinary differential equation

$$r^2 \frac{d^2 p}{dr^2} + 2r \frac{dp}{dr} + (\lambda r^2 - \mu)p = 0, \quad (12.99)$$

for the radial component $p(r)$, while the second is a familiar partial differential equation

$$\Delta_S w + \mu w = \frac{\partial^2 w}{\partial \varphi^2} + \frac{\cos \varphi}{\sin \varphi} \frac{\partial w}{\partial \varphi} + \frac{1}{\sin^2 \varphi} \frac{\partial^2 w}{\partial \theta^2} + \mu w = 0, \quad (12.100)$$

for its angular counterpart $w(\varphi, \theta)$. The operator Δ_S is the *spherical Laplacian* from (12.19). In Section 12.2, we showed that its eigenvalues are

$$\mu_m = m(m+1) \quad \text{for} \quad m = 0, 1, 2, 3, \dots$$

The m^{th} eigenvalue admits $2m+1$ linearly independent eigenfunctions: the spherical harmonics $Y_m^0, \dots, Y_m^m, \tilde{Y}_m^1, \dots, \tilde{Y}_m^m$ defined in (12.38).

Spherical Bessel Functions

The radial ordinary differential equation (12.99) can be solved by setting

$$q(r) = \sqrt{r} p(r). \quad (12.101)$$

We use the product rule to relate the derivatives of q and p , whereby

$$p = \frac{q}{r^{1/2}}, \quad \frac{dp}{dr} = \frac{1}{r^{1/2}} \frac{dq}{dr} - \frac{q}{2r^{3/2}}, \quad \frac{d^2 p}{dr^2} = \frac{1}{r^{1/2}} \frac{d^2 q}{dr^2} - \frac{1}{r^{3/2}} \frac{dq}{dr} + \frac{3q}{4r^{5/2}}.$$

Substituting these expressions back into (12.99) with $\mu = \mu_m = m(m+1)$ and multiplying the resulting equation by \sqrt{r} , we discover that $q(r)$ must solve the differential equation

$$r^2 \frac{d^2 q}{dr^2} + r \frac{dq}{dr} + [\lambda r^2 - (m + \frac{1}{2})^2] q = 0, \quad (12.102)$$

which we recognize as the rescaled Bessel equation (11.56) of half-integer order $m + \frac{1}{2}$. Consequently, the solution to (12.102) that remains bounded at $r = 0$ is (up to a scalar multiple) the rescaled Bessel function

$$q(r) = J_{m+1/2}(\sqrt{\lambda} r).$$

The corresponding solution

$$p(r) = r^{-1/2} J_{m+1/2}(\sqrt{\lambda} r) \tag{12.103}$$

to (12.99) is important enough to warrant a special name.

Definition 12.13. The *spherical Bessel function* of order $m \geq 0$ is defined by the formula

$$S_m(x) = \sqrt{\frac{\pi}{2x}} J_{m+1/2}(x). \tag{12.104}$$

Remark: The multiplicative factor $\sqrt{\pi/2}$ is included in the definition so as to avoid annoying factors of $\sqrt{\pi}$ and $\sqrt{2}$ in the subsequent formulas.

Surprisingly, unlike the Bessel functions of integer order, the spherical Bessel functions are all elementary functions! Comparing (12.104) with (11.105), we see that the spherical Bessel function of order 0 is

$$S_0(x) = \frac{\sin x}{x}. \tag{12.105}$$

The corresponding explicit formulas for the higher-order spherical Bessel functions can be obtained through the general recurrence relation

$$S_{m+1}(x) = -\frac{dS_m}{dx} + \frac{m}{x} S_m(x), \tag{12.106}$$

which is a consequence of the Bessel function recurrence formula (11.111). Indeed,

$$\begin{aligned} \frac{dS_m}{dx} &= \sqrt{\frac{\pi}{2x}} \frac{dJ_{m+1/2}}{dx} - \frac{1}{2} \sqrt{\frac{\pi}{2}} \frac{1}{x^{3/2}} J_{m+1/2}(x) \\ &= -\sqrt{\frac{\pi}{2x}} \left[J_{m+3/2}(x) + \frac{m + \frac{1}{2}}{x} J_{m+1/2}(x) \right] - \frac{1}{2} \sqrt{\frac{\pi}{2}} \frac{1}{x^{3/2}} J_{m+1/2}(x) \\ &= -\sqrt{\frac{\pi}{2x}} J_{m+3/2}(x) + \frac{m}{x} \sqrt{\frac{\pi}{2x}} J_{m+1/2}(x) = -S_{m+1}(x) + \frac{m}{x} S_m(x). \end{aligned}$$

The next few spherical Bessel functions are, therefore,

$$\begin{aligned} S_1(x) &= -\frac{dS_0}{dx} = -\frac{\cos x}{x} + \frac{\sin x}{x^2}, \\ S_2(x) &= -\frac{dS_1}{dx} + \frac{S_1}{x} = -\frac{\sin x}{x} - \frac{3 \cos x}{x^2} + \frac{3 \sin x}{x^3}, \\ S_3(x) &= -\frac{dS_2}{dx} + \frac{2S_2}{x} = \frac{\cos x}{x} - \frac{6 \sin x}{x^2} - \frac{15 \cos x}{x^3} + \frac{15 \sin x}{x^4}, \end{aligned} \tag{12.107}$$

and so on. **Figure 11.4** provides graphs of the first four spherical Bessel functions on the interval $0 \leq x \leq 20$; the vertical axes range from -0.5 to 1.0 . We note that

$$S_0(0) = 1, \quad \text{whereas} \quad S_m(0) = 0 \quad \text{for} \quad m > 0, \tag{12.108}$$

whose proof is the task of Exercise 12.4.26. Thus, our radial solution (12.103) is, apart from an inessential constant multiple, a rescaled spherical Bessel function of order m :

$$p(r) = S_m(\sqrt{\lambda} r).$$

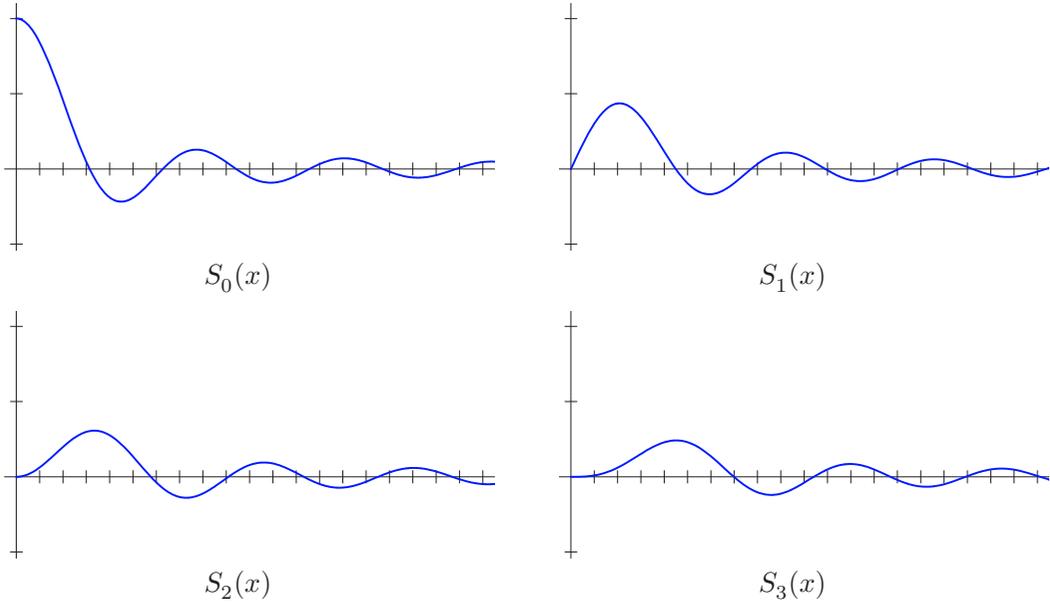


Figure 12.8. Spherical Bessel functions.

So far, we have not taken into account the (homogeneous) Dirichlet boundary condition at $r = 1$. This requires

$$p(1) = 0, \quad \text{and hence} \quad S_m(\sqrt{\lambda}) = 0.$$

Therefore, $\sqrt{\lambda}$ must be a root of the m^{th} order spherical Bessel function. We introduce the notation

$$0 < \sigma_{m,1} < \sigma_{m,2} < \sigma_{m,3} < \dots$$

to denote the successive (positive) *spherical Bessel roots*, satisfying

$$S_m(\sigma_{m,n}) = 0 \quad \text{for} \quad n = 1, 2, \dots \tag{12.109}$$

In particular the roots of the zeroth order spherical Bessel function $S_0(x) = x^{-1} \sin x$ are just the integer multiples of π :

$$\sigma_{0,n} = n\pi \quad \text{for} \quad n = 1, 2, \dots$$

The higher-order roots are not expressible in terms of known constants. A table of all spherical Bessel roots that are < 13 appears below. The columns of the table are indexed by m , the order, while the rows are indexed by n , the root number.

Re-assembling the individual constituents, we have now demonstrated that the separable eigenfunctions of the Helmholtz equation on a solid ball of radius 1, when subject to homogeneous Dirichlet boundary conditions, are products of spherical Bessel functions and spherical harmonics,

$$\begin{aligned} v_{k,m,n}(r, \varphi, \theta) &= S_m(\sigma_{m,n} r) Y_m^k(\varphi, \theta), & m &= 0, 1, 2, \dots, \\ \tilde{v}_{k,m,n}(r, \varphi, \theta) &= S_m(\sigma_{m,n} r) \tilde{Y}_m^k(\varphi, \theta), & k &= 0, \dots, m, \\ & & n &= 1, 2, 3, \dots \end{aligned} \tag{12.110}$$

Spherical Bessel Roots $\sigma_{m,n}$

| $n \backslash m$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|------------------|---------|---------|---------|---------|---------|---------|---------|---------|-------------|
| 1 | 3.1416 | 4.4934 | 5.7635 | 6.9879 | 8.1826 | 9.3558 | 10.5128 | 11.6570 | 12.7908 ... |
| 2 | 6.2832 | 7.7253 | 9.0950 | 10.4171 | 11.7049 | 12.9665 | ⋮ | ⋮ | ⋮ |
| 3 | 9.4248 | 10.9041 | 12.3229 | ⋮ | ⋮ | ⋮ | | | |
| 4 | 12.5664 | ⋮ | ⋮ | | | | | | |
| ⋮ | ⋮ | | | | | | | | |

The corresponding eigenvalues

$$\lambda_{m,n} = \sigma_{m,n}^2, \quad m = 0, 1, 2, \dots, \quad n = 1, 2, 3, \dots, \quad (12.111)$$

are the squared spherical Bessel roots. Since there are $2m + 1$ independent spherical harmonics of order m , the eigenvalue $\lambda_{m,n}$ admits $2m + 1$ linearly independent eigenfunctions, namely $v_{0,m,n}, \dots, v_{m,m,n}, \tilde{v}_{1,m,n}, \dots, \tilde{v}_{m,m,n}$. In particular, the radially symmetric solutions are the eigenfunctions with $k = m = 0$:

$$v_n(r) = v_{0,0,n}(r) = S_0(\sigma_{0,n} r) = \frac{\sin n\pi r}{n\pi r}, \quad n = 1, 2, \dots. \quad (12.112)$$

Further analysis, cf. [34], demonstrates that the separable solutions (12.110) form a complete system of eigenfunctions for the Helmholtz equation on the unit ball with homogeneous Dirichlet boundary conditions.

We have thus completely determined the basic separable solutions to the heat equation on a solid unit ball subject to homogeneous Dirichlet boundary conditions. They are products of exponential functions of time, spherical Bessel functions of the radius, and spherical harmonics:

$$\begin{aligned} u_{k,m,n}(t, r, \varphi, \theta) &= e^{-\sigma_{m,n}^2 t} S_m(\sigma_{m,n} r) Y_m^k(\varphi, \theta), \\ \tilde{u}_{k,m,n}(t, r, \varphi, \theta) &= e^{-\sigma_{m,n}^2 t} S_m(\sigma_{m,n} r) \tilde{Y}_m^k(\varphi, \theta). \end{aligned} \quad (12.113)$$

The general solution can be written as an infinite ‘‘Fourier–Bessel–spherical harmonic’’ series in these fundamental modes:

$$\begin{aligned} u(t, r, \varphi, \theta) &= \sum_{m=0}^{\infty} \sum_{n=1}^{\infty} e^{-\sigma_{m,n}^2 t} S_m(\sigma_{m,n} r) \left(\frac{c_{0,m,n}}{2} Y_m^0(\varphi, \theta) \right. \\ &\quad \left. + \sum_{k=1}^m [c_{k,m,n} Y_m^k(\varphi, \theta) + \tilde{c}_{k,m,n} \tilde{Y}_m^k(\varphi, \theta)] \right). \end{aligned} \quad (12.114)$$

The series’ coefficients are uniquely prescribed by the initial data $u(0, r, \varphi, \theta) = f(r, \varphi, \theta)$,

and their explicit formulae[†]

$$\begin{aligned}
 c_{k,m,n} &= \frac{(2m+1)(m-k)!}{\pi(m+k)! S_{m+1}(\sigma_{m,n})^2} \int_{-\pi}^{\pi} \int_0^{\pi} \int_0^1 f(r, \varphi, \theta) v_{k,m,n}(r, \varphi, \theta) r^2 \sin \varphi \, dr \, d\varphi \, d\theta, \\
 \tilde{c}_{k,m,n} &= \frac{(2m+1)(m-k)!}{\pi(m+k)! S_{m+1}(\sigma_{m,n})^2} \int_{-\pi}^{\pi} \int_0^{\pi} \int_0^1 f(r, \varphi, \theta) \tilde{v}_{k,m,n}(r, \varphi, \theta) r^2 \sin \varphi \, dr \, d\varphi \, d\theta,
 \end{aligned}
 \tag{12.115}$$

follow from the usual orthogonality relations among the eigenfunctions, combined with the formulas

$$\begin{aligned}
 \|v_{0,m,n}\| &= \sqrt{\frac{2\pi}{2m+1}} S_{m+1}(\sigma_{m,n}), \\
 \|v_{k,m,n}\| = \|\tilde{v}_{k,m,n}\| &= \sqrt{\frac{\pi(m+k)!}{(2m+1)(m-k)!}} S_{m+1}(\sigma_{m,n}), \quad k > 0,
 \end{aligned}
 \tag{12.116}$$

for their norms, to be established in Exercise 12.4.29. In particular, the slowest-decaying mode is the spherically symmetric function

$$u_{0,0,1}(t, r) = \frac{e^{-\pi^2 t} \sin \pi r}{\pi r}, \tag{12.117}$$

corresponding to the smallest eigenvalue $\lambda_{0,1} = \sigma_{0,1}^2 = \pi^2$. Therefore, typically, the decay to thermal equilibrium of a unit sphere is at an exponential rate of $\pi^2 \approx 9.8696$, or, to a very rough approximation, 10.

