Yichao Zhu

Equations and Analytical Tools in Mathematical Physics

A Concise Introduction

Science Press
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ISBN 978-981-16-5440-4 ISBN 978-981-16-5441-1 (eBook)
https://doi.org/10.1007/978-981-16-5441-1

Jointly published with Science Press
The print edition is not for sale in China (Mainland). Customers from China (Mainland) please order the print book from: Science Press.

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Preface

The core contents of the present book are partial differential equation (PDE). The essence of PDE as a modelling tool can be perceived from summarising several key fundamental features underlying various physical processes. We are living in a world where things and states are normally spatially varying and temporally evolving. From a mathematical viewpoint, differentiation can be employed to describe variation or evolution. Meanwhile, certain physical quantities, such as energy, are conserved during evolution, and equation or identity can be used to capture conservation. Therefore, differential equations naturally become an effective tool for describing evolving physical processes with certain quantities conserved. When multiple free variables are needed, one normally ends up with partial differential equations.

The procedure of analysing a physical process with PDE can be generally divided into three stages. The first stage can be termed as "modelling" (from physics to mathematics), which seeks to represent the physical processes of interest through the mathematical formulation of PDE. The second stage can be termed as "analysis", which seeks to mathematically solve the derived PDE problems. The third stage can be termed as "interpretation" (from mathematics back to physics), which seeks to gain physical insights out of the mathematical results. The main goal of the present book is to help the reader develop a habit of such a chained way of thinking, i.e. "starting from physics, digging in mathematics, and return to physics". Moreover, several mathematical concepts and methods, which have been proven to be effective in solving PDE problems, are also discussed. It has to be mentioned that the mathematical tools that are originally devised for solving PDEs are quite vast in number, and some of them have already evolved to individual topics, such as functional analysis. Therefore, perhaps due to the author's limited understanding over the subject, it is quite difficult to use more specific terms than "analytical tools" to summarise those various mathematical tools. This is how the title of the book emerges, and only selected topics are discussed here.

Part I of this book is aimed to introduce three typical PDEs: the wave equation, the heat equation and Poisson's equation. They are discussed in parallel in the first three chapters. In each chapter, the contents cover the physical phenomena that can be described by the corresponding PDE, the solution strategies designated for solving the resulting PDE problems, as well as what can be interpreted from the

derived solutions. In such an illustrative manner, the essential links between a physical phenomenon and the mathematical structures underlying its corresponding PDE can be addressed. Awareness of such insightful linkages has proven to be crucial for implementing PDE tools, both theoretically and numerically, for solving real-world problems. For instance, implementation of the central difference scheme for approximating functional derivatives is likely to give rise to (unphysical) oscillation when simulating fluid mechanics problems. But such behaviour does not appear in the computation of linear elastostatic problems. This is because the governing equation in fluid mechanics are usually (first-order) hyperbolic, where the information is transmitted downstream. Mathematically, this is implied by the so-called characteristics. In contrast, the governing differential equations for elastostatic problems are generalised elliptic systems, which do not exhibit the behaviour of characteristics. Hence, using the central difference for discretising them becomes effective. Therefore, understanding the mathematical structures behind PDEs should enable one to choose appropriate numerical schemes, even facing with brand new PDE models. To this end, the classification of general second-order linear PDEs is discussed in Chap. 4.

Part II of this book covers topics on special functions, a powerful tool especially for analysing PDE problems defined in cylindrical/spherical domains. Attentions are first paid to two representative classes of special functions, namely Bessel functions and Legendre functions. Part II of this book concludes with a brief discussion on hypergeometric functions, which is aimed to address the commonalities of many special functions intensively used in the field of mathematical physics.

The book is suitable for undergraduates of science and engineering, who have accomplished their courses on calculus and linear algebra. A common impression about courses on PDEs and related topics is, given their importance in the sense of their applicability, they are quite challenging for students to manage. In the author's opinion, the difficulties can be summarised as follows. Firstly, solid understanding of the course materials entails an intensive use of the prerequisite knowledge on calculus, linear algebra, etc. As a result, students often get frustrated when the necessary prerequisite knowledge slips their minds. Secondly, some related concepts in the course are quite abstruse, while the derivations involved are often cumbersome. These intrinsic features of the course tend to discourage students, which could further prevent their absorption of advanced knowledge on using PDEs in their own fields.

To cope with such challenging issues, actions are taken in writing this book. Firstly, when certain prerequisite knowledge is expected to be intensively used for elaborating the contents of a section, a subsection which concisely summarises the key prerequisite knowledge is included, aiming to awake one's memory over the prerequisite topic. Secondly, when new concepts are to be introduced, addressing their linkages with the known (if applicable) is always prioritised. For example, when the properties of Bessel functions are introduced, a comparative discussion with that of sinusoidal functions is made. Thirdly, a road map is charted at the beginning of each chapter. The aim is to develop an overview of the contents about the chapter and their interrelationships. Fourthly, a set of online videos are also devised in parallel with the book, so as to make the best use of multimedia tools to

present the course contents. In summary, acquiring knowledge on PDEs and related topics is technically challenging for students, but one should also see its bright side. It offers an opportunity to (re-)consolidate the understanding of one's mathematical knowledge system in an application-oriented manner, and thus gets the reader ready for taking advanced courses on quantitative analysis.

It has to be emphasised that as a subject, "PDEs" itself has a very wide coverage in contents. Here only representative topics on PDEs are mentioned at a fairly elementary level. Hence, the present book is recommended as an introductory tool to familiarise readers with PDEs and special functions. Besides, technical terms are written in the *italic* font when they appear for the first time.

On writing this book, a number of classical textbooks on PDEs and special functions are referred to, and they are listed in the references with my great gratitude. I would like to thank my colleagues in Dalian University of Technology (DUT), in particular, Prof. Xu Guo and Prof. Yonggang Zheng, for their valuable suggestions. The hard works from several students at DUT, Dingchuan Xue, Jing Luo, Chuang Ma, Qian Xiang and Zhengcheng Zhou, on helping me arranging the book materials are gratefully acknowledged. All the students of Yunchuang 1901 class at DUT also have my gratitude, as they were forced to trial on the book manuscript, and nice comments regarding its revision are reported from them. Among them, Hongyu Ma and Qikai Zhu who have pointed several typos appearing in the book manuscript have my especial gratitude. Moreover, the financial support from the Department of Engineering Mechanics of DUT is acknowledged. Finally, I must thank my family for their constant support on my work, in particular my daughter Peien, without whom the book should have already been published, but of course, with far less fun.

Dalian, China Yichao Zhu

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Part I
Second-Order Linear Partial Differential Equations

Chapter 1
The Wave Equation

In this chapter, partial differential equations that govern many featured wave propagation phenomena are discussed. We start with modelling the process of string vibration through a partial differential equation, known as the wave equation, or the equation for string vibration. Then the concepts of initial and boundary conditions are introduced. This is followed by the presentation of a number of relevant methods widely used for solving problems governed by the wave equation. Our scope is then extended to cover two-/three-dimensional cases of wave propagation. The chapter concludes with discussion over the properties of solutions for problems governed by the wave equation.

The contents in this chapter are summarised in the knowledge map given in Fig. 1.1. Note that the contents in Fig. 1.1 are classified into several groups identified by the shapes of their frames. "Modelling" corresponds to a stage where a physical phenomenon is being represented by means of certain mathematical formulations. "Analysis" corresponds to a stage where certain mathematical tools are introduced so as to analyse the derived formulations (from physics). "Interpretation" corresponds to a stage where the mathematical results obtained through the analysis stage are employed to offer (often more insightful) interpretations to the physical phenomena that are modelled. For developing solid understanding of the course materials, certain mathematical knowledge that is supposed to be covered in the prerequisite courses, e.g. calculus, linear algebra, etc., is required, and these contents are summarised in the "prerequisite" stage. The linkages of the introduced contents with other topics likely to appear for future studies are also mentioned, and these "related topics" are identified in hexagonal frames. The setting here also applies for the knowledge map charted for other chapters in this book.

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Y. Zhu, *Equations and Analytical Tools in Mathematical Physics*,
https://doi.org/10.1007/978-981-16-5441-1_1

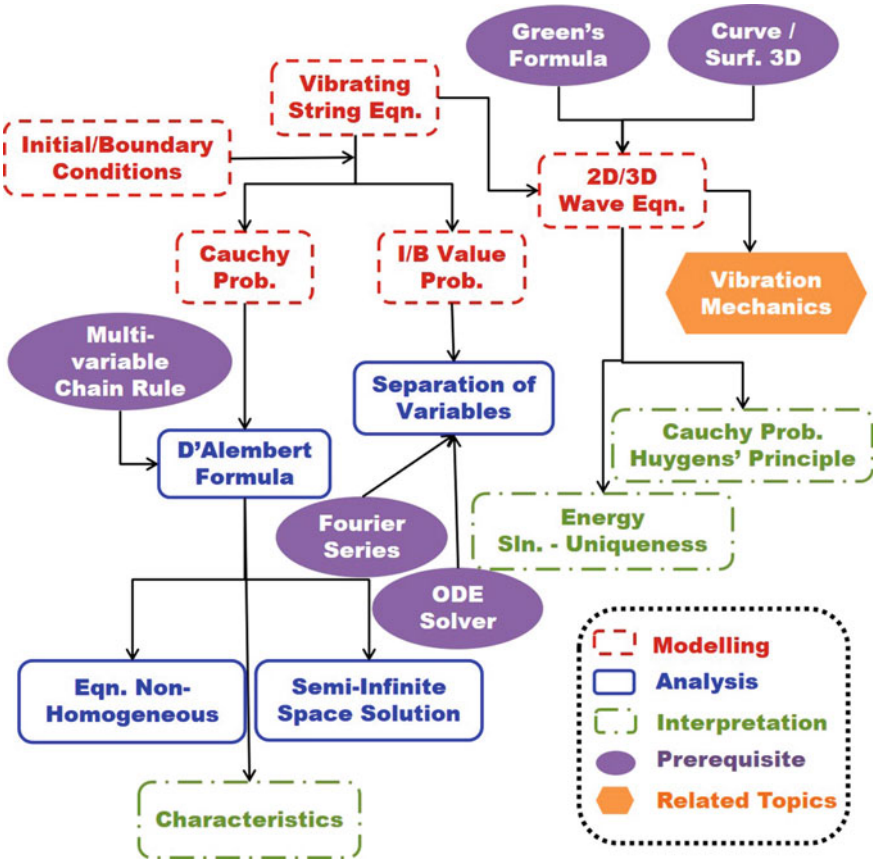


Fig. 1.1 Knowledge map—wave equation

1.1 Equation for String Vibration

1.1.1 Derivation of the Equation for String Vibration

In this section, we consider deriving a mathematical model to describe string vibration. To this end, we refer to a string, as shown in Fig. 1.2, of initial length L and of (linear) mass density ρ. As for modelling, one often needs to specify certain physically reasonable presumptions from the key features of the process of interest. For the case of string vibration, three assumptions are given as follows.