Exercises

- 12.4.13. It takes a solid ball of radius 1 cm ten minutes to return to (approximate) thermal equilibrium. How long does it take a similar ball of radius 2?
- 12.4.14. If a 200-gram potato served hot from the oven takes 15 minutes until its maximum temperature is less than 40°C , how long does it take a 300-gram potato of the same shape to cool off?
- ♡ 12.4.15. A uniform solid metal ball of radius 1 meter, with diffusion coefficient $\gamma = 2$, is taken from a 300° oven and immersed in a bucket of ice water. (a) Write down an initial-boundary value problem that describes the temperature of the ball. (b) Find a series solution for the temperature. (c) At what time is the temperature $\leq 50^\circ$ throughout the ball?
- ◇ 12.4.16. Find the decay rate to thermal equilibrium of a solid spherical ball of radius R and diffusion coefficient γ when subject to homogeneous Dirichlet boundary conditions.
- 12.4.17. *True or false:* A heated solid hemisphere placed in a 0° environment cools down twice as fast as a solid sphere of the same radius made out of the same material.
- 12.4.18. A fully insulated solid spherical ball of radius 1 has initial temperature distribution $f(r, \varphi, \theta)$. (a) Write down a formula for the equilibrium temperature of the ball. (b) What is the rate of decay of the ball to thermal equilibrium?

[†] We use the spherical coordinate form of the L^2 inner product on the ball.

- 12.4.19. Which cools down to equilibrium faster: a fully insulated solid ball or one whose boundary is held fixed at 0° ? How much faster?
- 12.4.20. A solid sphere and solid cube are made out of the same material and have the same volume. Both are heated in an oven and then submerged in a large vat of water. Which will cool down faster? Explain and justify your answer.
- 12.4.21. Answer Exercise 12.4.20 when the two solids have the same surface area.
- 12.4.22. Suppose the solid spherical shell in Exercise 12.2.7 starts off at room temperature. Assuming that the water in the center remains at 100° , find the rate at which the shell tends to thermal equilibrium.
- ♡ 12.4.23. The thermodynamics of a thin, uniform, spherical shell of unit radius is governed by the *spherical heat equation* $u_t = \gamma \Delta_S u$, $u(0, \varphi, \theta) = f(\varphi, \theta)$, in which Δ_S is the spherical Laplacian (12.19). The solution $u(t, \varphi, \theta)$ represents the temperature of the point on the unit sphere with angular coordinates φ, θ , while $f(\varphi, \theta)$ is the initial temperature distribution. (a) Find the eigensolutions. (b) Write down the solution to the initial value problem as a series in eigensolutions. (c) What is the final equilibrium temperature of the spherical shell? (d) What is its rate of decay to equilibrium? (e) Find the solution and the final equilibrium temperature when $f(\varphi, \theta) = (i) \sin \varphi \cos \theta$; $(ii) \cos 2\varphi$.
- 12.4.24. A spherical potato, of radius $R = 7.5$ cm and thermal diffusivity $\gamma = .3 \text{ cm}^2/\text{sec}$, is initially at room temperature, 25°C , and is placed in a pot of boiling water at 100°C . The potato is cooked when it has reached the temperature of at least 90°C throughout. How long do you have to wait until the potato is done?
- 12.4.25. (a) Explain why the spherical Bessel function $S_1(x)$ is bounded at $x = 0$. What is $S_1(0)$? (b) Answer the same question for $S_2(x)$.
- ◇ 12.4.26. Prove the formulae (12.108).
- ◇ 12.4.27. (a) Find a recurrence relation expressing the spherical Bessel function $S_{m-1}(x)$ in terms of $S_m(x)$. (b) Prove that
- $$\frac{d}{dx} [x^3 (S_m(x)^2 - S_{m-1}(x) S_{m+1}(x))] = 2x^2 S_m(x)^2.$$
- ◇ 12.4.28. Let $m \geq 0$ be a fixed integer. (a) Prove that the rescaled spherical Bessel functions $v_n(r) = S_m(\sigma_{m,n} r)$, $n = 1, 2, \dots$, are mutually orthogonal under the inner product $\langle f, g \rangle = \int_0^1 f(r) g(r) r^2 dr$. (b) Prove that $\|v_n\| = \frac{1}{\sqrt{2}} |S_{m+1}(\sigma_{m,n})|$. *Hint*: Mimic the method outlined in Exercise 11.4.22, using the identity in Exercise 12.4.27(b).
- ◇ 12.4.29. (a) Use the result of Exercise 12.4.28 to prove the formulae (12.116) for the L^2 norms of the eigenfunctions (12.110). (b) Justify the formulae (12.115).

The Fundamental Solution to the Heat Equation in Space

For the heat equation (as well as more general diffusion equations), the fundamental solution measures the response of the body to an instantaneously applied concentrated unit heat source. Thus, given a point $\boldsymbol{\xi} = (\xi, \eta, \zeta) \in \Omega$ within the body, the *fundamental solution*

$$u(t, \mathbf{x}) = F(t, \mathbf{x}; \boldsymbol{\xi}) = F(t, x, y, z; \xi, \eta, \zeta)$$

solves the initial-boundary value problem

$$u_t = \Delta u, \quad u(0, \mathbf{x}) = \delta(\mathbf{x} - \boldsymbol{\xi}), \quad \text{for } \mathbf{x} \in \Omega, \quad t > 0, \quad (12.118)$$

subject to the selected homogeneous boundary conditions — Dirichlet, Neumann, or mixed.

Explicit formulas for the fundamental solution are rare, although in bounded domains it is possible to construct it as an eigenfunction series, as described in Section 9.5. The one case amenable to a complete analysis is that in which the heat is distributed over all of three-dimensional space, so $\Omega = \mathbb{R}^3$. We recall that Lemma 11.11 showed how to construct solutions of the two-dimensional heat equation as products of one-dimensional solutions. In a similar manner, if $p(t, x)$, $q(t, x)$, and $r(t, x)$ are any three solutions to the one-dimensional heat equation $u_t = \gamma u_{xx}$, then their product

$$u(t, x, y, z) = p(t, x) q(t, y) r(t, z) \quad (12.119)$$

is a solution to the three-dimensional heat equation

$$u_t = \gamma (u_{xx} + u_{yy} + u_{zz}).$$

In particular, choosing

$$p(t, x) = \frac{e^{-(x-\xi)^2/4\gamma t}}{2\sqrt{\pi\gamma t}}, \quad q(t, y) = \frac{e^{-(y-\eta)^2/4\gamma t}}{2\sqrt{\pi\gamma t}}, \quad r(t, z) = \frac{e^{-(z-\zeta)^2/4\gamma t}}{2\sqrt{\pi\gamma t}},$$

to all be one-dimensional fundamental solutions, we are immediately led to the fundamental solution in the form of a three-dimensional *Gaussian filter*.

Theorem 12.14. *The fundamental solution*

$$F(t, \mathbf{x}; \boldsymbol{\xi}) = F(t, \mathbf{x} - \boldsymbol{\xi}) = \frac{e^{-\|\mathbf{x}-\boldsymbol{\xi}\|^2/(4\gamma t)}}{8(\pi\gamma t)^{3/2}} \quad (12.120)$$

solves the three-dimensional heat equation $u_t = \gamma \Delta u$ on \mathbb{R}^3 for $t > 0$, with an initial temperature equal to a delta function concentrated at the point $\mathbf{x} = \boldsymbol{\xi}$.

Thus, the initially concentrated heat energy immediately begins to spread out in a spherically symmetric manner, with a minuscule, but nonzero effect that is felt immediately arbitrarily far away from the initial concentration. At each individual point $\mathbf{x} \in \mathbb{R}^3$, after an initial warm-up, the temperature decays back to zero at a rate proportional to $t^{-3/2}$ — more rapidly than in two dimensions, because, intuitively, there are more directions in which the heat energy can disperse.

To solve a more general initial value problem with the initial temperature distributed over all of space, we first write

$$u(0, \mathbf{x}) = f(\mathbf{x}) = \iiint f(\boldsymbol{\xi}) \delta(\mathbf{x} - \boldsymbol{\xi}) d\xi d\eta d\zeta$$

as a linear superposition of delta functions. By linearity, the solution to the initial value problem is given by the corresponding superposition

$$u(t, \mathbf{x}) = \frac{1}{8(\pi\gamma t)^{3/2}} \iiint f(\boldsymbol{\xi}) e^{-\|\mathbf{x}-\boldsymbol{\xi}\|^2/(4\gamma t)} d\xi d\eta d\zeta \quad (12.121)$$

of the fundamental solutions. Since the fundamental solution has exponential decay as $\|\mathbf{x}\| \rightarrow \infty$, the superposition formula is valid even for initial temperature distributions that are moderately increasing at large distances. We remark that the integral (12.121) has the form of a three-dimensional convolution

$$u(t, \mathbf{x}) = F(t, \mathbf{x}) * f(\mathbf{x}) = \iiint f(\boldsymbol{\xi}) F(t, \mathbf{x} - \boldsymbol{\xi}) d\xi d\eta d\zeta \quad (12.122)$$

of the initial data with a one-parameter family of increasingly spread-out Gaussian filters. Thus, as before, convolution with a Gaussian filter has a smoothing effect on the initial temperature distribution.

Exercises

- 12.4.30. *True or false:* In a three-dimensional medium, heat energy propagates at infinite speed.
- 12.4.31. A solid spherical ball of radius 1 is heated to 100° and inserted into a three-dimensional medium filling the rest of \mathbb{R}^3 with uniform temperature 0° .
- (a) Write down an integral formula for the subsequent temperature distribution over \mathbb{R}^3 at time $t > 0$, assuming a common diffusion coefficient $\gamma = 1$.
- (b) Evaluate the resulting integral using spherical coordinates.
- 12.4.32. (a) Prove that $u(t, r)$ is a spherically symmetric solution to the three-dimensional heat equation if and only if $w(t, r) = r u(t, r)$ solves the one-dimensional heat equation: $w_t = w_{rr}$.
- (b) *True or false:* If $w(t, r)$ is the fundamental solution for the one-dimensional heat equation based at $r = 0$, then $u(t, r) = w(t, r)/r$ is the fundamental solution for the three-dimensional heat equation based at the origin.
- 12.4.33. Construct the solution to the initial value problem in Exercise 12.4.31 using radial symmetry and Exercise 12.4.32.
- ♥ 12.4.34. Suppose that, as Earth orbits the sun, its surface is subject to yearly periodic temperature variations $a \cos \omega t$, where the frequency ω is given by (4.56). (a) Assuming, for simplicity, that the Earth is a homogeneous solid ball, of radius R , formulate an initial-boundary value problem that governs the temperature fluctuations within the Earth due to its orbiting the sun. (b) At what depth does the temperature vary out of phase with the surface, i.e., is the warmest in winter and coldest in summer? Compare your answer with the root cellar computation at the end of Section 4.1. *Hint:* Use Exercise 12.4.32.
- 12.4.35. (a) Prove that if $u(t, x)$ is any (sufficiently smooth) solution to the heat equation, so is its time derivative $v = \partial u / \partial t$. (b) Write out the time derivative of the fundamental solution, and the initial value problem it satisfies.
- 12.4.36. Write down an explicit eigenfunction series for the fundamental solution $F(t, \mathbf{x}; \boldsymbol{\xi})$ to the heat equation in a unit cube with thermal diffusivity $\gamma = 1$ that is subject to homogeneous Dirichlet boundary conditions.
- 12.4.37. Write down an explicit eigenfunction series for the fundamental solution $F(t, \mathbf{x}; \boldsymbol{\xi})$ to the heat equation in a ball of radius 1 that has thermal diffusivity $\gamma = 1$ and is subject to homogeneous Dirichlet boundary conditions.
- ◇ 12.4.38. Justify the statement that formula (12.119) provides a solution to the three-dimensional heat equation.
- 12.4.39. Fill in the details of the proof of Theorem 12.14.

12.5 The Wave Equation for Three-Dimensional Media

The *three-dimensional wave equation*

$$u_{tt} = c^2 \Delta u = c^2 (u_{xx} + u_{yy} + u_{zz}), \quad (12.123)$$

in which $c > 0$ denotes the speed of light, governs the propagation of waves in a homogeneous isotropic three-dimensional medium, e.g., electromagnetic waves (light, X-rays, radio waves, etc.) in empty space. In this context, while the electric and magnetic vector fields \mathbf{E} , \mathbf{B} are intrinsically coupled by the more complicated system of Maxwell's equations, each individual component satisfies the wave equation; see Exercise 12.5.14 for details.

The wave equation also models certain restricted classes of vibrations of a uniform solid body. The solution $u(t, \mathbf{x}) = u(t, x, y, z)$ represents a scalar-valued displacement of the body at time t and position $\mathbf{x} = (x, y, z) \in \Omega \subset \mathbb{R}^3$. For example, $u(t, \mathbf{x})$ might represent the radial displacement of the body. One imposes suitable boundary conditions, e.g., Dirichlet, Neumann, or mixed, on $\partial\Omega$, along with a pair of initial conditions

$$u(0, \mathbf{x}) = f(\mathbf{x}), \quad \frac{\partial u}{\partial t}(0, \mathbf{x}) = g(\mathbf{x}), \quad \mathbf{x} \in \Omega, \quad (12.124)$$

that specify the body's initial displacement and initial velocity. As long as the initial and boundary data are reasonably nice, there exists a unique classical solution to the initial-boundary value problem for all $-\infty < t < \infty$, cf. [38, 61, 99]. Thus, in contrast to the heat equation, one can follow solutions to the wave equation both forwards and backwards in time.

Let us focus our attention on the homogeneous boundary value problem. The fundamental vibrational modes are found by imposing our usual trigonometric ansatz

$$u(t, x, y, z) = \cos(\omega t) v(x, y, z) \quad \text{or} \quad \sin(\omega t) v(x, y, z).$$

Substituting into the wave equation (12.123), we discover (yet again) that $v(x, y, z)$ must be an eigenfunction for the associated Helmholtz eigenvalue problem

$$\Delta v + \lambda v = 0, \quad \text{where} \quad \lambda = \frac{\omega^2}{c^2}, \quad (12.125)$$

coupled to the relevant boundary conditions. In the positive definite cases, i.e., Dirichlet and mixed boundary conditions, the eigenvalues $\lambda_k = \omega_k^2/c^2 > 0$ are all positive. Each eigenfunction $v_k(x, y, z)$ yields two normal vibrational modes

$$u_k(t, x, y, z) = \cos(\omega_k t) v_k(x, y, z), \quad \tilde{u}_k(t, x, y, z) = \sin(\omega_k t) v_k(x, y, z),$$

of frequency $\omega_k = c\sqrt{\lambda_k}$ equal to the square root of the corresponding eigenvalue multiplied by the wave speed. The general solution is a quasiperiodic linear combination,

$$u(t, x, y, z) = \sum_{k=1}^{\infty} [a_k \cos(\omega_k t) + b_k \sin(\omega_k t)] v_k(x, y, z), \quad (12.126)$$

of the eigenmodes. The coefficients a_k, b_k are uniquely prescribed by the initial conditions (12.124). Thus,

$$u(0, x, y, z) = \sum_{k=1}^{\infty} a_k v_k(x, y, z) = f(x, y, z),$$

$$\frac{\partial u}{\partial t}(0, x, y, z) = \sum_{k=1}^{\infty} \omega_k b_k v_k(x, y, z) = g(x, y, z).$$

The explicit formulas follow immediately from the orthogonality of the eigenfunctions:

$$a_k = \frac{\langle f, v_k \rangle}{\|v_k\|^2} = \frac{\iiint_{\Omega} f v_k \, dx \, dy \, dz}{\iiint_{\Omega} v_k^2 \, dx \, dy \, dz}, \quad b_k = \frac{1}{\omega_k} \frac{\langle g, v_k \rangle}{\|v_k\|^2} = \frac{\iiint_{\Omega} g v_k \, dx \, dy \, dz}{\omega_k \iiint_{\Omega} v_k^2 \, dx \, dy \, dz}. \tag{12.127}$$

In the positive semi-definite Neumann case, there is an additional zero eigenvalue $\lambda_0 = 0$ corresponding to the constant null eigenfunction $v_0(x, y, z) \equiv 1$. This results in two additional terms in the eigenfunction expansion — a constant term

$$a_0 = \frac{1}{\text{vol } \Omega} \iiint_{\Omega} f(x, y, z) \, dx \, dy \, dz$$

that equals the average initial displacement, and an unstable mode $b_0 t$ that grows linearly in time, whose speed

$$b_0 = \frac{1}{\text{vol } \Omega} \iiint_{\Omega} g(x, y, z) \, dx \, dy \, dz$$

is the average initial velocity over the entire body. Thus, the unstable mode will be excited if and only if there is a nonzero net initial velocity: $b_0 \neq 0$.

Most of the basic solution techniques we learned in the two-dimensional case apply here, and we will not dwell on the details. The case of a rectangular box is a particularly straightforward application of the method of separation of variables, and is outlined in the exercises. A similar analysis, now in cylindrical coordinates, can be applied to the case of a vibrating cylinder. The most interesting case is that of a solid spherical ball, which is the subject of the next subsection.

Vibration of Balls and Spheres

Let us focus on the radial vibrations of a solid ball, as modeled by the three-dimensional wave equation (12.123). The solution $u(t, x, y, z)$ represents the radial displacement of the “atom” that is situated at position (x, y, z) when the ball is at rest.

For simplicity, we look at the Dirichlet boundary value problem on the unit ball $B_1 = \{\|\mathbf{x}\| < 1\}$. The normal modes of vibration are governed by the Helmholtz equation (12.125) subject to homogeneous Dirichlet boundary conditions. According to (12.110), the eigenfunctions are

$$\begin{aligned} v_{0,m,n}(r, \varphi, \theta) &= S_m(\sigma_{m,n} r) Y_m^0(\varphi, \theta), & n &= 1, 2, 3, \dots, \\ v_{k,m,n}(r, \varphi, \theta) &= S_n(\sigma_{n,m} r) Y_m^k(\varphi, \theta), & \text{for } m &= 0, 1, 2, \dots, \\ \tilde{v}_{k,m,n}(r, \varphi, \theta) &= S_m(\sigma_{m,n} r) \tilde{Y}_m^k(\varphi, \theta), & k &= 1, 2, \dots, m. \end{aligned} \tag{12.128}$$

Here S_m denotes the m^{th} order spherical Bessel function (12.104), $\sigma_{m,n}$ is its n^{th} root, as in (12.109), while Y_n^m, \tilde{Y}_n^m are the spherical harmonics (12.38). Each eigenvalue

$$\lambda_{m,n} = \sigma_{m,n}^2, \quad m = 0, 1, 2, \dots, \quad n = 1, 2, 3, \dots,$$

corresponds to $2m + 1$ independent eigenfunctions, namely

$$v_{k,m,0}(r, \varphi, \theta), \quad v_{k,m,1}(r, \varphi, \theta), \quad \dots, \quad v_{k,m,m}(r, \varphi, \theta), \quad \tilde{v}_{k,m,1}(r, \varphi, \theta), \quad \dots, \quad \tilde{v}_{k,m,m}(r, \varphi, \theta).$$

The purely radial modes of vibration (12.131) have individual frequencies

$$\omega_{0,n} = \frac{n\pi c}{R}, \quad \text{so} \quad \frac{\omega_{0,n}}{\omega_{0,1}} = n,$$

which appear in the first column of the table. The lowest frequency is $\omega_{0,1} = \pi c/R$, corresponding to a vibration with period $2\pi/\omega_{0,1} = 2R/c$. In particular, for the Earth, the radius $R \approx 6000$ km, and the wave speed in rock is, on average, $c \approx 5$ km/sec, so that the fundamental mode of vibration has period $2R/c \approx 2400$ seconds, or 40 minutes. Of course, we have suppressed almost all interesting terrestrial geology in this very crude approximation, which has been based on the assumption that the Earth is a uniform spherical body, globally vibrating only in its radial direction. A more realistic modeling of the vibrations of the Earth requires an understanding of the basic partial differential equations of linear and nonlinear elastodynamics, [7, 49]. Nonuniformities in the Earth lead to scattering of the vibrational waves, which are then used to locate subterranean geological structures, e.g., oil and gas deposits. Localized vibrations of the Earth are also known as *seismic waves*, and, of course, earthquakes are their most severe manifestation. We refer the interested reader to [5] for an introduction to mathematical seismology. Understanding terrestrial vibrations is an issue of critical importance in geophysics and civil engineering, including the design of structures, buildings, and bridges, requiring the avoidance of potentially catastrophic resonant frequencies.

Example 12.15. The radial vibrations of a hollow thin spherical shell (e.g., an elastic balloon) are governed by the differential equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \Delta_S[u] = c^2 \left(\frac{\partial^2 u}{\partial \varphi^2} + \frac{\cos \varphi}{\sin \varphi} \frac{\partial u}{\partial \varphi} + \frac{1}{\sin^2 \varphi} \frac{\partial^2 u}{\partial \theta^2} \right), \quad (12.133)$$

where Δ_S denotes the spherical Laplacian (12.19). The radial displacement $u(t, \varphi, \theta)$ of a point on the sphere depends only on time t and the angular coordinates φ, θ . The solution $u(t, \varphi, \theta)$ is required to be 2π -periodic in the azimuthal angle θ and bounded at the poles, where $\varphi = 0$ and π .

According to (12.38), the n^{th} eigenvalue of the spherical Laplacian, $\lambda_n = n(n + 1)$, possesses $2n + 1$ linearly independent eigenfunctions, namely, the spherical harmonics

$$Y_n^0(\varphi, \theta), \quad Y_n^1(\varphi, \theta), \quad \dots, \quad Y_n^n(\varphi, \theta), \quad \tilde{Y}_n^1(\varphi, \theta), \quad \dots, \quad \tilde{Y}_n^n(\varphi, \theta).$$

As a consequence, the fundamental frequencies of vibration for a spherical shell are

$$\omega_n = c \sqrt{\lambda_n} = c \sqrt{n(n + 1)}, \quad n = 1, 2, \dots \quad (12.134)$$

The vibrational solutions are quasiperiodic combinations of the fundamental spherical harmonic modes

$$\begin{aligned} \cos(\sqrt{n(n + 1)} t) Y_n^m(\varphi, \theta), & \quad \sin(\sqrt{n(n + 1)} t) Y_n^m(\varphi, \theta), \\ \cos(\sqrt{n(n + 1)} t) \tilde{Y}_n^m(\varphi, \theta), & \quad \sin(\sqrt{n(n + 1)} t) \tilde{Y}_n^m(\varphi, \theta). \end{aligned} \quad (12.135)$$

Representative graphs can be seen in [Figure 12.5](#). The smallest positive eigenvalue is $\lambda_1 = 2$, yielding a lowest tone of frequency $\omega_1 = c\sqrt{2}$. The higher-order frequencies are irrational multiples of the fundamental frequency, implying that a vibrating spherical bell sounds dissonant to our ears.

One further remark is in order. The spherical Laplacian operator is only positive semi-definite, since the lowest mode has eigenvalue $\lambda_0 = 0$, which corresponds to the constant

null eigenfunction $v_0(\varphi, \theta) = Y_0^0(\varphi, \theta) \equiv 1$. Therefore, the wave equation (12.133) admits an unstable mode $b_{0,0} t$, corresponding to a uniform radial inflation; its coefficient

$$b_{0,0} = \frac{3}{4\pi} \iint_{S_1} \frac{\partial u}{\partial t}(0, \varphi, \theta) dS$$

represents the shell's average initial velocity. The existence of such an unstable mode is an artifact of the simplified linear model we are using, which fails to account for nonlinearly elastic effects that serve to constrain the inflation of a spherical balloon.

Exercises

- 12.5.1. Find the eigenfunction series solution to the initial-boundary value problem for the wave equation $u_{tt} = \Delta u$ on a unit cube $C = \{0 < x, y, z < 1\}$, subject to homogeneous Dirichlet boundary conditions and one of the following sets of initial conditions:
 (a) $u(0, x, y, z) = 1$, $u_t(0, x, y, z) = 0$; (b) $u(0, x, y, z) = 0$, $u_t(0, x, y, z) = 1$;
 (c) $u(0, x, y, z) = \sin \pi x \sin \pi y \sin \pi z$, $u_t(0, x, y, z) = 0$; (d) $u(0, x, y, z) = \sin 3\pi x$, $u_t(0, x, y, z) = \sin 2\pi y$; (e) $u(0, x, y, z) = 0$, $u_t(0, x, y, z) = xyz(1-x)(1-y)(1-z)$.
- 12.5.2. Suppose the cube in Exercise 12.5.1 is subject to homogeneous Neumann boundary conditions. Which of the preceding initial value problems leads to an unstable motion of the cube?
- 12.5.3. (a) Find the separable periodic vibrations of a unit cube subject to homogeneous Dirichlet boundary conditions. (b) Can you find a periodic mode that is not separable?
- 12.5.4. Answer Exercise 12.5.3 when one face of the cube is left free, while the other five faces are fixed.
- 12.5.5. Given a material with wave speed $c = 1.5$ cm/sec, find the natural vibrational frequencies of a solid rectangular box of size 1 cm \times 2 cm \times 3 cm whose sides are held fixed. List the lowest five such frequencies in order. Does the box vibrate periodically?
- 12.5.6. Find the natural vibrational frequencies of a solid cylinder of height 2, radius 1, and wave speed $c = 1$, when (a) all sides are fixed; (b) the top and bottom of the cylinder are free, while the curved side is fixed; (c) the curved side of the cylinder is free, while the top and bottom are fixed.
- 12.5.7. Among all solid cylinders of unit volume with fixed boundary, find the one that vibrates the slowest.
- 12.5.8. Does a solid spherical ball that is subject to homogeneous Neumann boundary conditions vibrate (i) faster, (ii) slower, or (iii) at the same rate as the same ball subject to homogeneous Dirichlet conditions. If your answer is (i) or (ii), estimate how much faster or slower.
- 12.5.9. A solid cube and solid sphere are made of the same material and have the same volume. Which vibrates faster when subject to homogeneous Dirichlet boundary conditions?
- 12.5.10. Assuming that they both have the same wave speed and fixed boundaries, which vibrates faster: a solid sphere or a circular membrane of the same radius?
- 12.5.11. A uniform, solid spherical planet is floating freely in outer space. Find its three slowest resonant frequencies.
- 12.5.12. *True or false:* Suppose we have two uniform solid bodies composed of the same material. If the first body cools down to thermal equilibrium the fastest, then it also vibrates the fastest. Explain your answer.