1. **The diameter of a string should be far shorter than its length**. This agrees with the common understanding of a "string". But we need to express such a fact in mathematical terms. If we use d to denote the string diameter, then $d \ll L$. Hence, the string can be fully represented by one spatial variable, say, x. As shown

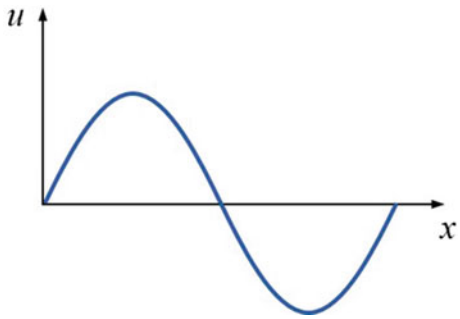


Fig. 1.2 To set up a model describing string vibration

in Fig. 1.2, the x-axis is set in parallel with the configuration when the string is straight, and any point on the string should correspond to a value of $x \in [0, L]$.

2. **The string undergoes small and transverse vibration**. Here the term "transverse" means that each point on the string only moves along the direction that is perpendicular to the x-axis. Thus, a function $u(x, t)$ can be introduced to denote the (transverse) displacement of the string section around x, away from the x-axis at time t. The term "small vibration" means that the magnitude of the displacement u is far smaller than that of the string length L. Note that "small" is meant in a relative sense. For instance, if the string of interest is from a guitar, then a displacement of 1 dm is quite large. But if the string of interest is a cable upholding a suspension bridge, then a displacement of 1 dm can still be considered as "small". Mathematically, the non-dimensional quantity of $\frac{\partial u}{\partial x}$ is employed to measure the degree of string vibration. Under small vibration, we write $|\frac{\partial u}{\partial x}| \ll 1$, indicating that $\left|\frac{\partial u}{\partial x}\right|$ is small in magnitude, or we can simply require

$$\left|\frac{\partial u}{\partial x}\right|^2 \approx 0. \tag{1.1}$$

3. **A string resists elongation by a line tension following Hooke's law**. A string is expected to resist elongation, leading to a state of tension. The resisting force, or the line tension denoted by $T(x, t)$, is supposed to follow Hooke's law, i.e. the magnitude of the line tension at (x, t) is proportional to the local increment in the string arc-length denoted by $s(x, t)$.

Moreover, a transversely vibrating string may also experience an external driving force, whose distribution can be denoted by $F(x, t)$. Here $F(x, t)$ is measured in unit "Newton per metre". In Fig. 1.1, the key physical quantities that are needed for modelling string vibration are summarised.

For a transversely vibrating string, its behaviour can be dictated through the displacement function $u(x, t)$. Thus, our modelling target is to set up mathematical formulations for $u(x, t)$. Here the modelling procedure encompasses the use of the above-listed three assumptions and the law of conservation in momentum. Our strategy here, as shown in Fig. 1.3, is to be focused on the behaviour of an arbitrarily

Table 1.1 Physical quantities needed for modelling string vibration

Symbol	Physical meaning	Dimension
x	Spatial variable	Metre (m)
t	Temporal variable	Second (s)
$u(x, t)$	Transverse displacement	m
$s(x, t)$	String arc-length	m
$T(x, t)$	Line tension	Newton (N)
$F(x, t)$	External force	N/m
ρ	Mass density	kg/m

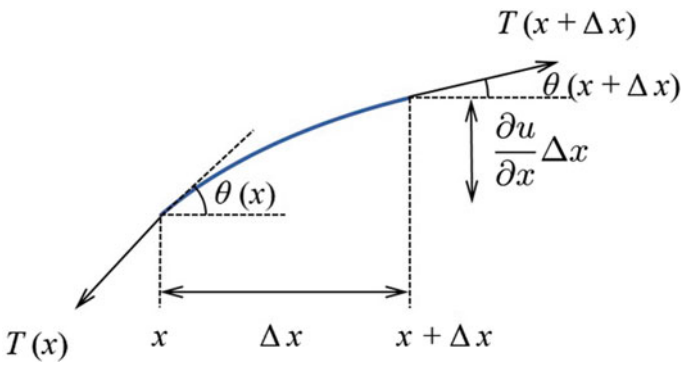


Fig. 1.3 Infinitesimally short string segment

chosen string segment of infinitesimally short length, say, $[x, x + \Delta x]$ with $\Delta x \to 0$. In order to set up the model, it takes three steps detailed as follows.

1. **To show that the line tension T is independent of time t**. For the string segment shown in Fig. 1.3, its arc-length can be formulated by

$$\Delta s \approx \sqrt{1 + \left(\frac{\partial u}{\partial x}\right)^2}\,\Delta x \approx \Delta x, \tag{1.2}$$

where the second approximation comes from the presumption that $\frac{\partial u}{\partial x}$ is small as from Eq. (1.1). Thus, the local arc-length of the string segment stays the same as the initial state. Based on the third assumption above, the line tension T should not evolve in time near the spatial point x. Since this infinitesimally short segment is selected arbitrarily on the string, the line tension T stays constant in time everywhere on the string. In other words, T is a unary function of the spatial variable x.

2. **To show that the line tension is uniform in space**. From the second assumption above, the infinitesimally small string segment does not experience any longitudinal displacement. To formulate the force equilibrium in the longitudinal direction, we

introduce $\theta(x)$ to denote the angle of the line target of the infinitesimal segment about the x-axis, as shown in Fig. 1.3, and the following identity should hold:

$$T(x)\cos[\theta(x)] = T(x+\Delta x)\cos[\theta(x+\Delta x)]\,.$$

For simplicity, throughout the book, a functional symbol affiliated with a bar and a subscript is always employed to denote the function evaluated at the variable indicated by the subscript. For example, $T(x)$ appearing in the identity above can be expressed by $T(x) = T|_x$.

The identity above is thus rewritten by

$$T|_x \cos\theta|_x = T|_{x+\Delta x}\cos\theta|_{x+\Delta x}\,. \tag{1.3}$$

Note that the angle θ can be related to the displacement u by

$$\tan[\theta(x)] = \frac{\partial u}{\partial x} \ll 1,$$

which suggests that $\tan[\theta(x)]$ is also an infinitesimally small quantity. Then we have

$$\cos\theta = (1+\tan^2\theta)^{-\frac{1}{2}} = \left(1+\left(\frac{\partial u}{\partial x}\right)^2\right)^{-\frac{1}{2}} \approx 1, \tag{1.4}$$

where Eq. (1.1) is adopted again. Inserting Eq. (1.4) into (1.3) suggests that

$$T|_x = T|_{x+\Delta x}\,.$$

Since our choice of the infinitesimally small string segment is arbitrary in x, the line tension should stay constant over the whole string.

Therefore, we conclude that the line tension is a constant, independent both of time and space.

A question may probably arise from the derivations above. If $\cos\theta$ approximately equals 1, then why $\tan\theta$ is not approximately 0? A quick answer to this question is about the order of the magnitude of an small quantity. Here $\tan\theta$ is a small quantity of the first order, while $\cos\theta$ deviates from 1 by a small number of second order. This can be clearly seen from the corresponding Taylor's series around $\theta = 0$, i.e.

$$\sin\theta \sim \theta - \frac{\theta^3}{6} + \cdots;$$
$$\cos\theta \sim 1 - \frac{\theta^2}{2} + \cdots;$$
$$\tan\theta \sim \theta + \frac{\theta^3}{3} + \cdots.$$

If we let the "truncation error" to be the second order, we see that

$$\sin\theta \approx \theta \approx \tan\theta \approx \frac{\partial u}{\partial x}, \tag{1.5}$$

but $\cos\theta \approx 1$. In other words, our modelling precision is up to the first order in terms of the small quantity $\frac{\partial u}{\partial x}$.

3. **To derive a differential equation governing string vibration**. Given the infinitesimally small string segment of $[x, x+\Delta x]$, the momentum in the transverse direction is conserved within any time period, say, $[t, t+\Delta t]$. To effectively express the momentum change over this short period, we introduce another short-form notation. If a function is affiliated with a subscript and a superscript, it means the difference in function values, e.g. $f|_a^b = f(b) - f(a)$.

Hence, the momentum change along the transverse direction over the time interval $[t, t+\Delta t]$ is formulated by

$$\rho\Delta x \left.\frac{\partial u}{\partial t}\right|_t^{t+\Delta t} = \rho\Delta x \left(\left.\frac{\partial u}{\partial t}\right|_{t+\Delta t} - \left.\frac{\partial u}{\partial t}\right|_t \right), \tag{1.6}$$

where $\rho\Delta x \approx \rho\Delta s$ measures the mass of the string segment.

Now we turn to formulating the impulse applied on this segment over $[t, t+\Delta t]$. The force acting on the segment comes from two sources. The first one is due to the external force, and the second one is from the line tensions at its two ends exerted by the rest parts of the string. As suggested in Fig. 1.3, the transverse component of the total line tension equals

$$T\sin\theta\,|_{x+\Delta x} - T\sin\theta\,|_x = T\sin\theta\,|_x^{x+\Delta x}.$$

Therefore, the total impulse applied on the infinitesimally small string segment is given by

$$\left(T\sin\theta|_x^{x+\Delta x} + F\Delta x\right)\Delta t = \left(T \left.\frac{\partial u}{\partial x}\right|_x^{x+\Delta x} + F\Delta x \right)\Delta t, \tag{1.7}$$

where Eq. (1.5) is used.

According to the law of momentum conservation, the momentum change given by Eq. (1.6) should be equated with the impulse formulated by Eq. (1.7), i.e.

$$\rho\Delta x \left.\frac{\partial u}{\partial t}\right|_t^{t+\Delta t} = T \left.\frac{\partial u}{\partial x}\right|_x^{x+\Delta x} \Delta t + F\Delta x\Delta t.$$

Dividing the identity above by $\rho\Delta x\Delta t$ on both sides gives

$$\frac{1}{\Delta t}\left(\left.\frac{\partial u}{\partial t}\right|_t^{t+\Delta t} \right) = \frac{T}{\rho}\cdot\frac{1}{\Delta x}\left.\frac{\partial u}{\partial x}\right|_x^{x+\Delta x} + \frac{F}{\rho}. \tag{1.8}$$

Note that as Δx and $\Delta t \to 0$, one obtains

$$\lim_{\Delta t \to 0} \frac{1}{\Delta t} \left(\left. \frac{\partial u}{\partial t} \right|_{t}^{t+\Delta t} \right) = \frac{\partial^2 u}{\partial t^2}, \qquad \lim_{\Delta x \to 0} \frac{1}{\Delta x} \left(\left. \frac{\partial u}{\partial x} \right|_{x}^{x+\Delta x} \right) = \frac{\partial^2 u}{\partial x^2}.$$

Thus, as both Δx and Δt tend to 0 in Eq. (1.8), we finally get

$$\frac{\partial^2 u}{\partial t^2} = \frac{T}{\rho} \frac{\partial^2 u}{\partial x^2} + \frac{F(x,t)}{\rho}. \tag{1.9}$$

If we further introduce $a^2 = \frac{T}{\rho}, f = \frac{F}{\rho}$, Eq. (1.9) becomes

$$\frac{\partial^2 u}{\partial t^2} - a^2 \frac{\partial^2 u}{\partial x^2} = f(x,t). \tag{1.10}$$

It can be checked that the parameter a in Eq. (1.10) is measured in "m/s", and it will be shown in Sec. 1.2.2 that a actually describes the wave propagation speed. Moreover, f in Eq. (1.10) is in unit "N/kg", and it measures the external load in the sense of "force per weight".

Equation (1.10) identifies a mathematical formulation which describes the behaviour of a string experiencing small and transverse vibration. It is, in fact, a **differential equation** for the unknown function $u(x,t)$, which represents the displacement field along the transverse direction. Since the equation is established through the partial differentiation of the unknown function, Eq. (1.10) is called a *partial differential equation*, or usually abbreviated as "PDE" for the displacement field $u(x,t)$. In particular, Eq. (1.10) is usually termed as the (one-dimensional) *wave equation*, or the *equation for string vibration* in this book so as to be distinguished from the wave equation defined for higher-dimensional cases. A function which makes a PDE hold is called a *solution* to this PDE.

1.1.2 Initial and Boundary Conditions

Similar as in the cases for ordinary differential equations, which are abbreviated as "ODEs" in this book, one needs to impose extra conditions so as to fully identify the physical process in consideration. For the cases with partial differential equations, initial and boundary conditions are usually needed. For example, in order to fully determine the behaviour of a vibrating string, one needs to know not only how it vibrates as formulated through Eq. (1.10), but also the initial state of the string, as well as how it is affected by the exterior through its two end points. The latter two issues are related to the concepts of initial/boundary conditions, respectively. Here to formulate a definite physical process, a *problem of partial differential equation* or shortly a *PDE problem* should be set up. A *definite* PDE problem should consist of a

governing PDE and appropriate initial and/or boundary conditions. The definiteness of a PDE problem is further discussed in Sect. 1.5. The *solution* for a PDE problem should satisfy not only the governing PDE, but also make the initial and boundary conditions hold.

An *initial condition* describes the system behaviour at $t = 0$. For modelling string vibration, we need two pieces of initial information: the initial profile of the string and the initial speed. Mathematically, they are formulated by

$$u\,|_{t=0} = \phi(x); \tag{1.11a}$$

$$\left.\frac{\partial u}{\partial t}\right|_{t=0} = \psi(x), \tag{1.11b}$$

where $\phi(x)$ and $\psi(x)$ are given functions. Here a key observation is that the initial conditions are given by functions independent of the temporal variable t. Moreover, $\phi(x)$ and $\psi(x)$ should exhibit certain smoothness over their input arguments in accordance with the actual physical situation.

When the string of interest is infinitely long, i.e. $x \in (-\infty, \infty)$, only initial conditions are needed, and the resulting PDE problem is termed as a *Cauchy Problem*. For instance, the Cauchy problem for the wave equation can be generally expressed by

$$\begin{cases} u_{tt} - a^2 u_{xx} = f(x,t), \;\; (x,t) \in \mathbb{R} \times \mathbb{R}^+; \\ u|_{t=0} = \phi(x), \quad u_t|_{t=0} = \psi(x). \end{cases} \tag{1.12}$$

Equation (1.12) offers a paradigm to represent a PDE problem. The first line indicates the governing equation and then the domain of definition for the independent variables x and t, which is expressed by means of the Descartes product. The second line of problem (1.12) outlines the initial conditions. Note that when the domain of definition becomes of finite size, boundary conditions to be introduced later should also be included.

When the string of interest is of finite length, a *boundary condition* should also be imposed at each of its ends. A PDE problem containing both initial and boundary conditions is called an *initial–boundary value problem*.

Suppose the string of interest ends at $x = a$. Three types of physically meaningful boundary conditions can be imposed.

When the (transverse) trajectory of the end point is known, we have

$$u|_{x=a} = g_1(t), \tag{1.13a}$$

which is called a *Dirichlet boundary condition*, or sometimes *the first type of boundary condition*. In particular, when $g_1(t)$ in Eq. (1.13a) becomes a constant, the end point at $x = a$ does not move, corresponding to a *fixed-value boundary condition*.

When the tangential direction of a string at one end is given, we write

$$\left.\frac{\partial u}{\partial x}\right|_{x=a} = g_2(t), \tag{1.13b}$$

which is called a *Neumann boundary condition*, or sometimes *the second type of boundary condition*. Note that $T\frac{\partial u}{\partial x}|_{x=a}$ measures the transverse component of the line tension at $x = a$. Thus, a Neumann boundary condition for string vibration may be achieved through force control at the string end.

The third type of boundary condition is formulated as a linear combination of the previous two cases. Mathematically, it is given by

$$\left.\left(ku \pm T\frac{\partial u}{\partial x}\right)\right|_{x=a} = g_3(t), \tag{1.13c}$$

which is called a *Robin boundary condition*. To obtain a Robin boundary condition, one may consider the case where the string end is attached with a spring. The term ku measures the restoring force of the spring, and $T\frac{\partial u}{\partial x}$ measures the line tension at the end point. Note that the sign in Eq. (1.13c) is determined by the case at which end the boundary condition is imposed. If $x = a$ marks the left end of a string, "$-$" should be taken; if $x = a$ marks the right end of a string, "+" should be taken. Finally, the first two types of boundary conditions can be treated as special cases of the third type. For instance, when $T = 0$, Eq. (1.13c) degenerates to Eq. (1.13a); when $k = 0$, Eq. (1.13c) degenerates to Eq. (1.13b).

1.1.3 Terminology

In the end of this section, several key concepts in association with partial differential equation are mentioned. Here we introduce another set of notations to make the mathematical expressions more concisely looking during the rest of the book. We add an independent variable as a subscript to a quantity, indicating its partial derivative with respect to the independent variable. For example, $u_t = \frac{\partial u}{\partial t}$, $u_{xx} = \frac{\partial^2 u}{\partial x^2}$.

Hence, the equation for string vibration, given by Eq. (1.10), can be reformulated by

$$u_{tt} - a^2 u_{xx} = f(x, t). \tag{1.14}$$

If we further introduce a "*differential operator*" $\mathcal{L}$, such that $\mathcal{L}[u] = u_{tt} - a^2 u_{xx}$, Eq. (1.14) becomes

$$\mathcal{L}[u] = f. \tag{1.15}$$

Equation (1.15) actually provides a general way to express a partial differential equation. The left side operates on the unknown function u, while the right side is a known function f.

The highest derivatives appearing in the differential operator $\mathcal{L}[u]$ define the *order* of a PDE. For example, the wave equation (1.14) is a second-order PDE both in time and space, because the highest derivatives are second order.

A PDE written in the form of Eq. (1.15) is termed as a *linear* PDE, provided that $\mathcal{L}[u]$ is a linear differential operator, that is, for any functions u and v, and for any real numbers α and β, the identity

$$\mathcal{L}[\alpha u_1 + \beta u_2] = \alpha \mathcal{L}[u_1] + \beta \mathcal{L}[u_2]$$

always holds. Examined with this rule, partial differentiation is a linear differential operator, because $\frac{\partial}{\partial t}(\alpha u_1 + \beta u_2) = \alpha(u_t) + \beta(u_t)$, and so is the linear combination of partial differentiations of u. Therefore, the equation for string vibration is a linear PDE. In contrast, when $\mathcal{L}[u]$ is not linear with u, the resulting PDE is called a *nonlinear* PDE.

A linear PDE given by Eq. (1.15) is *homogeneous*, provided that $f \equiv 0$. In contrast, if f is not uniformly zero, the string is in a state of *forced vibration*, and the resulting PDE is called an *inhomogeneous* PDE. In general, a homogeneous PDE is easier to solve than an inhomogeneous one.

The aforementioned terms, such as "linearity" and "homogeneity", also apply for initial and boundary conditions. For example, the initial/boundary conditions listed from Eqs. (1.11a) to (1.13c) are all *linear*. If the right side of certain conditions vanishes, we end up with a *homogeneous initial/boundary condition*.

When the governing differential equation, the initial and boundary conditions are all linear, the corresponding PDE problem is called a *linear PDE problem*. Generally speaking, there are far more methods proposed for solving a linear PDE problem than a nonlinear one. For instance, the superposition of several linear PDE problems is still linear. Hence, one can always decouple a complicated linear problem into several simple looking ones. In this book, almost all the methods presented are designated for solving linear PDE problems.

1.2 D'Alembert's Formula

In this section, we aim to solve the Cauchy problem governed by the wave equation, which can be generally formulated, according to Sect. 1.1.2, by

$$\begin{cases} u_{tt} - a^2 u_{xx} = f(x,t), \ \ (x,t) \in \mathbb{R} \times \mathbb{R}^+; \\ u|_{t=0} = \phi(x), \quad u_t|_{t=0} = \psi(x). \end{cases} \tag{1.16}$$

The PDEs and the initial conditions of problem (1.16) are all inhomogeneous. It can be readily verified that its solution u is equal to the superposition of two functions: $u = v + w$, where v and w satisfy

$$\text{(I)} \quad \begin{cases} v_{tt} - a^2 v_{xx} = 0, \ (x,t) \in \mathbb{R} \times \mathbb{R}^+; \\ v|_{t=0} = \phi(x), \quad v_t|_{t=0} = \psi(x) \end{cases} \tag{1.17}$$

and

$$\text{(II)} \quad \begin{cases} w_{tt} - a^2 w_{xx} = f(x,t), \ (x,t) \in \mathbb{R} \times \mathbb{R}^+; \\ w|_{t=0} = 0, \quad w_t|_{t=0} = 0. \end{cases} \tag{1.18}$$

respectively. Upon such decomposition, certain parts of problems (1.17) and (1.18) become homogeneous.

1.2.1 D'Alembert's Formula

First, we consider solving the first problem, i.e. problem (1.17), which consists of a linear homogeneous PDE and two inhomogeneous initial conditions. Our strategy is to introduce a new set of independent variables, under which the governing equation becomes simplified significantly.