- 12.5.13. (a) Define what is meant by a nodal curve and a nodal region on a vibrating thin spherical shell. (b) *True or false:* All the nodal curves are arcs of circles.
- ♡ 12.5.14. The propagation of electromagnetic waves (including light) is governed by the electric field $\mathbf{E}(t, \mathbf{x})$ and magnetic field $\mathbf{B}(t, \mathbf{x})$, which are both time-dependent vector fields defined for $\mathbf{x} = (x, y, z)$ in a domain $\Omega \subset \mathbb{R}^3$. In empty space, *Maxwell's equations* (as formulated by Heaviside) are

$$\nabla \cdot \mathbf{E} = 0, \quad \nabla \cdot \mathbf{B} = 0, \quad \frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}, \quad \frac{\partial \mathbf{E}}{\partial t} = \frac{1}{\mu_0 \epsilon_0} \nabla \times \mathbf{B}, \quad (12.136)$$

where μ_0, ϵ_0 are, respectively, the *permeability* and *permittivity* constants. Prove that all individual components of \mathbf{E} and \mathbf{B} satisfy the scalar wave equation. What is the wave speed, i.e., the speed of light in empty space?

12.6 Spherical Waves and Huygens' Principle

For any dynamical partial differential equation, the fundamental solution measures the effect of applying an instantaneous concentrated unit impulse at a single point. Two representative physical effects to keep in mind are the light waves emanating from a sudden concentrated blast, e.g., a lightning bolt or a stellar supernova, and the sound waves due to an explosion or thunderclap, propagating in air at a much slower speed. Linear superposition utilizes the fundamental solution to build up more general solutions to initial value problems. For the wave and other second-order vibrational equations, the impulse can be applied either to the initial displacement or to the initial velocity, resulting in two distinct types of fundamental solution. The general solution to the initial value problem will be obtained by a double superposition. In this section, we derive explicit formulas for the two fundamental solutions for the three-dimensional wave equation on all of space, leading to Kirchhoff's formula for the solution to the general initial value problem. An important consequence is Huygens' Principle, which states that, in three-dimensional space, localized initial disturbances remain localized as they propagate. In the final subsection, we apply the method of descent to our three-dimensional solution formulas in order to solve the two-dimensional wave equation, for which, surprisingly, Huygens' Principle is no longer valid.

Spherical Waves

In a uniform isotropic medium, an initial concentrated blast results in a spherically expanding wave, moving away at the speed of light (or sound) in all directions. Invoking translation invariance, we will assume, without loss of generality, that the source of the disturbance is at the origin, and so the solution $u(t, \mathbf{x})$ should depend only on the distance $r = \|\mathbf{x}\|$ from the source. We adopt spherical coordinates and look for a solution $u = u(t, r)$ to the three-dimensional wave equation (12.123) with no angular dependence. Substituting the formula (12.16) for the spherical Laplacian and setting both angular derivatives to 0, we are led to the partial differential equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \left(\frac{\partial^2 u}{\partial r^2} + \frac{2}{r} \frac{\partial u}{\partial r} \right), \quad (12.137)$$

which governs the propagation of spherically symmetric waves in three-dimensional space. Surprisingly, we can explicitly solve (12.137). The secret is to multiply both sides of the equation by r :

$$\frac{\partial^2(ru)}{\partial t^2} = r \frac{\partial^2 u}{\partial t^2} = c^2 \left(r \frac{\partial^2 u}{\partial r^2} + 2 \frac{\partial u}{\partial r} \right) = c^2 \frac{\partial^2}{\partial r^2} (ru).$$

Thus, the function

$$w(t, r) = ru(t, r)$$

satisfies the one-dimensional wave equation

$$\frac{\partial^2 w}{\partial t^2} = c^2 \frac{\partial^2 w}{\partial r^2}. \quad (12.138)$$

According to Theorem 2.14, the general solution to the one-dimensional wave equation (12.138) can be written in d'Alembert form

$$w(t, r) = p(r - ct) + q(r + ct),$$

where $p(\xi)$ and $q(\eta)$ are arbitrary functions of a single characteristic variable. Therefore, spherically symmetric solutions to the three-dimensional wave equation assume the form

$$u(t, r) = \frac{p(r - ct)}{r} + \frac{q(r + ct)}{r}. \quad (12.139)$$

The first summand,

$$u(t, r) = \frac{p(r - ct)}{r}, \quad (12.140)$$

represents a wave moving at speed c in the direction of increasing r , and so describes the illumination from a variable light source that is concentrated at the origin, e.g., a pulsating quasar in interstellar space. To highlight this interpretation, let us concentrate on the case that $p(\xi) = \delta(\xi - a)$ is a delta function, keeping in mind that more general solutions can then be assembled by linear superposition. The induced solution

$$u(t, r) = \frac{\delta(r - ct - a)}{r} = \frac{\delta(r - c(t - t_0))}{r}, \quad \text{where} \quad t_0 = -\frac{a}{c}, \quad (12.141)$$

represents a spherical wave propagating through space. At the instant $t = t_0$, the light is entirely concentrated at the origin, $r = 0$. The signal then moves away from the origin in all directions at speed c . At each later time $t > t_0$, the wave remains concentrated on the surface of a sphere of radius $r = c(t - t_0)$. Its intensity at each point on the sphere, however, has decreased by a factor $1/r$, and so, the farther the light travels away from the source, the dimmer it becomes. A stationary observer sitting at a fixed point in space will see only an instantaneous flash of light of intensity $1/r$ as the spherical wave passes by at time $t = t_0 + r/c$, where r is the observer's distance from the light source. A similar statement holds for sound waves — to an observer, the sound of a distant explosion will last momentarily. Thunder and lightning are the most familiar examples of this everyday phenomenon.

On the other hand, for $t < t_0$, the impulse is concentrated at a negative radius $r = c(t - t_0) < 0$. To interpret this, note that, for spherical coordinates (12.15), replacing r by $-r$ has the same effect as changing \mathbf{x} to the antipodal point $-\mathbf{x}$. Thus, the solution (12.141) represents a concentrated spherically symmetric light wave arriving from the edges

of the universe at speed c that strengthens in intensity as it collapses into the origin at $t = t_0$. After collapse, it immediately reappears and expands back out into the universe.

The second solution in the d'Alembert formula (12.139) has, in fact, exactly the same physical form under the antipodal identification. Indeed, if we set

$$\tilde{r} = -r, \quad \tilde{p}(\xi) = -q(-\xi), \quad \text{then} \quad \frac{q(r + ct)}{r} = \frac{\tilde{p}(\tilde{r} - ct)}{\tilde{r}}.$$

Thus, the second d'Alembert solution is redundant, and we only need to consider solutions of the form (12.140) from now on.

To effectively utilize such spherical wave solutions, we need to understand the nature of their originating singularity. For simplicity, we set $t_0 = 0$ in (12.141) and concentrate on the particular solution

$$u(t, r) = \frac{\delta(r - ct)}{r}, \tag{12.142}$$

which apparently has a bad singularity at the origin, $r = 0$, at the initial time $t = 0$. We need to pin down precisely which sort of distribution (generalized function) it represents. Invoking the limiting definition is tricky, and it will be easier to work with the dual characterization of a distribution as a linear functional. Thus, at a fixed time $t \geq 0$, we must evaluate the inner product[†]

$$\langle u(t, \cdot), f \rangle = \iiint u(t, x, y, z) f(x, y, z) dx dy dz$$

of the solution with a smooth test function $f(\mathbf{x}) = f(x, y, z)$. We rewrite the triple integral in spherical coordinates, whereby

$$\langle u(t, \cdot), f \rangle = \int_{-\pi}^{\pi} \int_0^{\pi} \int_0^{\infty} \frac{\delta(r - ct)}{r} f(r, \varphi, \theta) r^2 \sin \varphi dr d\varphi d\theta.$$

When $t \neq 0$, the r integration can be immediately evaluated, and so

$$\langle u(t, \cdot), f \rangle = ct \int_{-\pi}^{\pi} \int_0^{\pi} f(ct, \varphi, \theta) \sin \varphi d\varphi d\theta = 4\pi ct M_{ct}[f], \tag{12.143}$$

where

$$M_{ct}[f] = \frac{1}{4\pi} \int_{-\pi}^{\pi} \int_0^{\pi} f(ct, \varphi, \theta) \sin \varphi d\varphi d\theta = \frac{1}{4\pi c^2 t^2} \iint_{S_{ct}} f dS \tag{12.144}$$

is the *mean* or *average value* of the function f on the sphere $S_{ct} = \{ \|\mathbf{x}\| = ct \}$ of radius $r = ct$ and, hence, surface area $4\pi c^2 t^2$. In particular, in the limit as the sphere's radius $ct \rightarrow 0$, by continuity, the mean reduces to just the value of the function at the origin:

$$\lim_{t \rightarrow \infty} M_{ct}[f] = M_0[f] = f(\mathbf{0}). \tag{12.145}$$

Thus, (12.143) implies that

$$\lim_{t \rightarrow \infty} \langle u(t, \cdot), f \rangle = \langle u(0, \cdot), f \rangle = 0 \quad \text{for all functions } f,$$

[†] For fixed t , we use $u(t, \cdot)$ to indicate the real-valued function $(x, y, z) \mapsto u(t, x, y, z)$ on \mathbb{R}^3 .

and hence $u(0, x, y, z) \equiv 0$ represents a zero initial displacement. In other words, there is, in fact, *no singularity* in the solution at $t = 0$!

In the absence of any initial displacement, how, then, can the solution (12.142) be nonzero? Clearly, this must be the result of a nonzero initial velocity. To evaluate $\partial u / \partial t$, we differentiate (12.143), whereby

$$\begin{aligned} \left\langle \frac{\partial u}{\partial t}, f \right\rangle &= \frac{\partial}{\partial t} \langle u(t, \cdot), f \rangle = \frac{\partial}{\partial t} \left(ct \int_{-\pi}^{\pi} \int_0^{\pi} f(ct, \varphi, \theta) \sin \varphi \, d\varphi \, d\theta \right) \\ &= c \int_{-\pi}^{\pi} \int_0^{\pi} f(ct, \varphi, \theta) \sin \varphi \, d\varphi \, d\theta + c^2 t \int_{-\pi}^{\pi} \int_0^{\pi} \frac{\partial f}{\partial r}(ct, \varphi, \theta) \sin \varphi \, d\varphi \, d\theta \\ &= 4\pi c M_{ct} [f] + 4\pi c^2 t M_{ct} \left[\frac{\partial f}{\partial r} \right]. \end{aligned} \quad (12.146)$$

The result is a linear combination of the means of f and its radial derivative f_r over the sphere of radius ct . In the limit, the second term goes to 0, and so, by (12.145),

$$\lim_{t \rightarrow 0} \langle u_t, f \rangle = 4\pi c M_0 [f] = 4\pi c f(\mathbf{0}).$$

Since this holds for all test functions f , we conclude that the initial velocity of our solution is a multiple of a delta function at the origin:

$$u_t(0, r) = 4\pi c \delta(\mathbf{x}).$$

Dividing through by $4\pi c$, we find that the spherical expanding wave

$$u(t, r) = \frac{\delta(r - ct)}{4\pi c r} \quad (12.147)$$

solves the initial value problem

$$u(0, \mathbf{x}) \equiv 0, \quad \frac{\partial u}{\partial t}(0, \mathbf{x}) = \delta(\mathbf{x}),$$

corresponding to an initial unit-velocity impulse concentrated at the origin. This solution can be viewed as the three-dimensional version of the hammer-blow solution to the one-dimensional wave equation discussed in Exercise 6.3.28.