To this end, we let

$$\xi = x - at, \ \eta = x + at. \tag{1.19}$$

With reference to the multivariable differentiation chain rule, one can express the derivative of v with respect to x through that with respect to ξ and η, i.e.

$$v_x = v_\xi \xi_x + v_\eta \eta_x = v_\xi + v_\eta,$$

where Eq. (1.19) is used to evaluate ξ_x and η_x. Differentiating the above identity with respect to x again gives

$$v_{xx} = (v_\xi + v_\eta)_x = v_{\xi\xi}\xi_x + v_{\xi\eta}\eta_x + v_{\xi\eta}\xi_x + v_{\eta\eta}\eta_x = v_{\xi\xi} + 2v_{\xi\eta} + v_{\eta\eta}. \tag{1.20}$$

Similarly, v_{tt} in Eq. (1.17) can be reformulated by

$$v_{tt} = a^2 \left(v_{\xi\xi} - 2v_{\xi\eta} + v_{\eta\eta} \right). \tag{1.21}$$

Inserting Eqs. (1.20) and (1.21) into the governing equation of problem (1.17) gives

$$v_{\xi\eta} = 0. \tag{1.22}$$

It is observed that the governing equation gets simplified if ξ and η are used as the independent variables. To satisfy Eq. (1.22), the function v should be expressed by the sum of a function solely of ξ and a function solely of η, i.e.

$$v = F(\xi) + G(\eta). \tag{1.23}$$

Rewriting Eq. (1.23) in the original $x - t$ coordinate system expresses a general solution to the equation of string vibration, which reads

$$v(x, t) = F(x - at) + G(x + at). \tag{1.24}$$

To further determine the unknown unary functions F and G, we refer to the initial conditions of problem (1.17). Thus, we write

$$F(x) + G(x) = \phi(x), \tag{1.25a}$$

$$-aF'(x) + aG'(x) = \psi(x). \tag{1.25b}$$

Integrating Eq. (1.25b) with respect to x gives

$$-aF(x) + aG(x) = \int_{x_0}^{x} \psi(\alpha)\mathrm{d}\alpha + C, \tag{1.26}$$

where C is a constant depending on the choice of x_0.

Equations (1.25a) and (1.26) actually form a linear algebraic equation system for $F(x)$ and $G(x)$. On solving it, we reach

$$F(x) = \frac{\phi(x)}{2} - \frac{1}{2a}\int_{x_0}^{x} \psi(\alpha)\mathrm{d}\alpha - \frac{C}{2a};$$

$$G(x) = \frac{\phi(x)}{2} + \frac{1}{2a}\int_{x_0}^{x} \psi(\alpha)\mathrm{d}\alpha + \frac{C}{2a}.$$

On replacing the inputs of $F(\cdot)$ and $G(\cdot)$ by $x - at$ and $x + at$, respectively, and employing Eq. (1.24), we derive the solution for problem (1.17) to be

$$v(x, t) = \frac{1}{2}\left(\phi(x - at) + \phi(x + at)\right) + \frac{1}{2a}\int_{x-at}^{x+at} \psi(\alpha)\mathrm{d}\alpha. \tag{1.27}$$

Eq. (1.27) is called *D'Alembert's formula*.

When a solution for a PDE problem is derived, one often needs to insert it into the original problem for verification. In the present context, one needs to check that D'Alembert's formula (1.27) satisfies both the governing equation and the initial conditions of problem (1.17).

First we show that Eq. (1.27) satisfies the governing equation of problem (1.17). Differentiating Eq. (1.27) with respect to t gives

$$v_t = \frac{a}{2}\left(-\phi'(x-at)+\phi'(x+at)\right)+\frac{1}{2}\left(\psi(x-at)+\psi(x+at)\right), \tag{1.28}$$

where $\phi'(\cdot)$ stands for the first derivative of ϕ with respect to its input argument. Note that the derivation of Eq. (1.28) encompasses differentiating an integral containing parameters, which is briefly summarised in the prerequisite knowledge session successive to the present section.

Differentiating it again expresses the second-order temporal derivative by

$$v_{tt} = \frac{a^2}{2}\left(\phi''(x-at)+\phi''(x+at)\right)+\frac{a}{2}\left(-\psi'(x-at)+\psi'(x+at)\right),$$

where ϕ'' stands for its second derivative.

In a similar sense, we obtain

$$v_{xx} = \frac{1}{2}\left(\phi''(x-at)+\phi''(x+at)\right)+\frac{1}{2a}\left(-\psi'(x-at)+\psi'(x+at)\right).$$

Inserting the results above into the governing equation verifies that D'Alembert's formula (1.27) solves the equation of string vibration.

As for the initial conditions of problem (1.17), we let $t=0$ in Eq. (1.27), and quickly see that $v|_{t=0}=\phi(x)$. By letting $t=0$ in Eq. (1.28), we can also show that $v_t|_{t=0}=\psi(x)$.

1.2.2 Characteristics

To show the physical picture charted by D'Alembert's formula, we now consider an exemplified Cauchy problem given as follows:

$$\begin{cases} v_{tt}-a^2v_{xx}=0, \ (x,t)\in\mathbb{R}\times\mathbb{R}^+; \\ v|_{t=0}=\cos x, \quad v_t|_{t=0}=0. \end{cases}$$

By letting $\phi(x)=\cos x$ and $\psi(x)=0$ in D'Alembert's formula (1.27), we write its solution by

$$v(x,t)=\frac{1}{2}\left(\cos(x-at)+\cos(x+at)\right). \tag{1.29}$$

It implies that in the absence of external forces, an initially static cosine wave evolves by being decomposed into a rightward cosine wave of speed a, i.e. $v_1=\frac{1}{2}\cos(x-at)$, and a leftward cosine wave of speed a.

A contour plot for v_1 against x and t is shown in Fig. 1.4, where the regions where the values of v_1 are identical share a same colour. Actually for a rightward wave of constant speed of a, the function values always stay unchanged along any lines

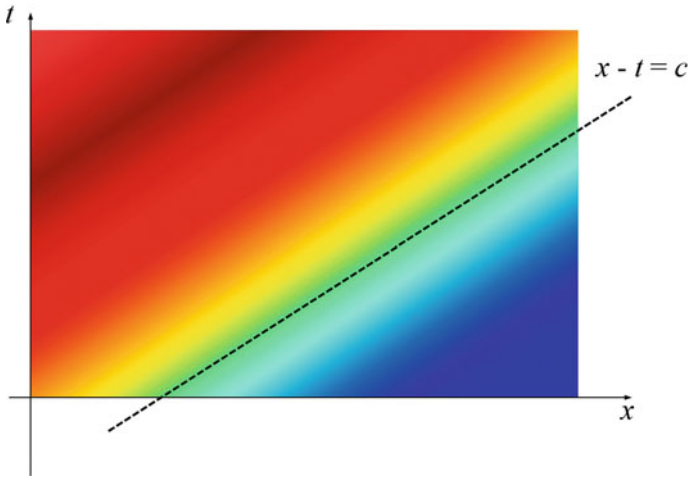


Fig. 1.4 Contour plot of the rightward cosine wave $v_1(x, t)$ defined by Eq. (1.29), where $a = 1$

of slope $\frac{1}{a}$ in the $x - t$ plane. In other words, a function in the form of $F(x - at)$ represents a wave propagating rightward at a constant speed a, and so does $G(x + at)$ for a leftward travelling wave.

From such a viewpoint, Eq. (1.24) implies that a solution to the wave equation consists of two travelling waves at a same speed of a, one to the right: $v_1 = F(x - at)$ and the other to the left: $v_2 = G(x + at)$. Hence, for a given constant C, the rightward wave function $F(\cdot)$ is invariant along the line of $x - at = C$, and so does the leftward wave function $G(\cdot)$ along $x + at = C$. Therefore, the two families of parametric curves $x \pm at = C$ (parameterised by C) play a central role in analysing the string vibration behaviour, and they are called the *characteristics* of the wave equation.

As a special case when the initial speed $\psi(x) = 0$, it is found that $F(x - at) = \frac{1}{2}\phi(x - at)$ and $G(x + at) = \frac{1}{2}\phi(x + at)$. In this scenario, the solution is given by the superposition of two initially identical waves, and they translate at a same speed, but in opposite directions.

The idea of wave decomposition is in fact generalisable. If a PDE describes a physical phenomenon involving wave propagation, one may search for a *travelling wave solution* in the form of $u = F(\mathbf{x} + \mathbf{v}t)$, where (1) $\mathbf{x}$ and $\mathbf{v}$ can be multidimensional; (2) the velocity $\mathbf{v}$ is often part of the solution. Extended theories on the characteristics can be applied to analyse PDEs sharing similar properties as the wave equation, and we will go back to this topic in Sect. 4.1.

More physical implications revealed by D'Alembert's formula are examined over how the initial conditions affect the whole string vibration process. As from Eq. (1.27), the initial information at $x = x_0$ should reach no farther than the points at $x_0 \pm at$ at time t. This means the function value at point x and time t is fully determined by the initial conditions taken from the spatial interval of $[x - at, x + at]$, as

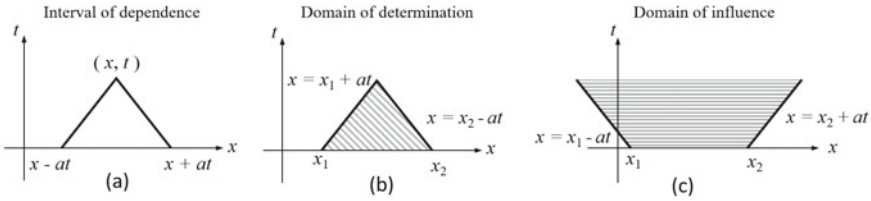


Fig. 1.5 Interval of dependence, domain of determination and domain of influence, respectively

shown in Fig. 1.5a. Thus, $[x - at, x + at]$ is known as the *interval of dependence* of the point (x, t).

For a given spatial interval, say, $[x_1, x_2]$, one may generate a triangle, whose two edges are parallel to the characteristics, as marked by the shaded region in Fig. 1.5b. Then the function values at any point (x, t) falling inside the triangle should be fully determined by the initial conditions taken from the interval $[x_1, x_2]$. The shaded region is thus termed as the *domain of determination* of the interval $[x_1, x_2]$.

Finally, for initial conditions taken within a spatial interval $[x_1, x_2]$, the largest region which they can cast their influence over is the shaded region shown in Fig. 1.5c, which is termed as the *domain of influence* of the interval $[x_1, x_2]$.