More generally, we use the translational symmetry of the wave equation to conclude that the function

$$G(t, \mathbf{x}; \boldsymbol{\xi}) = \frac{\delta(\|\mathbf{x} - \boldsymbol{\xi}\| - ct)}{4\pi c \|\mathbf{x} - \boldsymbol{\xi}\|}, \quad t \geq 0, \quad (12.148)$$

is the *fundamental solution* to the wave equation resulting from a unit-velocity impulse concentrated at the point $\boldsymbol{\xi}$ at the initial time $t = 0$:

$$G(0, \mathbf{x}; \boldsymbol{\xi}) = 0, \quad \frac{\partial G}{\partial t}(0, \mathbf{x}; \boldsymbol{\xi}) = \delta(\mathbf{x} - \boldsymbol{\xi}). \quad (12.149)$$

With this in hand, we can apply linear superposition to solve the zero initial displacement initial value problem

$$u(0, x, y, z) = 0, \quad \frac{\partial u}{\partial t}(0, x, y, z) = g(x, y, z). \quad (12.150)$$

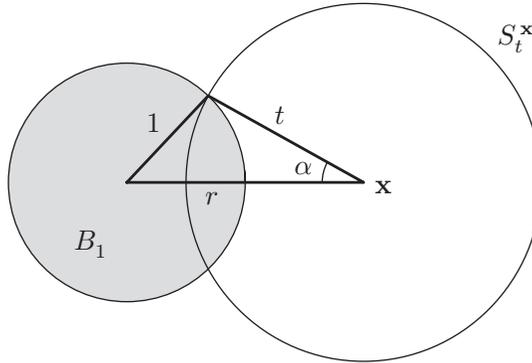


Figure 12.9. Cross-section of a sphere intersecting a ball.

Namely, we write the initial velocity

$$g(\mathbf{x}) = \iiint g(\boldsymbol{\xi}) \delta(\mathbf{x} - \boldsymbol{\xi}) \, d\xi \, d\eta \, d\zeta$$

as a superposition of impulses, and immediately conclude that the relevant solution is the selfsame superposition of spherical waves:

$$\begin{aligned} u(t, \mathbf{x}) &= \frac{1}{4\pi c} \iiint g(\boldsymbol{\xi}) \frac{\delta(\|\mathbf{x} - \boldsymbol{\xi}\| - ct)}{\|\mathbf{x} - \boldsymbol{\xi}\|} \, d\xi \, d\eta \, d\zeta \\ &= \frac{1}{4\pi c^2 t} \iint_{\|\boldsymbol{\xi} - \mathbf{x}\| = ct} g(\boldsymbol{\xi}) \, dS = t M_{ct}^{\mathbf{x}} [g]. \end{aligned} \tag{12.151}$$

Thus, the value of our solution at position \mathbf{x} and time $t > 0$ is equal to t times the *mean* of the initial velocity function g over the sphere of radius $r = ct$ centered at the point \mathbf{x} .

Example 12.16. Let us set the wave speed $c = 1$. Suppose that the initial velocity

$$g(\mathbf{x}) = \begin{cases} 1, & \|\mathbf{x}\| < 1, \\ 0, & \|\mathbf{x}\| > 1, \end{cases}$$

is 1 inside the unit ball B_1 centered at the origin and 0 outside. To solve the corresponding initial velocity problem, we must compute the average value of g over a sphere

$$S_t^{\mathbf{x}} = \{ \boldsymbol{\xi} \mid \|\boldsymbol{\xi} - \mathbf{x}\| = t \}$$

of radius $t > 0$ centered at a point $\mathbf{x} \in \mathbb{R}^3$. Since $g = 0$ outside the unit ball, its average will be equal to the surface area of that part of the sphere that is contained inside the unit ball, namely $S_t^{\mathbf{x}} \cap B_1$, divided by the total surface area of $S_t^{\mathbf{x}}$, namely $4\pi t^2$.

To compute this quantity, let $r = \|\mathbf{x}\|$. If $t > r + 1$ or $0 < t < r - 1$, then the sphere of radius t lies entirely outside the unit ball, and so the average is 0; if $0 < t < 1 - r$, which requires $r < 1$ and so $\mathbf{x} \in B_1$, then the sphere lies entirely within the unit ball, and so the average is 1. Otherwise, referring to [Figure 12.9](#) and [Exercise 12.6.7](#), we see that the area of the spherical cap $S_t^{\mathbf{x}} \cap B_1$ is given by

$$2\pi t^2(1 - \cos \alpha) = 2\pi t^2 \left(1 - \frac{r^2 + t^2 - 1}{2rt} \right) = \frac{\pi t}{r} [1 - (t - r)^2], \tag{12.152}$$

where α denotes the angle between the line joining the centers of the two spheres and the circle formed by their intersection, whose value is prescribed by the Law of Cosines. Assembling the different subcases, we conclude that

$$M_{ct}^{\mathbf{x}}[g] = \begin{cases} 1, & 0 \leq t \leq 1 - r, \\ \frac{1 - (t - r)^2}{4rt}, & |r - 1| \leq t \leq r + 1, \\ 0, & 0 \leq t \leq r - 1 \quad \text{or} \quad t \geq r + 1. \end{cases} \tag{12.153}$$

The solution (12.151) is obtained by multiplying by t , and hence for $t \geq 0$,

$$u(t, \mathbf{x}) = \begin{cases} t, & 0 \leq t \leq 1 - \|\mathbf{x}\|, \\ \frac{1 - (t - \|\mathbf{x}\|)^2}{4\|\mathbf{x}\|}, & \|\|\mathbf{x}\| - 1\| \leq t \leq \|\mathbf{x}\| + 1, \\ 0, & 0 \leq t \leq \|\mathbf{x}\| - 1 \quad \text{or} \quad t \geq \|\mathbf{x}\| + 1. \end{cases} \tag{12.154}$$

The resulting function is not smooth at the interfaces $t = \|\|\mathbf{x}\| - 1\|$ and $\|\mathbf{x}\| + 1$, and hence does not qualify as a classical solution. Nevertheless, it can be shown that (12.154) is a bona fide weak solution to the initial value problem.

The first two rows of [Figure 12.10](#) plot the solution as a function of time for several fixed values of $r = \|\mathbf{x}\|$. An observer sitting at the origin will see a linearly increasing light intensity followed by a sudden blackout. At other points inside the sphere, there is a similar linear increase, while the subsequent decrease follows a parabolic arc; if the observer is closer to the edge of the ball than its center, the parabolic portion will continue to increase for a while before eventually tapering off. On the other hand, an observer sitting outside the sphere will experience, after an initially dark period, a symmetric parabolic increase to a maximal intensity and then a decrease back to dark after a total time lapse of 2. The second two rows plot the solution as a function of r for various fixed times. Note that, up until time $t = 1$, the light spreads out while increasing in intensity near the origin, after which the solution is of gradually decreasing magnitude, supported within the domain lying between two concentric spheres of respective radii $t - 1$ and $t + 1$.

Returning to the general situation, we note that the solution formula (12.151) handles only nonzero initial velocities. What about solutions resulting from a nonzero initial displacement? Surprisingly, the answer comes from differentiation! The key observation is that if $u(t, \mathbf{x})$ is any (sufficiently smooth) solution to the wave equation, then so is its time derivative

$$v(t, \mathbf{x}) = \frac{\partial u}{\partial t}(t, \mathbf{x}). \tag{12.155}$$

This follows at once from differentiating both sides of the wave equation with respect to t and using the equality of mixed partial derivatives. Physically, this implies that the velocity of a wave obeys the same evolutionary principle as the wave itself, which is a manifestation of the linearity and time-independence (autonomy) of the equation.

Now, suppose u has initial conditions

$$u(0, \mathbf{x}) = f(\mathbf{x}), \quad u_t(0, \mathbf{x}) = g(\mathbf{x}). \tag{12.156}$$

What are the initial conditions for its derivative $v = u_t$? Clearly, its initial displacement

$$v(0, \mathbf{x}) = u_t(0, \mathbf{x}) = g(\mathbf{x}) \tag{12.157}$$

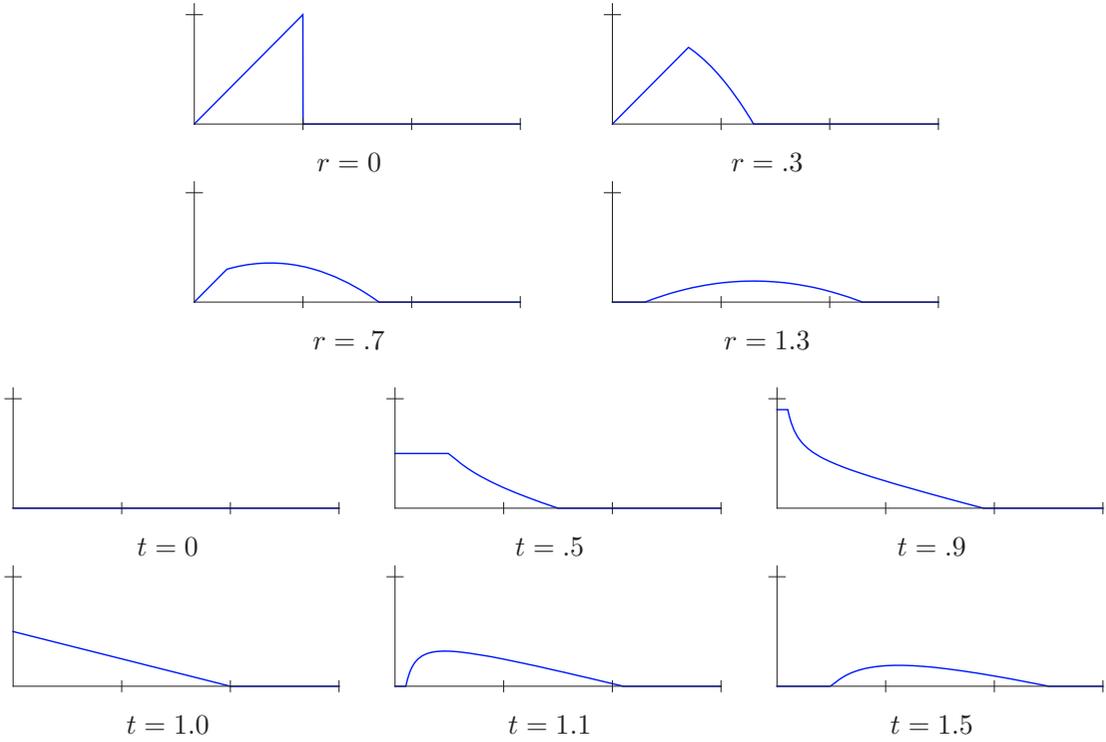


Figure 12.10. Wave equation solution $u(t, r)$ due to an initial velocity of the unit ball. $\boxed{+}$

equals the initial velocity of u . As for its initial velocity, we have

$$\frac{\partial v}{\partial t} = \frac{\partial^2 u}{\partial t^2} = c^2 \Delta u,$$

because we are assuming that u solves the wave equation. Thus, at the initial time, the velocity,

$$\frac{\partial v}{\partial t}(0, \mathbf{x}) = c^2 \Delta u(0, \mathbf{x}) = c^2 \Delta f(\mathbf{x}), \tag{12.158}$$

equals c^2 times the Laplacian of the initial displacement f . In particular, if u satisfies the initial conditions

$$u(0, \mathbf{x}) = 0, \quad u_t(0, \mathbf{x}) = g(\mathbf{x}), \tag{12.159}$$

then $v = u_t$ satisfies the initial conditions

$$v(0, \mathbf{x}) = g(\mathbf{x}), \quad v_t(0, \mathbf{x}) = 0. \tag{12.160}$$

Thus, paradoxically, to solve the initial displacement problem we differentiate the initial velocity solution (12.151) with respect to t , and hence

$$v(t, \mathbf{x}) = \frac{\partial u}{\partial t}(t, \mathbf{x}) = \frac{\partial}{\partial t} (t M_{ct}^{\mathbf{x}}[g]) = M_{ct}^{\mathbf{x}}[g] + ct M_{ct}^{\mathbf{x}} \left[\frac{\partial g}{\partial \mathbf{n}} \right], \tag{12.161}$$

where we have made use of our computation in (12.146). Therefore, $v(t, \mathbf{x})$ is a linear combination of the mean of the function g and the mean of its normal or radial derivative $\partial g/\partial \mathbf{n} = \partial g/\partial r$, taken over a sphere of radius ct centered at the point \mathbf{x} . In particular, to obtain the solution corresponding to a concentrated initial displacement,

$$F(0, \mathbf{x}; \boldsymbol{\xi}) = \delta(\mathbf{x} - \boldsymbol{\xi}), \quad \frac{\partial F}{\partial t}(0, \mathbf{x}; \boldsymbol{\xi}) = 0, \tag{12.162}$$

we differentiate the solution (12.148), resulting in

$$F(t, \mathbf{x}; \boldsymbol{\xi}) = \frac{\partial G}{\partial t}(t, \mathbf{x}; \boldsymbol{\xi}) = -\frac{\delta'(\|\mathbf{x} - \boldsymbol{\xi}\| - ct)}{4\pi\|\boldsymbol{\xi} - \mathbf{x}\|}, \tag{12.163}$$

which is the fundamental solution for the initial displacement problem. Thus, interestingly, a concentrated initial displacement spawns a spherically expanding doublet, cf. [Figure 6.6](#), whereas a concentrated initial velocity spawns an expanding spherical singlet or delta wave.

Example 12.17. Let $c = 1$. Consider the initial conditions

$$u(0, \mathbf{x}) = f(\mathbf{x}) = \begin{cases} 1, & \|\mathbf{x}\| < 1, \\ 0, & \|\mathbf{x}\| > 1, \end{cases} \quad \frac{\partial u}{\partial t}(0, \mathbf{x}) = 0, \tag{12.164}$$

modeling the effect of an instantaneously illuminated solid ball. To obtain the resulting solution, we differentiate (12.154) with respect to t , leading to

$$u(t, \mathbf{x}) = \begin{cases} 1, & 0 \leq t < 1 - \|\mathbf{x}\|, \\ \frac{\|\mathbf{x}\| - t}{2\|\mathbf{x}\|}, & \|\|\mathbf{x}\| - 1\| \leq t \leq \|\mathbf{x}\| + 1, \\ 0, & 0 \leq t < \|\mathbf{x}\| - 1 \quad \text{or} \quad t > 1 + \|\mathbf{x}\|. \end{cases} \tag{12.165}$$

As illustrated in the first two rows of [Figure 12.11](#), an observer sitting at the center of the ball will see a constant light intensity until $t = 1$, at which time the solution suddenly goes dark. At other points inside the ball, $0 < r < 1$, the downwards jump in intensity arrives sooner, and even goes below 0, followed by a further linear decrease, and finally a jump back to quiescence. An observer placed outside the ball, at radius $r = \|\mathbf{x}\| > 1$, will experience, after an initially dark period, a sudden increase in the light intensity at time $t = r - 1$, followed by a linear decrease to negative, followed by a jump back up to darkness at time $t = r + 1$. The farther away from the source, the fainter the light. In the second two rows, we plot the same solution as a function of r for different values of t . Note the sudden appearance of a $1/r$ singularity at the origin at time $t = 1$, which is the result of a focusing of the initial discontinuities of $u(0, \mathbf{x}) = f(\mathbf{x})$ on the surface of the unit sphere. Afterwards, the residual radially symmetric disturbance moves off to ∞ while gradually decreasing in intensity. Again, the discontinuities imply that (12.165) is not a classical solution, but it does qualify as a weak solution to the initial value problem.

Kirchhoff’s Formula and Huygens’ Principle

Linearly combining the two solution formulas (12.151) and (12.161) establishes *Kirchhoff’s formula* (first discovered by Poisson), which is the three-dimensional counterpart to d’Alembert’s solution formula for the wave equation.

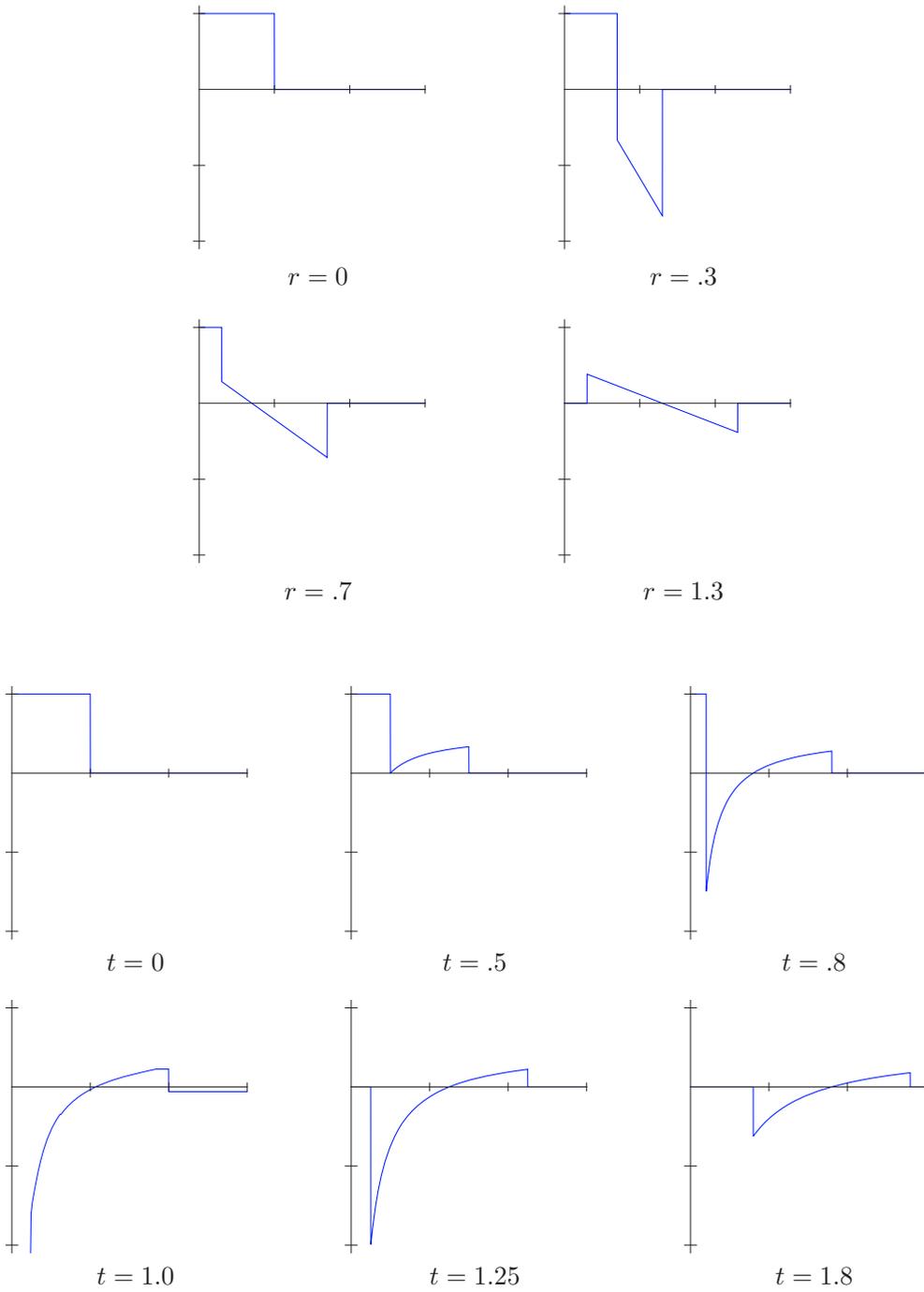


Figure 12.11. Wave equation solution $u(t, r)$ due to an initial displacement of the unit ball . 

Theorem 12.18. *The solution to the initial value problem*

$$u_{tt} = c^2 \Delta u, \quad u(0, \mathbf{x}) = f(\mathbf{x}), \quad \frac{\partial u}{\partial t}(0, \mathbf{x}) = g(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3, \quad (12.166)$$

for the wave equation in three-dimensional space is given by

$$u(t, \mathbf{x}) = \frac{\partial}{\partial t} (t M_{ct}^{\mathbf{x}}[f]) + t M_{ct}^{\mathbf{x}}[g] = M_{ct}^{\mathbf{x}}[f] + ct M_{ct}^{\mathbf{x}} \left[\frac{\partial f}{\partial \mathbf{n}} \right] + t M_{ct}^{\mathbf{x}}[g], \quad (12.167)$$

where $M_{ct}^{\mathbf{x}}[f]$ denotes the average of the function f over the sphere $S_{ct}^{\mathbf{x}} = \{\|\boldsymbol{\xi} - \mathbf{x}\| = ct\}$ of radius ct centered at the point \mathbf{x} .

A crucially important consequence of the Kirchhoff solution formula is a celebrated physical principle first set out by the pioneering seventeenth century Dutch scientist Christiaan Huygens.[†] Roughly, *Huygens' Principle* states that, in three-dimensional space, localized solutions to the wave equation remain localized. More concretely, (12.167) implies that the value of the solution at a point \mathbf{x} and time t depends only on the values of the initial displacements and velocities at a distance ct away. Thus, all signals propagate along the relativistic light cone

$$c^2 t^2 = x^2 + y^2 + z^2$$

in four-dimensional Minkowski space-time. Physically, Huygens' Principle assures us that any light that we witness at time t arrived from points that lie a distance exactly $d = c(t - t_0)$ away at an earlier time $t_0 < t$. In particular, a localized initial signal, whether initial displacement or initial velocity, that is concentrated near a point produces a response that remains concentrated on an ever expanding sphere surrounding the point. In our three-dimensional universe, we witness the light from a sudden explosion or lightning bolt for only a brief moment, after which the view returns to darkness. Similarly, a sharp sound, e.g., a thunderclap, remains sharply concentrated with diminishing magnitude as it propagates through space. Huygens' Principle is responsible for the important astronomical fact that the light we now observe from a distant star was generated at a single past time that is directly proportional to the star's distance from the Earth. Remarkably, as we will show in the following subsection, Huygens' Principle *does not hold* in a two-dimensional universe! There, initially concentrated light and sound impulses will spread out as time progresses, and their effect will be experienced over an extended time range; see below for details.

Exercises

12.6.1. Solve the wave equation in three-dimensional space for the following initial conditions:

- (a) $u(0, x, y, z) = x + z$, $u_t(0, x, y, z) = 0$; (b) $u(0, x, y, z) = 0$, $u_t(0, x, y, z) = y$;
 (c) $u(0, x, y, z) = 1/(1 + x^2 + y^2 + z^2)$, $u_t(0, x, y, z) = 0$,
 (d) $u(0, x, y, z) = 0$, $u_t(0, x, y, z) = 1/(1 + x^2 + y^2 + z^2)$.

12.6.2. At what points in space-time does a three-dimensional wave vanish if it vanishes outside a sphere of radius R at the initial time $t = 0$?

[†] Don't even bother trying to pronounce his name correctly unless you are Dutch!

12.6.3. Consider the initial value problem

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}, \quad u(0, x, y, z) = 0, \quad \frac{\partial u}{\partial t}(0, x, y, z) = \begin{cases} 1, & 0 < x, y, z < 1, \\ 0, & \text{otherwise,} \end{cases}$$

i.e., the initial velocity is 1 inside a unit cube and 0 outside the cube. We interpret the solution $u(t, x, y, z)$ as the intensity of light at a given point in space-time, measured in units that make the speed of light $c = 1$. (a) Write down an integral formula for $u(t, x, y, z)$. (b) Suppose a light sensor is placed at the point $(2, 2, 1)$. For which values of $t > 0$ will the sensor register a nonzero signal? Sketch a rough graph of what the sensor measures. (You do not need to find the precise formula, but explain how you obtained your graph.) (c) *True or false:* The solution $u(t, x, y, z) \geq 0$ at all points in space-time.

12.6.4. Is (12.151) a solution to the wave equation for $t < 0$? If not, write down a solution formula that is valid for negative t .

12.6.5. *True or false:* The function $u(t, x, y, z)$ defined by (12.154) is everywhere continuous.

12.6.6. A thermonuclear explosion occurs at the center of the Earth. Would you feel the effect first through a motion at the surface or a change in temperature at the surface? Discuss.

◇ 12.6.7. Prove that the area of the spherical cap $S_t^x \cap B_1$ is given by formula (12.152).

Descent to Two Dimensions

So far, we have found explicit formulas for the solution to the wave equation on the one-dimensional line, and in three-dimensional space. The two-dimensional case

$$u_{tt} = c^2 \Delta u = c^2 (u_{xx} + u_{yy}) \tag{12.168}$$

is, counterintuitively, more complicated! For instance, seeking a radially symmetric solution $u(t, r)$ requires solving the partial differential equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \left(\frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} \right), \tag{12.169}$$

which, unlike its three-dimensional counterpart (12.137), is not so easily integrated.

However, our solution to the three-dimensional problem can be adapted to construct a solution to the two-dimensional problem using the so-called *Method of Descent*. Observe that any solution $u(t, x, y)$ to the two-dimensional wave equation (12.168) can be viewed as a solution to the three-dimensional wave equation (12.123) that does not depend upon the vertical z coordinate, whence $\partial u / \partial z = 0$. Clearly, if the three-dimensional initial data does not depend on z , then the resulting solution $u(t, x, y)$ will also be independent of z .

Consider first the zero initial displacement condition

$$u(0, x, y) = 0, \quad \frac{\partial u}{\partial t}(0, x, y) = g(x, y). \tag{12.170}$$

In the three-dimensional solution formula (12.151), if $g(x, y)$ does not depend on the z -coordinate, then the integrals over the upper and lower hemispheres

$$S_{ct}^+ = \{ \|\boldsymbol{\xi} - \mathbf{x}\| = ct, \quad \zeta \geq z \}, \quad S_{ct}^- = \{ \|\boldsymbol{\xi} - \mathbf{x}\| = ct, \quad \zeta \leq z \},$$

are identical. To evaluate these integrals, we parametrize the upper hemisphere as the graph of

$$\zeta = z + \sqrt{c^2 t^2 - (\xi - x)^2 - (\eta - y)^2} \quad \text{over the disk} \quad D_{ct}^{\mathbf{x}} = \{ (\xi - x)^2 + (\eta - y)^2 \leq c^2 t^2 \},$$

concluding that

$$\begin{aligned} u(t, x, y) &= \frac{1}{4\pi c^2 t} \iint_{S_{ct}} g(\xi, \eta) dS = \frac{1}{2\pi c^2 t} \iint_{S_{ct}^+} g(\xi, \eta) dS \\ &= \frac{1}{2\pi c} \iint_{D_{ct}^{\mathbf{x}}} \frac{g(\xi, \eta)}{\sqrt{c^2 t^2 - (\xi - x)^2 - (\eta - y)^2}} d\xi d\eta \end{aligned} \tag{12.171}$$

solves the initial value problem (12.170). In particular, if we take the initial velocity

$$\frac{\partial u}{\partial t}(0, x, y) = g(x, y) = \delta(x) \delta(y)$$

to be a unit impulse concentrated at the origin, then the resulting solution is

$$u(t, x, y) = \begin{cases} \frac{1}{2\pi c \sqrt{c^2 t^2 - x^2 - y^2}}, & x^2 + y^2 < c^2 t^2, \\ 0, & x^2 + y^2 > c^2 t^2. \end{cases} \tag{12.172}$$

An observer sitting at distance $r = \|\mathbf{x}\| = \sqrt{x^2 + y^2}$ from the origin will first witness a concentrated displacement singularity at time $t = r/c$. However, in contrast to the three-dimensional solution, even after the impulse passes by, there will continue to be a decreasing, but nonzero, signal of magnitude roughly proportional to $1/t$. In Figure 12.12, we plot the solution (12.172) for unit wave speed $c = 1$. The first row plots intensity as a function of t at three different radii; note that the initial singularity, indicated by a spike in the graph, is followed by a progressively smaller residual displacement, which never entirely disappears. The second row shows the displacement at three different times as a function of $r = \|\mathbf{x}\|$.