It needs to be noted that infinitely long strings do not actually exist. The value of the Cauchy problem for the wave equation lies in the fact that it clearly reveals the propagating behaviour as discussed above. It is shown in the next case that the presence of the string ends affects the observation of this propagating behaviour by means of wave deflection. Therefore, Cauchy problems are normally analysed to reveal the intrinsic behaviour shown by their governing differential equations.

1.2.3 The Case of a Semi-infinitely Long String

Now we investigate the vibrating process of a semi-infinitely long string, as shown in Fig. 1.6. The domain of definition for the spatial variable then becomes $x \in (0, \infty)$. To set up the corresponding PDE problem, a boundary condition is necessary at $x = 0$. Here we require that the string stays tangentially horizontal at the origin, i.e. $u_x|_{x=0} = 0$, as shown in Fig. 1.6. As from Sect. 1.1, $T\frac{\partial u}{\partial x}$ measures the local line tension. The boundary condition at $x = 0$ means that the string is free from external driving force at the string end.

A PDE problem is thus established as

$$\begin{cases} u_{tt} - a^2 u_{xx} = 0, \ (x, t) \in \mathbb{R}^+ \times \mathbb{R}^+; \\ u|_{t=0} = \phi(x), \ u_t|_{t=0} = \psi(x); \\ u_x|_{x=0} = 0. \end{cases} \tag{1.30}$$

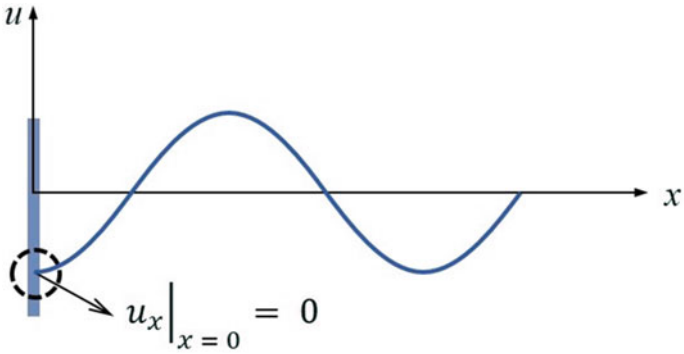


Fig. 1.6 Illustration of a semi-infinitely long string

Our strategy for solving problem (1.30) is to extend it to a problem defined over the whole domain of $x \in (-\infty, +\infty)$, such that D'Alembert's formula can be utilised. For this purpose, we first extend the initial conditions by

$$\Phi(x) = \begin{cases} \phi(x), & x > 0; \\ p(-x), & x < 0, \end{cases}$$

$$\Psi(x) = \begin{cases} \psi(x), & x > 0; \\ q(-x), & x < 0, \end{cases}$$

where $p(\cdot)$ and $q(\cdot)$ are functions to be determined. Note that $\Phi(x)$ and $\Psi(x) = 0$ should continuous across $x = 0$, leading to

$$\begin{cases} \lim_{x\to 0^+} \phi(x) = \lim_{x\to 0^-} p(-x) = \lim_{x\to 0^+} p(x); \\ \lim_{x\to 0^+} \psi(x) = \lim_{x\to 0^-} q(-x) = \lim_{x\to 0^+} q(x). \end{cases} \tag{1.31}$$

In certain occasions, the differentiability of $\Phi(x)$ and $\Psi(x)$ at $x = 0$ is desired to several times. Therefore,

$$\begin{cases} \lim_{x\to 0^+} \phi^{(n)}(x) = (-1)^n \lim_{x\to 0^-} p^{(n)}(-x) = (-1)^n \lim_{x\to 0^+} p^{(n)}(x); \\ \lim_{x\to 0^+} \psi^{(n)}(x) = (-1)^n \lim_{x\to 0^-} q^{(n)}(-x) = (-1)^n \lim_{x\to 0^+} q^{(n)}(x), \end{cases} \tag{1.32}$$

where $f^{(n)}(x)$ denotes the nth derivatives of $f(x)$.

As $\Phi(x)$ and $\Psi(x)$ are well defined for all $x \in (-\infty, +\infty)$, one may set up a Cauchy problem for $U(x, t)$ to be

$$\begin{cases} U_{tt} - a^2 U_{xx} = 0, \ (x, t) \in \mathbb{R} \times \mathbb{R}^+; \\ U|_{t=0} = \Phi(x), \ U_t|_{t=0} = \Psi(x). \end{cases} \tag{1.33}$$

Once the expression for $U(x,t)$ becomes available, the solution for the original problem (1.30) is determined by $u(x,t) = U|_{x>0}$.

With reference to D'Alembert's formula (1.27), we have

$$U(x,t) = \frac{1}{2}\left(\Phi(x-at) + \Phi(x+at)\right) + \frac{1}{2a}\int_{x-at}^{x+at} \Psi(\alpha)\mathrm{d}\alpha. \tag{1.34}$$

Since both Φ and Ψ are piecewisely defined, the evaluation of U in Eq. (1.34) should be carried out case by case, depending on the sign of $x \pm at$.

When $x > at$, both $x \pm at$ assume positive values. One can replace $\Phi(\cdot)$ and $\Psi(\cdot)$ in Eq. (1.34) directly by $\phi(\cdot)$ and $\psi(\cdot)$, respectively.

When $x < at$, we are only interested in situations where $0 < x < at$. Hence,

$$\Phi(x+at) = \phi(x+at);$$

$$\Phi(x-at) = p(at-x);$$

$$\int_{x-at}^{x+at} \Psi(\alpha)\,\mathrm{d}\alpha = \int_{0}^{x+at} \psi(\alpha)\mathrm{d}\alpha + \int_{x-at}^{0} q(-\alpha)\mathrm{d}\alpha.$$

Note that the second integral on the right side of the identity above can be reformulated by introducing $s = -\alpha$, that is,

$$\int_{x-at}^{0} q(-\alpha)\,\mathrm{d}\alpha = \int_{0}^{at-x} q(s)\,\mathrm{d}s.$$

Inserting these into Eq. (1.34) gives

$$U(x,t) = \begin{cases} \dfrac{\phi(x-at)+\phi(x+at)}{2} + \dfrac{1}{2a}\displaystyle\int_{x-at}^{x+at} \psi(\alpha)\mathrm{d}\alpha, & x > at; \\ \dfrac{p(at-x)+\phi(x+at)}{2} + \dfrac{1}{2a}\left(\displaystyle\int_{0}^{x+at} \psi(\alpha)\mathrm{d}\alpha + \int_{0}^{at-x} q(\alpha)\mathrm{d}\alpha\right), & 0 < x < at. \end{cases} \tag{1.35}$$

Up to this stage, we have not yet specified what $p(x)$ and $q(x)$ are. They are determined by making use of the boundary condition $u_x|_{x=0} = 0$. To calculate $u_x|_{x=0}$, attentions should be paid to the expression of $U(x,t)$ defined in the region of $x \in (0, at)$. Differentiating the second identity of Eq. (1.35) gives

$$U_x = \frac{1}{2}\left(-p'(at-x) + \phi'(at+x)\right) + \frac{1}{2a}\left(-q(at-x) + \psi(at+x)\right),$$

where p' and ϕ' denote the first derivatives of p and ϕ, respectively. Then the boundary condition $u_x|_{x=0} = 0$ reads

$$U_x|_{x=0} = \frac{1}{2}\left(-p'(at) + \phi'(at)\right) + \frac{1}{2a}\left(-q(at) + \psi(at)\right) = 0.$$

Since the identity above holds for any time t, we should require

$$p'(s) = \phi'(s), \;\; q(s) = \psi(s).$$

Integrating the first identity with respect to s, we have

$$p(s) = \phi(s) + C,$$

where C is a constant. Given the continuity condition (1.31), we have $C = 0$. Therefore, to ensure that the (extended) string is smooth at $x = 0$, one should choose

$$p(s) = \phi(s), \;\; q(s) = \psi(s). \tag{1.36}$$

Thus, to meet the boundary condition $u_x|_{x=0} = 0$, one simply needs to extend the initial conditions as even functions. This is not surprising because $u_x|_{x=0} = 0$ is effectively a property of even functions.

Inserting Eq. (1.36) into (1.35) finally expresses the solution for problem (1.30) by

$$u(x,t) = \begin{cases} \dfrac{\phi(x-at)+\phi(x+at)}{2} + \dfrac{1}{2a}\displaystyle\int_{x-at}^{x+at} \psi(\alpha)\mathrm{d}\alpha, & x > at; \\ \dfrac{\phi(at-x)+\phi(x+at)}{2} + \dfrac{1}{2a}\left(\displaystyle\int_{0}^{x+at} \psi(\alpha)\mathrm{d}\alpha + \int_{0}^{at-x} \psi(\alpha)\mathrm{d}\alpha\right), & 0 < x < at. \end{cases} \tag{1.37}$$

Now we interpret the physical meaning suggested by Eq. (1.37). Note that the expression for $u(x,t)$ switches as moving across the line $x = at$ in the $x - t$ space, as shown in Fig. 1.7. Here the region of $x > at$ is denoted by zone I, and the region of $0 < x < at$ by zone II.

For simplicity, we let $\psi(\alpha) = 0$ in Eq. (1.37). Then we have

$$u(x,t) = \begin{cases} \dfrac{1}{2}\left(\phi(x-at)+\phi(x+at)\right), & x > at; \\ \dfrac{1}{2}\left(\phi(at-x)+\phi(x+at)\right), & 0 < x < at. \end{cases} \tag{1.38}$$

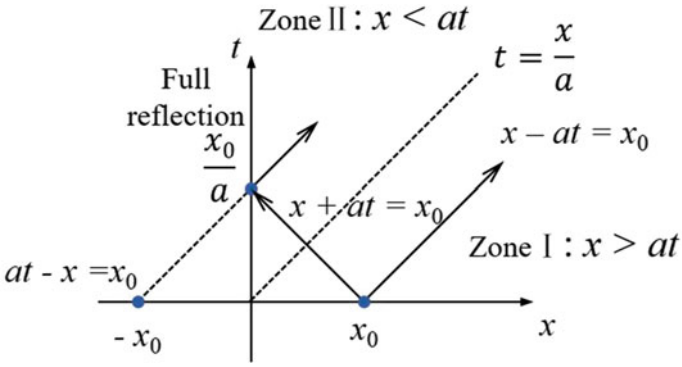


Fig. 1.7 Wave propagation behaviour shown by the solution given by (1.37) on the $x - t$ plane

Based on the discussion conducted in Sect. 1.2.2, the function of $u(x, t)$ given by Eq. (1.38) for both cases can be considered as a superposition of a rightward wave (of speed a) and a leftward wave (also of speed a). The corresponding characteristics can then be drawn as two families of mutually parallel straight lines in both zones, as shown in Fig. 1.7.

In domain I where $x > at$, the expression for u by Eq. (1.38) is exactly the same as D'Alembert's formula (1.27) with $\psi = 0$. Hence, the information initially at $x = x_0$ propagates to both sides at a same speed a. As suggested by Fig. 1.7, the rightward wave corresponds to the characteristics of $x - at = x_0$, which is parallel to the region boundary given by $x = at$. Thus, rightward waves never enter zone II. In contrast, the leftward characteristics, say, starting from $x = x_0$, cross the zone boundary at $t = \frac{x_0}{2a}$.

As for the leftward characteristics in zone II, they always find their origins from zone I, since the initial line $t = 0$ fully falls in zone I. As indicated by Fig. 1.7, a leftward characteristics observed in zone II is just the continuation of the corresponding characteristics in domain I across the zone boundary.

As for the rightward characteristics in zone II, they can be envisaged as waves virtually initialised on $x < 0$, as marked by the dash line in Fig. 1.7. But the actual starting points of the rightward characteristics lie on the left end of the string at $x = 0$. For instance, as shown in Fig. 1.7, the rightward wave virtually initialised at $x = -x_0$ corresponds to the characteristics of $at - x = x_0$. The function value on the characteristics, if inserting $x = 0$ and $t = \frac{x_0}{a}$ into the second formula of Eq. (1.38), stays the same as $\frac{1}{2}\phi(x_0)$. But at $x = 0$ and $t = \frac{x_0}{a}$, this rightward characteristic intersects with the leftward characteristics originating at $x = x_0$. The function value on this leftward characteristics is also founded to be $\frac{1}{2}\phi(x_0)$.

In a physical viewpoint, therefore, a leftward characteristic carrying a function value of $\frac{1}{2}\phi(x_0)$ is emitted from $x = x_0$ at $t = 0$. When it hits the free end at $t = \frac{x_0}{a}$, the leftward wave gets reflected by the boundary at $x = 0$ (through $u_x|_{x=0} = 0$), and then becomes a rightward wave. Since the function value stays the same after reflection, the free end governed by homogeneous Neumann boundary condition actually serves as a fully deflecting boundary to wave propagation.

1.2.4 Duhamel's Principle

The Cauchy problem (1.17) governed by the homogeneous equation for string vibration can be solved by D'Alembert's formula (1.27). Now we consider solving problem (1.18), which is governed by an inhomogeneous PDE, i.e.

$$\text{(II)} \quad \begin{cases} w_{tt} - a^2 w_{xx} = f(x,t), \ \ (x,t) \in \mathbb{R} \times \mathbb{R}^+; \\ w|_{t=0} = 0, \quad w_t|_{t=0} = 0. \end{cases} \tag{1.39}$$

The strategy is to make the governing PDE of problem (1.39) be homogeneous, and D'Alembert's formula can then be employed. For this purpose, we introduce Duhamel's principle.

Duhamel's principle: Suppose that $W(x,t;\tau)$ is a function of x and t, and of parameter τ. If it satisfies

$$\begin{cases} W_{tt} - a^2 W_{xx} = 0, \ x \in \mathbb{R}, \ t > \tau; \\ W|_{t=\tau} = 0, \ \ W_t|_{t=\tau} = f(x,\tau), \end{cases} \tag{1.40}$$

then

$$w(x,t) = \int_0^t W(x,t;\tau)\,\mathrm{d}\tau \tag{1.41}$$

solves problem (1.39).

For its verification, one simply inserts Eq. (1.41) into (1.39), and the proof is left for homeworks (see Exercise 1.10).

In fact, Duhamel's principle has physical implications. To this end, we divide the time axis into (infinitely) many short intervals $[0, t_1]$, $[t_1, t_2]$, $\cdots$. Then correspondingly, we introduce a family of functions $f_j(x,t)$, $j = 1, 2, \ldots$, such that

$$f_j(x,t) = \begin{cases} f(x,t), & t \in [t_{j-1}, t_j]; \\ 0, & \text{otherwise}. \end{cases}$$

It can be checked that the external force f appearing in the governing equation of problem (1.39) equals the superposition of f_j over all j. Note that for the jth section of the external force f, it is at $t = t_{j-1}$ that f_j begins to affect the string vibration. Since the problem is linear, the whole process can be formulated by supposing the vibrating processes caused solely by f_j, for $j = 1, 2, \ldots$. During the infinitesimal time interval $[t_{j-1}, t_j]$, f_j serves to accelerate the string system to an initial speed at $t = t_j$. Then f_j vanishes, and free vibration takes place afterwards. Hence, the role of f_j can be summarised as follows. It kicks off the vibration of a free string at t_j by providing an initial speed to it. The overall vibrating behaviour is then formulated by superposition over all j. The physical implication may help one better understand Duhamel's principle in the following two aspects. First, the external force

f_j arises in the initial condition of problem (1.40). Second, summation over these infinitesimally short intervals leads to an integral, which just appears in Eq. (1.41). In fact, the differential $W(x, t; \tau)\mathrm{d}\tau$ formulates the vibrating behaviour caused solely by $f(x, \tau)\mathrm{d}\tau$.

From Duhamel's principle, we end up with a PDE problem (1.39) for $W(x, t; \tau)$, where the governing equation becomes homogeneous. On introducing a shifted temporal variable $\tilde{t} = t - \tau$, problem (1.39) can be transformed into a standard Cauchy problem in $(x, \tilde{t})$, i.e.

$$\begin{cases} W_{\tilde{t}\tilde{t}} - a^2 W_{xx} = 0, \ (x, \tilde{t}) \in \mathbb{R} \times \mathbb{R}^+; \\ W|_{\tilde{t}=0} = 0, \ W_t|_{\tilde{t}=0} = f(x, \tau). \end{cases} \tag{1.42}$$

With reference to D'Alembert's formula (1.27), we have

$$W(x, t; \tau) = \frac{1}{2a} \int_{x-a\tilde{t}}^{x+a\tilde{t}} f(\alpha, \tau)\mathrm{d}\alpha = \frac{1}{2a} \int_{x-a(t-\tau)}^{x+a(t-\tau)} f(\alpha, \tau)\mathrm{d}\alpha, \tag{1.43}$$

where the temporal variable is transformed back to t. Incorporating Eq. (1.43) into (1.41), we derive an expression for the solution for problem (1.39), given by

$$w(x, t) = \frac{1}{2a} \int_0^t \int_{x-a(t-\tau)}^{x+a(t-\tau)} f(\alpha, \tau)\mathrm{d}\alpha\mathrm{d}\tau. \tag{1.44}$$

Eq. (1.44) is defined by a double integral containing two parameters.

Prerequisite knowledge

Differentiation of an integral containing parameters

When searching for PDE solutions, we are often encountered with functions defined through integrals containing parameters. For instance,

$$F(x) = \int_{a(x)}^{b(x)} f(x, t)\,\mathrm{d}t.$$

Suppose that the integrand $f(x, t)$ and its partial derivatives exhibit certain degree of smoothness. Thus, the derivative of $F(x)$ can be calculated by

$$\frac{\mathrm{d}F}{\mathrm{d}x} = b'(x)f(x, b(x)) - a'(x)f(x, a(x)) + \int_{a(x)}^{b(x)} \frac{\partial f}{\partial x}\,\mathrm{d}t, \tag{1.45}$$

where $a'(\cdot)$ and $b'(\cdot)$ denote the derivatives of functions $a(\cdot)$ and $b(\cdot)$, respectively.

1.3 Method of Separation of Variables

In this section, we consider solving initial–boundary value problems governed by the wave equation. And an extremely useful approach for solving PDE problems, known as the *method of separation of variables*, is introduced.

Given a string ending at $x = 0$ and $x = l$, we consider an initial–boundary value problem which is formulated by

$$\begin{cases} u_{tt} - a^2 u_{xx} = f(x,t), \ (x,t) \in (0,l) \times \mathbb{R}^+; \\ u|_{t=0} = \phi(x), \quad u_t|_{t=0} = \psi(x); \\ u|_{x=0} = \mu_1(t), \quad u|_{x=l} = \mu_2(t). \end{cases} \tag{1.46}$$

Note that Dirichlet boundary conditions are imposed at both ends, indicating that the displacements at the two ends are pre-given by $\mu_1(t)$ and $\mu_2(t)$, both of which are unary functions of time t.

1.3.1 Making Boundary Conditions Homogeneous

Note that the governing equation and the initial–boundary conditions constituting problem (1.46) are all inhomogeneous. As already demonstrated in the case for the Cauchy problem investigated in Sect. 1.2, making certain parts of a linear PDE problem be homogeneous may effectively enhance its solvability.

To this end, boundary conditions are made homogenous with the procedure detailed as follows. A new function $h(x,t)$ is firstly introduced through interpolating the two boundary conditions of problem (1.46), i.e.

$$h(x,t) = \frac{l-x}{l}\mu_1(t) + \frac{x}{l}\mu_2(t).$$

It can be readily checked that $h(0,t) = \mu_1(t)$ and $h(l,t) = \mu_2(t)$.

Now consider a new unknown function $v(x,t)$ defined by $v(x,t) = u(x,t) - h(x,t)$. Inserting this expression for $v(x,t)$ into problem (1.46) leads to

$$\begin{cases} v_{tt} - a^2 v_{xx} = f - \dfrac{l-x}{l}\mu_1''(t) - \dfrac{x}{l}\mu_2''(t), \ (x,t) \in (0,l) \times \mathbb{R}^+; \\ v|_{t=0} = \phi(x) - \dfrac{l-x}{l}\mu_1(0) - \dfrac{x}{l}\mu_2(0), v_t|_{t=0} = \psi(x) - \dfrac{l-x}{l}\mu_1'(0) - \dfrac{x}{l}\mu_2'(0); \\ v|_{x=0} = 0, \quad v|_{x=l} = 0. \end{cases} \tag{1.47}$$

To this stage, the boundary conditions of the PDE problem (1.47) for $v(x,t)$ become homogeneous. As for the solution for the original problem (1.46), it can be calculated by $u(x,t) = v(x,t) + h(x,t)$, soon after the expression for $v(x,t)$ is obtained.

It is worth nothing that the aforementioned treatments also work with other types of boundary conditions introduced in Sect. 1.1.2. But the interpolating function $h(x, t)$ should be constructed in accordance (see Exercise 1.12).