As in the three-dimensional case, the solution to the initial displacement conditions

$$u(0, x, y) = f(x, y), \quad \frac{\partial u}{\partial t}(0, x, y) = 0, \tag{12.173}$$

can then be obtained by differentiation of (12.171) with respect to t , and so

$$u(t, x, y) = \frac{1}{2\pi c} \frac{\partial}{\partial t} \iint_{D_{ct}^{\mathbf{x}}} \frac{f(\xi, \eta)}{\sqrt{c^2 t^2 - (\xi - x)^2 - (\eta - y)^2}} d\xi d\eta. \tag{12.174}$$

As before, starting with a concentrated impulse, an observer will witness, after a time lapse $t = r/c$, an abrupt impulse passing by, followed by a progressively decaying residual wave. The general solution to the two-dimensional wave equation on all of \mathbb{R}^2 is a linear combination of these two types of solutions (12.171, 174).

As a consequence of these considerations, we discover that Huygens' Principle is *not* valid in a two-dimensional universe. The solution to the two-dimensional wave equation at a point \mathbf{x} at time t depends on the initial displacement and velocity on the entire disk of radius ct centered at the point, and not just on the points lying a distance ct away. So a two-dimensional creature would experience not just an initial effect of a concentrated sound or light wave, but also an "afterglow" of slowly diminishing magnitude. It would be

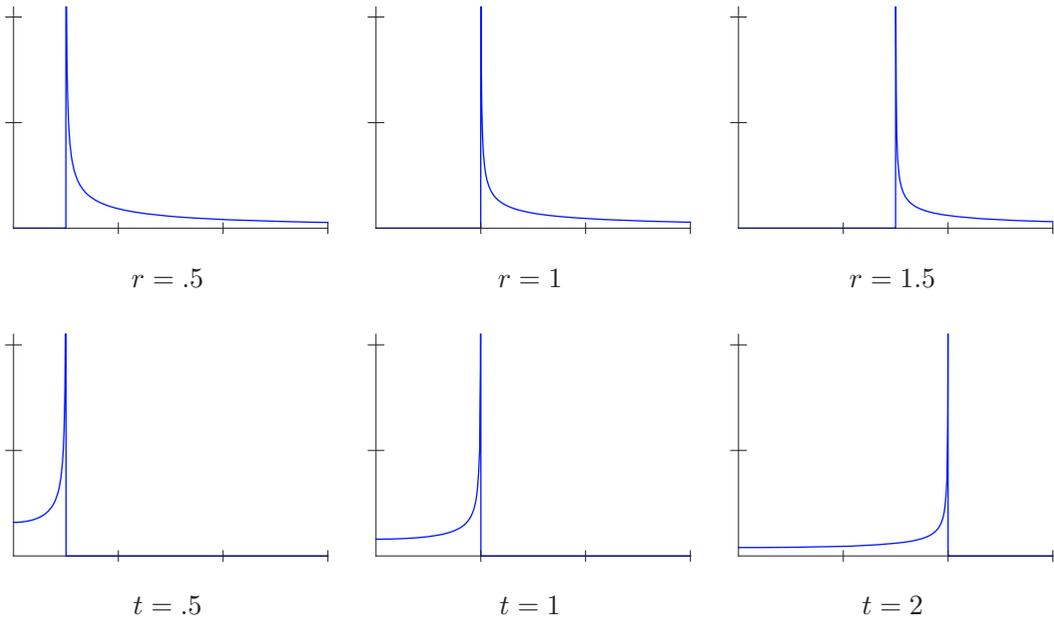


Figure 12.12. Solution to the two-dimensional wave equation \square for a concentrated impulse.

like living in a permanent echo chamber, and so understanding and acting upon sensory phenomena would be considerably more challenging. In general, it can be proved that Huygens' Principle for the wave equation is valid only in spaces of odd dimension $n = 2k + 1 \geq 3$; see also [15] for recent advances in the classification of partial differential equations that admit a Huygens' Principle.

Remark: Since the solutions to the two-dimensional wave equation can be interpreted as three-dimensional solutions with no z dependence, a concentrated delta impulse for the two-dimensional wave equation would correspond to a three-dimensional initial impulse that is concentrated along an entire vertical line, e.g., an instantaneous lightning bolt in the form of an infinite straight line. An observer fixed in space will first encounter the light flash arriving from the closest point on the line, but will subsequently experience the gradually decreasing effect of the light emitted by points that lie progressively farther away along the line. This accounts for the two-dimensional afterglow in formula (12.172).

Exercises

12.6.8. Solve initial value problem for the two-dimensional wave equation with the following initial data (a) $u(0, x, y) = x - y, u_t(0, x, y) = 0$; (b) $u(0, x, y) = 0, u_t(0, x, y) = y$.

- 12.6.9. (a) Prove that $u(t, x, y) = 1/\sqrt{x^2 + y^2 - c^2t^2}$ is a solution to the two-dimensional wave equation on the domain $\Omega = \{x^2 + y^2 > c^2t^2\}$ exterior to the light cone passing through the origin. What is the corresponding initial data at $t = 0$? (b) Use part (a) to solve the initial value problem $u(0, x, y) = 0$, $u_t(0, x, y) = 1/\sqrt{x^2 + y^2}$, on Ω .
- 12.6.10. Consider the two-dimensional wave equation on \mathbb{R}^2 with wave speed $c = 1$. Write down an integral formula for the solution to the following initial value problems. You need not evaluate the integrals. (a) $u(0, x, y) = x^3 - y^3$, $u_t(0, x, y) = 0$; (b) $u(0, x, y) = 0$, $u_t(0, x, y) = y^2$; (c) $u(0, x, y) = x^2 + y^2$, $u_t(0, x, y) = -x^2 - y^2$.
- 12.6.11. (a) Find the solution to the two-dimensional wave equation whose initial displacement is a concentrated delta impulse at the origin and whose initial velocity is zero. (b) Is your expression a classical solution when $t > 0$? (c) *True or false:* The solution tends to 0 uniformly as $t \rightarrow \infty$.
- 12.6.12. Use separation of variables to write down an eigenfunction series solution to the partial differential equation (12.169) when subject to homogeneous Dirichlet boundary conditions at $r = 1$ and bounded at $r = 0$.
- ◇ 12.6.13. Write down the fundamental solution for the one-dimensional wave equation with (a) a concentrated initial displacement at the origin; (b) a concentrated initial velocity at the origin. (c) Discuss the validity of Huygens' Principle in a one-dimensional universe.
- 12.6.14. Discuss how you can construct solutions to the one-dimensional wave equation by descent from the three-dimensional wave equation.

12.7 The Hydrogen Atom

A *hydrogen atom* consists of a single electron circling an atomic nucleus that contains a single proton, which, owing to its relatively tiny size, is assumed to be entirely concentrated at the origin. As a result of quantization of the corresponding classical Coulomb problem, the Schrödinger equation[†] governing the dynamical behavior of the electron moving around the nucleus takes the explicit form

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2M} \Delta \psi - \frac{\alpha^2}{r} \psi = -\frac{\hbar^2}{2M} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) - \frac{\alpha^2 \psi}{\sqrt{x^2 + y^2 + z^2}}. \quad (12.175)$$

Here $\psi(t, x, y, z)$ denotes the electron's time-dependent wave function, which, at each time t , prescribes its quantum probability density as it circles the nucleus. In the quantized Hamiltonian operator $K = -\frac{1}{2}(\hbar^2/M)\Delta - \alpha^2/r$, the coefficient of the Laplacian depends on Planck's constant \hbar and the electron's mass M . The final term represents the three-dimensional electromagnetic (Coulomb) potential function $V(\mathbf{x}) = \alpha^2/r$ attracting the electron to the nucleus, with α representing the electron's (and proton's) charge, while $r = \|\mathbf{x}\|$ is its distance from the nucleus. Incidentally, the quantum-mechanical Schrödinger equation for multi-electron atoms or even molecules is not so difficult to write down, but its solution, even for, say, the helium atom, is *much* more difficult, and, in general, is still

[†] The reader is referred to (9.151) and the subsequent discussion for generalities regarding the Schrödinger equation and quantum mechanics.

a major challenge for numerical analysts, even on today's supercomputers, [116]. Thus, to keep matters as simple as possible, we will consider only the case of a single electron hydrogen atom here.

Bound States

According to the analysis in Section 9.5, the normal mode solutions to the Schrödinger equation are of the form

$$\psi(t, x, y, z) = e^{i\lambda t/\hbar} v(x, y, z),$$

where v is an eigenfunction of the Hamiltonian operator with eigenvalue λ , and hence satisfies

$$\frac{\hbar^2}{2M} \Delta v + \left(\lambda + \frac{\alpha^2}{r} \right) v = 0. \quad (12.176)$$

The *bound states* of the atom, in which the electron remains trapped by the nucleus, are represented by the nonzero solutions to the eigenvalue problem (12.176) with unit L^2 norm:

$$\|v\|^2 = \iiint |v(x, y, z)|^2 dx dy dz = 1.$$

The eigenvalue λ specifies the bound state's energy, and is necessarily negative: $\lambda < 0$. Since we are working on an unbounded domain, the bound states do *not* form a complete system of eigenfunctions, and so not every wave function $\varphi \in L^2(\mathbb{R}^3)$ can be approximated by an eigenfunction series. The missing data are the so-called *scattering states* arising from the *continuous spectrum* of the Schrödinger operator; these represent electrons that scatter off the nucleus, and so do not remain trapped in an orbit. (For the classical Kepler problem of a planet circling a sun, the bound states would correspond to planets following bounded elliptic orbits, while the scattering states correspond to interstellar comets and the like moving along unbounded hyperbolic or parabolic trajectories.) We will leave the discussion of the quantum-mechanical scattering states and the associated continuous spectrum to a more advanced treatment of the subject, [72, 95].

To understand the bound states, we will apply the method of separation of variables. We begin by rewriting the eigenvalue problem (12.176) in spherical coordinates:

$$\frac{\hbar^2}{2M} \left(\frac{\partial^2 v}{\partial r^2} + \frac{2}{r} \frac{\partial v}{\partial r} + \frac{1}{r^2} \frac{\partial^2 v}{\partial \varphi^2} + \frac{\cos \varphi}{r^2 \sin \varphi} \frac{\partial v}{\partial \varphi} + \frac{1}{r^2 \sin^2 \varphi} \frac{\partial^2 v}{\partial \theta^2} \right) + \left(\lambda + \frac{\alpha^2}{r} \right) v = 0. \quad (12.177)$$

We then separate off the radial coordinate, setting

$$v(r, \varphi, \theta) = p(r) w(\varphi, \theta).$$

The angular component satisfies the spherical Helmholtz equation

$$\Delta_S w + \mu w = \frac{\partial^2 w}{\partial \varphi^2} + \frac{\cos \varphi}{\sin \varphi} \frac{\partial w}{\partial \varphi} + \frac{1}{\sin^2 \varphi} \frac{\partial^2 w}{\partial \theta^2} + \mu w = 0,$$

which we have already solved; see (12.21) and the ensuing discussion. The eigensolutions are spherical harmonics, which, because the quantum-mechanical solutions are intrinsically complex-valued, we take in their complex form (12.46). The associated eigenvalue

$$\mu = l(l+1), \quad \text{where the integer} \quad l = 0, 1, 2, \dots \quad (12.178)$$

is known as the *angular quantum number*, admits a total of $2l + 1$ linearly independent eigenfunctions

$$\mathcal{Y}_l^m(\varphi, \theta) = P_l^m(\cos \varphi) e^{im\theta}, \quad m = -l, -l + 1, \dots, l - 1, l. \quad (12.179)$$

The radial equation with the separation constant (12.178) is

$$\frac{\hbar^2}{2M} \left(\frac{d^2 p}{dr^2} + \frac{2}{r} \frac{dp}{dr} \right) + \left(\lambda + \frac{\alpha^2}{r} - \frac{l(l+1)}{r^2} \right) p = 0. \quad (12.180)$$

To eliminate the physical parameters, let us rescale the radial coordinate by setting

$$s = \sigma r, \quad \text{where} \quad \sigma = \frac{2\sqrt{-2M\lambda}}{\hbar}, \quad (12.181)$$

given that $\lambda < 0$. The resulting ordinary differential equation for the rescaled function

$$P(s) = p\left(\frac{s}{\sigma}\right)$$

is

$$\frac{d^2 P}{ds^2} + \frac{2}{s} \frac{dP}{ds} - \left(\frac{1}{4} - \frac{n}{s} + \frac{l(l+1)}{s^2} \right) P = 0, \quad (12.182)$$

where

$$n = \frac{2M\alpha^2}{\sigma\hbar^2} = \frac{\alpha^2}{\hbar} \sqrt{-\frac{M}{2\lambda}}. \quad (12.183)$$

Equation (12.182) is a version of the *generalized Laguerre differential equation* — see Exercise 12.7.4 below — named after the nineteenth-century French mathematician Edmond Laguerre, who studied its solutions well before the appearance of quantum mechanics. Since we are searching for bound states, the relevant solutions should be defined on $0 \leq s < \infty$, remain bounded at $s = 0$, and go to zero as $s \rightarrow \infty$:

$$\lim_{s \rightarrow 0^+} P(s) < \infty, \quad \lim_{s \rightarrow \infty} P(s) = 0. \quad (12.184)$$

The proof of the following key result is outlined in Exercises 12.7.4–5.