Therefore, we can always start with problem (1.46) for the case where $\mu_1(t) = \mu_2(t) = 0$. Similar as the case for the Cauchy problem investigated in Sect. 1.2, the initial–boundary value problem imposed with homogeneous boundary conditions [$\mu_1(t) = \mu_2(t) = 0$ in problem (1.46)] can be decomposed as the superposition of two slightly simplified problems given by

$$\text{(I)} \quad \begin{cases} v_{tt} - a^2 v_{xx} = 0, \ (x, t) \in (0, l) \times \mathbb{R}^+; \\ v|_{t=0} = \phi(x), \quad v_t|_{t=0} = \psi(x); \\ v|_{x=0} = 0, \quad v|_{x=l} = 0, \end{cases} \tag{1.48}$$

and

$$\text{(II)} \quad \begin{cases} w_{tt} - a^2 w_{xx} = f, \ (x, t) \in (0, l) \times \mathbb{R}^+; \\ w|_{t=0} = 0, \quad w_t|_{t=0} = 0; \\ w|_{x=0} = 0, \quad w|_{x=l} = 0. \end{cases} \tag{1.49}$$

The solution for problem (1.46) is then calculated by $u = v + w$.

1.3.2 Method of Separation of Variables—Its Procedure

Now we consider solving problem (1.48) using the method of separation of variables. It always starts with seeking solutions taking a "variable-separated" form. For problem (1.48), we look for solutions taking the form of

$$v(x, t) = X(x)T(t), \tag{1.50}$$

where $X(x)$ and $T(t)$ are two unary functions of x and t, respectively. Here $X(x)$ is termed as the "spatial function" and $T(t)$ as the "temporal function".

Inserting Eq. (1.50) into the governing PDE of problem (1.48) gives

$$T''X = a^2 TX'',$$

where T'' denotes the second derivative of T with respect to its input argument and so does X''.

Dividing the above identity by $a^2 X(x)T(t)$, we find that the left side becomes T''/a^2T, a function solely of t, and the right side becomes X''/X, a function solely of x. This means, if they are equal to each other, they must both be equal to a constant, say, $-\lambda$. Thus, we obtain

$$\frac{T''}{a^2 T} = \frac{X''}{X} = -\lambda. \tag{1.51}$$

For Eq. (1.51) to hold, $T(t)$ and $X(x)$ should satisfy

$$T'' + a^2\lambda T = 0; \tag{1.52a}$$

$$X'' + \lambda X = 0, \tag{1.52b}$$

respectively. Therefore, we derive two ordinary differential equations for $T(t)$ and $X(x)$, respectively. And for their definite problems, initial or boundary conditions are needed.

Here the case with the spatial function $X(x)$ is considered first. Inserting the expression of Eq. (1.50) into the (homogeneous) boundary conditions of problem (1.48) implies that $X(0) = X(l) = 0$. A definite problem for the spatial function $X(x)$ is thus set up by

$$\begin{cases} X'' + \lambda X = 0, \ x \in (0, l); \\ X(0) = X(l) = 0. \end{cases} \tag{1.53}$$

Note that $X(x) \equiv 0$ is naturally a solution for problem (1.53). But its *non-trivial solutions*, which are not uniformly zero, are of our interest.

Note that the governing equation of problem (1.53) is a second-order, linear and homogeneous ODE whose coefficients take constant values. The general solution to such ODEs, or alternatively its fundamental solution system is summarised in the prerequisite knowledge for this section. For the present case, the form of its general solution should depend on the sign of λ.

Case 1 with $\lambda < 0$. The general solution to the ODE of problem (1.53) is given by

$$X(x) = C_1 e^{\sqrt{-\lambda}x} + C_2 e^{-\sqrt{-\lambda}x}, \tag{1.54}$$

where C_1 and C_2 are constants to be determined.

Incorporating Eq. (1.54) with the boundary conditions of problem (1.53) renders an algebraic equation for C_1 and C_2, that is,

$$\begin{pmatrix} 1 & 1 \\ e^{\sqrt{-\lambda}l} & e^{-\sqrt{-\lambda}l} \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Note that the matrix appearing above is invertible for any $\lambda < 0$. Thus, $C_1 = C_2 = 0$ is the only solution to this algebraic equation system. Therefore, for $\lambda < 0$, problem (1.53) only yields a trivial solution.

Case 2 with $\lambda = 0$. Then the general solution for problem (1.53) reads

$$X(x) = C_1 x + C_2. \tag{1.55}$$

Incorporating it with the boundary conditions gives

$$\begin{pmatrix} 0 & 1 \\ l & 1 \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Since $l > 0$, problem (1.53) with $\lambda = 0$ only yields a trivial solution too.

Case 3 with $\lambda > 0$. The general solution now reads

$$X(x) = C_1 \cos(\sqrt{\lambda}x) + C_2 \sin(\sqrt{\lambda}x). \tag{1.56}$$

Incorporating it with the boundary conditions gives

$$\begin{pmatrix} 1 & 0 \\ \cos(\sqrt{\lambda}l) & \sin(\sqrt{\lambda}l) \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

which implies $C_1 = 0$, and $C_2 \sin(\sqrt{\lambda}l) = 0$. If $\sin(\sqrt{\lambda}l) = 0$, then C_2 can be nonzero, and non-trivial solutions exist. This suggests that the evaluation of λ is not arbitrary, but $\lambda = \left(\frac{k\pi}{l}\right)^2$, $k = 1, 2, \ldots$.

This introduces a set of $\{\lambda_k\}_{k=1}^{\infty}$, such that

$$\lambda_k = \left(\frac{k\pi}{l}\right)^2, \; k = 1, 2, \ldots. \tag{1.57}$$

For any λ_k, an ODE problem is identified to be

$$\begin{cases} X_k'' + \lambda_k X_k = 0, \; x \in (0, l); \\ X_k(0) = X_k(l) = 0, \end{cases} \tag{1.58}$$

which yields a non-trivial solution of

$$X_k(x) = \sin \frac{k\pi x}{l}. \tag{1.59}$$

Note that $X_k(x)$ of Eq. (1.59) multiplied by a scalar is still a solution for problem (1.58).

The set of $\{\lambda_k\}_{k=1}^{\infty}$ defined by Eq. (1.57) are called the *eigenvalues* of problem (1.53), and $X_k(x)$ defined by Eq. (1.59) is called the *eigenfunction* corresponding to λ_k. It is noted that the distribution of eigenvalues $\{\lambda_k\}_{k=1}^{\infty}$ is not continuous but discrete.

Here the definition of eigenvalue echoes with the same term introduced in the course of linear algebra ($A\mathbf{x} = \lambda x$). They both arise when solving for non-trivial solutions for a linear problem. Further generalisation over the concept of eigenvalues will be discussed in Sect. 2.3.

From Eq. (1.51), the spatial function $X(x)$ is linked with its corresponding temporal function $T(t)$ through λ. Now we restrict our attentions to the case where $\lambda = \lambda_k$,

and the ODE for the resulting temporal function $T_k(t)$ then becomes

$$T_k'' + a^2\lambda_k T_k = 0, \tag{1.60}$$

whose general solution reads

$$T_k = A_k \cos\frac{ak\pi t}{l} + B_k \sin\frac{ak\pi t}{l}, \tag{1.61}$$

where A_k and B_k are coefficients to be determined.

Incorporating Eqs. (1.59) and (1.61) with (1.50), we obtain a family of solutions to the equation for string vibration, which is expressed by

$$v_k(x,t) = X_k(x)T_k(t), \quad k = 1, 2, \ldots. \tag{1.62}$$

Note that $v_k(x,t)$ satisfies both the governing equation and the homogeneous boundary conditions. Naturally, we can presume that the solution for problem (1.48) can be expressed as the linear combination about all v_k, i.e.

$$v(x,t) = \sum_{k=1}^{\infty} v_k(x,t) = \sum_{k=1}^{\infty}\left(A_k \cos\frac{ak\pi t}{l} + B_k \sin\frac{ak\pi t}{l}\right)\cdot \sin\frac{k\pi x}{l}. \tag{1.63}$$

For determining the unspecified coefficients A_k and B_k, we refer to the initial conditions of problem (1.48).

Note that Eq. (1.63) effectively expresses the solution for problem (1.48) by means of a functional series. Thus, its validity roots in the fact that the series should be uniformly convergent. At this stage, we simply assume that this is the case, and the issue about its uniform convergence will be revisited later.

Letting $t = 0$ in Eq. (1.63) and inserting it into the first initial condition of problem (1.48), we obtain

$$\phi(x) = u|_{t=0} = \sum_{k=1}^{\infty} A_k \sin\frac{k\pi x}{l}. \tag{1.64a}$$

Differentiating Eq. (1.63) with respect to t, and inserting it to the second initial condition, we obtain

$$\psi(x) = u_t|_{t=0} = \sum_{k=1}^{\infty} X_k(x)T_k'(0) = \sum_{k=1}^{\infty} B_k \frac{ak\pi}{l} \sin\frac{k\pi x}{l}. \tag{1.64b}$$

Both Eqs. (1.64a) and (1.64b) are expressed by means of series consisting of odd sine functions, which is a special case of Fourier series. Concise discussion on sine series can be found in the prerequisite part concluding this section, and more thorough discussion over the issue should be found in general calculus textbooks.

Table 1.2 Comparison of some concepts of vectors in Euclidean spaces and their counterparts in functional spaces

	Vector in $\mathbb{R}^n$	Function
Inner product	$(\mathbf{u}, \mathbf{v}) = \sum_{k=1}^{n} u_k v_k$	$< f(x), g(x) >= \int_0^l f(x)g(x)\mathrm{d}x$
Orthogonal basis	$(\mathbf{e}^j, \mathbf{e}^k) = 0, j \neq k$	$\int_0^l \sin\frac{j\pi x}{l} \sin\frac{k\pi x}{l}\mathrm{d}x = 0, j \neq k$
Decomposition	$\mathbf{v} = \sum_{k=1}^{n} \alpha_k \mathbf{e}^k$	$\phi(x) = \sum_{k=1}^{\infty} A_k \sin\frac{k\pi x}{l}$
Coefficient	$\alpha_k = \frac{(\mathbf{v}, \mathbf{e}^k)}{(\mathbf{e}^k, \mathbf{e}^k)}$	$A_k = \frac{2}{l}\int_0^l \phi(x) \sin\frac{k\pi x}{l}\mathrm{d}x$

Applying the results of sine series given by Eq. (1.74) to Eqs. (1.64a) and (1.64b), we obtain

$$A_k = \frac{2}{l}\int_0^l \phi(x) \sin\frac{k\pi x}{l}\,\mathrm{d}x, \quad B_k = \frac{2}{ak\pi}\int_0^l \psi(x) \sin\frac{k\pi x}{l}\,\mathrm{d}x. \tag{1.65}$$

Therefore, the solution for problem (1.48) is finally expressed by

$$v(x,t) = \sum_{k=1}^{\infty}\left(A_k \cos\frac{ak\pi t}{l} + B_k \sin\frac{ak\pi t}{l}\right)\cdot \sin\frac{k\pi x}{l}, \tag{1.66}$$

with A_k and B_k determined by Eq. (1.65).