Theorem 12.19. *For each pair of nonnegative integers $0 \leq l < n$, the boundary value problem (12.182, 184) has the eigensolution*

$$P_l^n(s) = s^l e^{-s/2} L_{n-l-1}^{2l+1}(s), \quad (12.185)$$

where

$$L_k^j(s) = \frac{s^{-j} e^s}{k!} \frac{d^k}{ds^k} [s^{j+k} e^{-s}] = \sum_{i=0}^k \frac{(-1)^i}{i!} \binom{j+k}{j+i} s^i, \quad j, k = 0, 1, 2, \dots, \quad (12.186)$$

are known as generalized[†] Laguerre polynomials.

[†] The ordinary *Laguerre polynomials* are $L_k(s) = L_k^0(s)$.

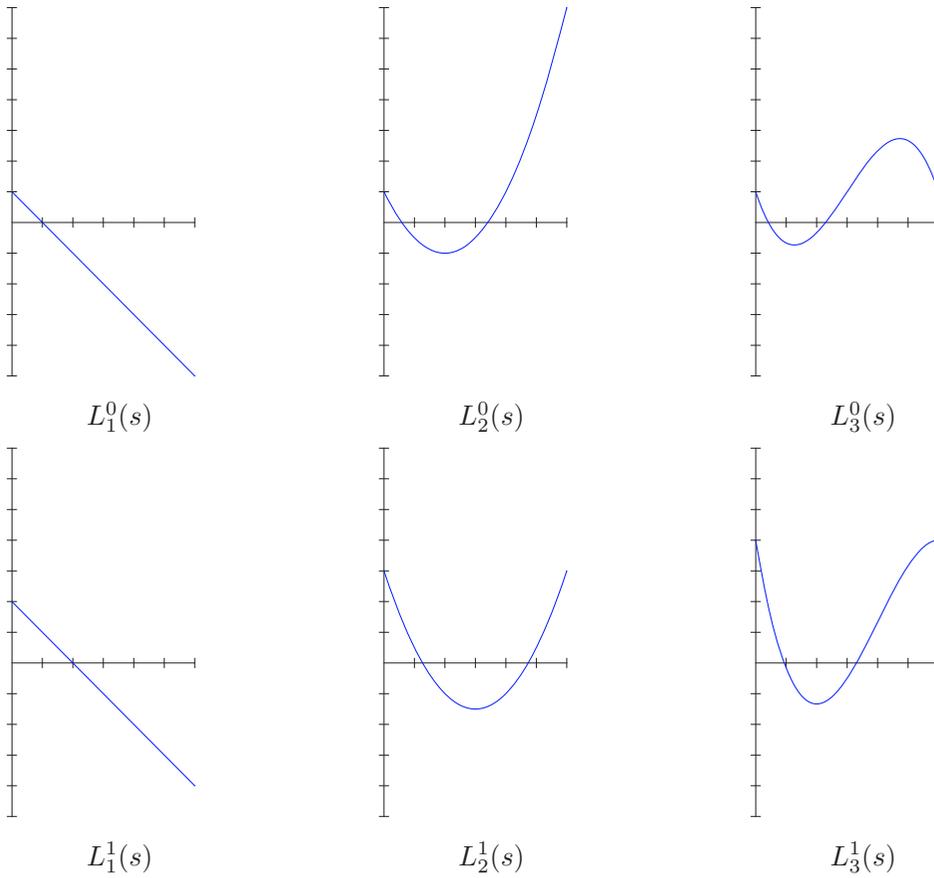


Figure 12.13. Generalized Laguerre polynomials.

The first few generalized Laguerre polynomials are

$$\begin{aligned}
 L_0^0(s) &= 1, & L_1^0(s) &= 1 - s, & L_2^0(s) &= 1 - 2s + \frac{1}{2}s^2, & L_3^0(s) &= 1 - 3s + \frac{3}{2}s^2 - \frac{1}{6}s^3, \\
 L_0^1(s) &= 1, & L_1^1(s) &= 2 - s, & L_2^1(s) &= 3 - 3s + \frac{1}{2}s^2, & L_3^1(s) &= 4 - 6s + 2s^2 - \frac{1}{6}s^3, \\
 L_0^2(s) &= 1, & L_1^2(s) &= 3 - s, & L_2^2(s) &= 6 - 4s + \frac{1}{2}s^2, & L_3^2(s) &= 10 - 10s + \frac{5}{2}s^2 - \frac{1}{6}s^3.
 \end{aligned}$$

Note that $L_k^j(s)$ has degree k . A few graphs, on the interval $0 \leq t \leq 6$, appear in [Figure 12.13](#). See [\[86\]](#) for details on their properties.

Atomic Eigenstates and Quantum Numbers

The integer n , whose physical value was noted in (12.183), is known as the *principal quantum number*. We further note that the scaling factor in (12.181) can be written as

$$\sigma = \frac{2M\alpha^2}{n\hbar^2} = \frac{2}{na}, \quad \text{where} \quad a = \frac{\hbar^2}{M\alpha^2} \approx .529 \times 10^{-10} \text{ meter},$$

which approximates the radius of the electron's lowest energy level, is known as the *Bohr radius*, in honor of the pioneering Danish quantum physicist Niels Bohr. Reverting to phys-

ical coordinates, the bound state solutions (12.185) become, up to an inessential constant multiple, the *radial wave functions*

$$\beta_l^n(r) = \left(\frac{2r}{na}\right)^l e^{-r/(na)} L_{n-l-1}^{2l+1} \left(\frac{2r}{na}\right). \quad (12.187)$$

Combining them with the spherical harmonics (12.179) yields the *atomic eigenfunctions* or *eigenstates*

$$v_{lmn}(r, \varphi, \theta) = \sqrt{\frac{(2l+1)(l-m)!(n-l-1)!}{\pi a^3 n^4 (l+m)!(l+n)!}} \beta_l^n(r) \mathcal{Y}_l^m(\varphi, \theta), \quad (12.188)$$

where the initial factor is selected so as to make $\|v_{lmn}\| = 1$, and hence a bona fide wave function. (A proof of this fact is outlined in Exercise 12.7.8.) The eigenstates depend on three integers, which have the following physical designations:

- $n = 1, 2, 3, \dots$: the *principal quantum number*;
- $l = 0, 1, \dots, n-1$: the *angular quantum number*;
- $m = -l, -l+1, \dots, l-1, l$: the *magnetic quantum number*.

The energy is the associated eigenvalue:

$$\lambda_n = -\frac{\alpha^4 M}{2\hbar^2} \frac{1}{n^2} = -\frac{\alpha^2}{2a} \frac{1}{n^2}, \quad n = 1, 2, 3, \dots \quad (12.189)$$

The fact that the ratios $\lambda_n/\lambda_1 = 1/n^2$ between the energy levels of an atom are inverse squares of integers was one of the key experimental discoveries that precipitated the discovery of quantum mechanics. Observe that the n^{th} energy level has a total of

$$\sum_{l=0}^{n-1} (2l+1) = n^2 \quad (12.190)$$

linearly independent bound states (12.188). The dimension of the eigenspace corresponds to the number of orbital subshells in the atom for the corresponding energy level. The shells indexed by the angular quantum number, i.e., the order $l = 0, 1, 2, \dots$ of the spherical harmonic, are traditionally labeled by a letter in the sequence s, p, d, f, g, \dots , where each successive shell contains $2l+1$ individual subshells, indexed by the magnetic quantum number m .

The one missing ingredient in this simple model is the electron's *spin*. Since electrons can have one of two possible spins, the *Pauli Exclusion Principle*, first formulated by the Austrian physicist Wolfgang Pauli, tells us that each atomic energy shell can be occupied by at most two electrons. Consequently, the atomic shell with angular quantum number l may contain up to $2(2l+1)$ electrons. Keep in mind that, since $0 \leq l < n$, the l^{th} shell appears only when n is sufficiently large, so that, according to (12.190), the n^{th} energy level contains up to $2n^2$ electrons.

The resulting atomic configuration of electronic energy shells is the explanation for Mendeleev's periodic table. Its rows are indexed by the principal quantum number n , while the columns are labeled by the angular and magnetic quantum numbers l, m , and the spin. As one moves up the periodic table, the electrons in each successive element's atom progressively fill up the lower energy levels, each new shell containing first a single electron, then two electrons with opposite spins. Thus, hydrogen (in its ground state) has a single electron in the $1s$ shell. Helium has two electrons in the $1s$ shell. Lithium has

three electrons, with two of them filling the $1s$ shell and the third in the $2s$ shell. Neon has ten electrons filling the first two energy levels, with two electrons in the $1s$ shell, two in the $2s$ shell, and six in the $2p$ shell. And so on. The one complication is that, owing to the orbital's geometry, as prescribed by the associated spherical harmonic, the angular and, to a lesser extent, magnetic quantum numbers also affect the physically observed energy, and this can cause shells to fill later than might initially be expected. For example, in potassium and calcium, the $4s$ shell is successively filled, followed by scandium, which begins the process of filling the $3d$ subshells. The chemical properties of the elements are, to a very large extent, determined by the placement of their atom's electrons within the outermost energy level. The interested reader can consult, for example, [67, 79] for further details.

Exercises

- 12.7.1. If the nucleus contains Z protons circled by a single electron, then its atomic potential $V(\mathbf{x})$ is rescaled accordingly, replacing α^2/r by $Z\alpha^2/r$. Discuss the induced effect on the energy levels of such an atomic ion.
- ♡ 12.7.2. (a) Write down the time-dependent wave function for a single electron atom when the electron is in its ground state, i.e., the lowest energy level. (b) What is the probability density of the electron? (c) What is the probability of finding the electron within 1 Bohr radius of the atom? (d) Find the distance d (measured in Bohr radii) so that there is a 95% probability of finding the electron within a distance d of the nucleus.
- ◇ 12.7.3. Prove that the two expressions for the Laguerre polynomials in (12.186) agree.
- ◇ 12.7.4. (a) Let $k = 0, 1, 2, \dots$ be a nonnegative integer. The *Laguerre differential equation of order k* is

$$x u'' + (1-x) u' + k u = 0. \quad (12.191)$$

Show that $x = 0$ is a regular singular point. Then prove that the Frobenius solution based at $x = 0$ is a polynomial of degree j that coincides with the Laguerre polynomial $L_k^0(x)$.

- (b) Given nonnegative integers $j, k \geq 0$, use the Frobenius method to prove that the *generalized Laguerre differential equation*

$$x u'' + (j+1-x) u' + k u = 0 \quad (12.192)$$

has a polynomial solution that can be identified with the generalized Laguerre polynomial $L_k^j(x)$ in (12.186).

- ◇ 12.7.5. Suppose that $P(s)$ solves the ordinary differential equation (12.182). Prove that $Q(s) = s^{-l} e^{s/2} P(s)$ solves the differential equation

$$s \frac{d^2 Q}{ds^2} + [2(l+1) - s] \frac{dQ}{ds} + (n-l-1)Q = 0. \quad (12.193)$$

Then apply the result of Exercise 12.7.4 to complete the proof of Theorem 12.19.

- ♡ 12.7.6. Suppose $f(x)$ is a polynomial, and let $L_k^j(s)$ denote the generalized Laguerre polynomials (12.186). (a) Prove that, for $j, k \geq 0$,

$$\int_0^\infty f(s) L_k^j(s) s^j e^{-s} ds = \frac{(-1)^k}{k!} \int_0^\infty f^{(k)}(s) s^{j+k} e^{-s} ds.$$

- (b) For fixed j , prove that the generalized Laguerre polynomials $L_k^j(s)$, $k = 0, 1, 2, \dots$, are orthogonal with respect to the weighted inner product $\langle f, g \rangle = \int_0^\infty f(s) g(s) s^j e^{-s} ds$.

- (c) Prove the formula for their corresponding norms: $\|L_k^j\| = \sqrt{\frac{(j+k)!}{k!}}$.

- ◇ 12.7.7.(a) Prove that the generalized Laguerre polynomials satisfy the following recurrence relation:

$$(k+1)L_{k+1}^j(s) - (j+2k+1-s)L_k^j(s) + (j+k)L_{k-1}^j(s) = 0. \quad (12.194)$$

- (b) Prove that

$$\int_0^\infty s^{j+1} e^{-s} [L_k^j(s)]^2 ds = \frac{(j+2k+1)(j+k)!}{k!}. \quad (12.195)$$

Hint: Use part (a) and Exercise 12.7.6.

- ♡ 12.7.8. Prove that the atomic eigenfunctions (12.188) form an orthonormal system of wave functions with respect to the L^2 inner product on \mathbb{R}^3 .

Hint: Use Theorem 9.33 and equation (12.195).