Now the conditions ensuring that Eq. (1.66) is effectively the solution for problem (1.48) are discussed. First, to guarantee solution smoothness, $\phi(x)$ and $\psi(x)$ appearing in the initial conditions should be sufficiently smooth. Second, the initial and the boundary conditions should be mutually consistent. For problem (1.48), the initial displacement and speed at the two fixed ends should vanish, i.e.$\phi(0) = \phi(l) = \psi(0) = \psi(l) = 0$. Third, being a solution for problem (1.48), as discussed above, the series by Eq. (1.66) must be uniformly convergent for all $x \in (0, l)$ and $t > 0$. In fact, with A_k and B_k given by Eqs. (1.65), the uniform convergence about the series defined by Eq. (1.66) can be demonstrated, with its proof omitted here.

Note that A_k and B_k of Eq. (1.66) are determined through Fourier series, which actually does not work for many other cases where the method of separation of variables is applicable. For wider applications of the method, we consider determining A_k and B_k of Eq. (1.66) from a different angle of "function orthogonality". The concept of "orthogonality" has been covered in the course of linear algebra, where the objectives are vectors in Euclidean space $\mathbb{R}^n$. Terminology in association with vector orthogonality in $\mathbb{R}^n$ is summarised in Table. 1.2.

Given two vectors $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$, one may first introduce the concept of inner product, defined by $(\mathbf{u}, \mathbf{v}) = \sum_{k=1}^{n} u_k v_k$, where u_k is the kth entry of $\mathbf{u}$ and so on for v_k. When $(\mathbf{u}, \mathbf{v}) = 0$, they are called mutually orthogonal. Besides, one can always find n

mutually orthogonal vectors, say, $\mathbf{e}^1, \cdots, \mathbf{e}^n$, which form a set of orthogonal basis in $\mathbb{R}^n$. Mathematically, it is described by $(\mathbf{e}^j, \mathbf{e}^k) = 0$, given $j \neq k$. Then any vector $\mathbf{v} \in \mathbb{R}^n$ can be expressed as the linear combination of the orthogonal basis, i.e.

$$\mathbf{v} = \sum_{k=1}^{n} \alpha_k \mathbf{e}^k, \tag{1.67}$$

and the kth coefficient α_k is simply expressed as the quotient of two inner products

$$\alpha_k = \frac{(\mathbf{v}, \mathbf{e}^k)}{(\mathbf{e}^k, \mathbf{e}^k)}.$$

The idea on orthogonality in $\mathbb{R}^n$ can actually be generalised to "spaces" consisting of functions. Take the case of Eq. (1.64a) as an example. The function $\phi(x)$ can be treated as the linear combination of infinitely many sinusoidal functions, which actually form a set of "basis functions". The corresponding inner product between functions, as shown in Table 1.2, can be defined as their product integrated over the domain of definition $[0, l]$. It can be verified that

$$\int_0^l \sin\frac{k\pi x}{l} \sin\frac{j\pi x}{l}\,\mathrm{d}x = \begin{cases} l/2, & \text{if } j = k; \\ 0, & \text{if } j \neq k. \end{cases} \tag{1.68}$$

Any two of the "basis functions" from the set formed by $\left\{y_k(x) = \sin\frac{k\pi x}{l}\right\}_{k=1}^{\infty}$ return a zero inner product, and they are thus mutually "orthogonal".

Now if we multiply Eq. (1.64a) by $\sin\frac{j\pi x}{l}$ and then integrate the result from 0 to l, we have

$$\int_0^l \phi(x) \sin\frac{j\pi x}{l}\,\mathrm{d}x = \sum_{k=1}^{\infty} A_k \int_0^l \sin\frac{k\pi x}{l} \sin\frac{j\pi x}{l}\,\mathrm{d}x, \tag{1.69}$$

where the operations of integration and summation are interchanged, because the involved series has been justified to be uniformly convergent. As from Eq. (1.68), all the integrals appearing on the right side of Eq. (1.69) vanish except when $j = k$. Thus, Eq. (1.69) is reduced to

$$\int_0^l \phi(x) \sin\frac{j\pi x}{l}\mathrm{d}x = A_j \int_0^l \left(\sin\frac{j\pi x}{l}\right)^2 \mathrm{d}x = \frac{A_j l}{2}.$$

After changing the indexation from j to k, we reach the expression for A_k as given by Eq. (1.65).

The concept of function orthogonality is key to the utilisation of the method of separation of variables, and this topic will be examined in a more systematic manner in Sect. 2.3.

1.3.3 Physical Implications

To reveal the physical implications of the series solution given by Eq. (1.63), we rearrange the right side of $v_k(x, t)$ given by Eq. (1.62) and obtain

$$v_k(x, t) = N_k \cos(\omega_k t + \theta_k) \sin \frac{k\pi x}{l}, \tag{1.70}$$

where $N_k = \sqrt{A_k^2 + B_k^2}$, $\omega_k = a\sqrt{\lambda_k} = \frac{ak\pi}{l}$, $\cos\theta_k = \frac{A_k}{\sqrt{A_k^2+B_k^2}}$, $\sin\theta_k = \frac{-B_k}{\sqrt{A_k^2+B_k^2}}$.

The vibrating behaviour formulated by v_k shows a profile of a *standing wave* or a *stationary wave*, as shown in Fig. 1.8.

At each moment (with t fixed), the string takes a sinusoidal shape. As time evolves, the profile stays in a sinusoidal shape with its amplitude oscillating dictated by $\cos(\omega_k t + \theta_k)$. Moreover, there exist certain points on the string, which are kept still during vibration, as marked in Fig. 1.8. They are known as the *nodes* or the *standing points*, which are implied by the zeros of the eigenfunction $y_k(x) = \sin \frac{k\pi x}{l}$.

Another key observation here is that both the eigenfunction $X_k(x)$ by Eq. (1.59) and the corresponding wave frequency ω_k only depend on the intrinsic properties of the string, such as its length, its mass density and its line tension (via $a^2 = T/\rho$), as

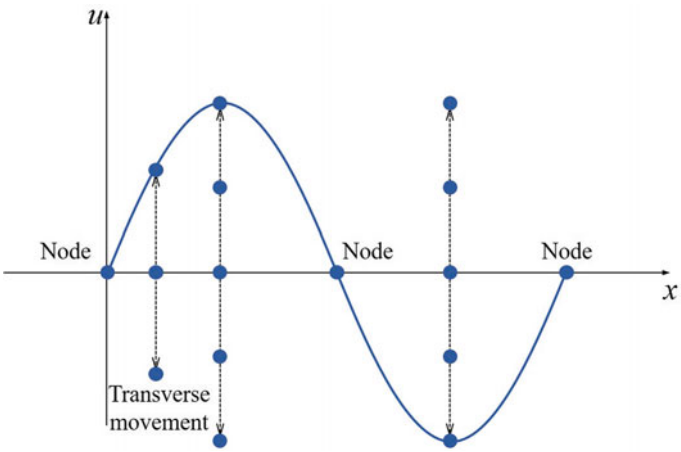


Fig. 1.8 Trajectories of selected points on the string based on the expression for v_k defined through Eq. (1.70). Here $k = 2$ as an example

well as the types of boundary conditions applied. They are independent of the initial conditions. Such observation offers insights into the initial–boundary value problem studied here. Any vibrating behaviour of a given string (with its two ends fixed), as suggested by Eq. (1.63), is merely a superposition of waves that are intrinsic to the string itself (and how their end points are treated). A change in initial conditions simply alters the values of the coefficients of A_k and B_k.

The aforementioned features should also be found in other cases, as long as the solution for a linear PDE problem can be expressed as a series formed by functions taking the variable-separated form (1.50). The nodes naturally come from the zeros of the spatial $X(x)$. When setting up the problem for $X(x)$ [as in Eq. (1.53)], it only relies on the spatial domain of definition $(0, l)$ and the homogeneous boundary conditions and thus do the eigenvalues [as in Eq. (1.57)] and the resulting non-trivial solutions or the eigenfunctions [as in Eq. (1.59)].

Therefore, the method of separation of variables actually reveals certain fundamental physical features of a system, and its applicability is thus quite wide. In the subject of quantum mechanics, for instance, it is employed to analyse the differential equation governing the behaviour of electrons, known as the Schrödinger equation. In that scenario, one is expected to end up with a set of eigenfunctions [as in the case of Eq. (1.59)], which, as discussed above, should correspond to a discretised number of electron states intrinsic to the nucleus configuration and the boundary conditions. This implies that an electron can only stay in one of those "quantised" states. And the actual system behaviour we see is just a superposition of these quantised states. More mathematical theorems underpinning the method of separation of variables will be discussed in Sect. 2.3.

1.3.4 Inhomogeneous Governing Equations

Finally, we consider problem (1.49), where the governing PDE is inhomogeneous. Naturally, we refer to the concept of Duhamel's principle that was introduced for transforming the Cauchy problem in Sect. 1.2. But in this case, the boundary conditions should also be taken into account.

Duhamel's principle. For a function $W(x, t; \tau)$ with τ being its parameter, if it solves

$$\begin{cases} W_{tt} - a^2 W_{xx} = 0, \ x \in (0, l), \ t > \tau; \\ W|_{t=\tau} = 0, \ W_t|_{t=\tau} = f(x, \tau); \\ W|_{x=0} = 0, \ W|_{x=l} = 0, \end{cases} \tag{1.71}$$

then

$$w(x, t) = \int_0^t W(x, t; \tau) \mathrm{d}\tau \tag{1.72}$$

solves problem (1.49).

Applying the method of separation of variables to solve problem (1.71), we obtain

$$W(x,t;\tau)=\sum_{k=1}^{\infty}B_k\sin\frac{ak\pi(t-\tau)}{l}\sin\frac{k\pi x}{l},$$

where the coefficient B_k is calculated by

$$B_k=\frac{2}{ak\pi}\int_0^l f(s,\tau)\sin\frac{k\pi s}{l}\,\mathrm{d}s.$$

Inserting it into Eq. (1.72), we derive the solution for problem (1.49) as

$$w(x,t)=\sum_{k=1}^{\infty}\frac{2}{ak\pi}\cdot\sin\frac{k\pi x}{l}\cdot\int_0^t\int_0^l f(s,\tau)\sin\frac{k\pi s}{l}\sin\frac{ak\pi(t-\tau)}{l}\,\mathrm{d}s\mathrm{d}\tau.$$

Prerequisite knowledge

About Fourier series

For a function $f(x)$ that is integrable over its domain of definition $x\in(-l,l)$, its Fourier series is expressed by

$$f(x)\sim\frac{a_0}{2}+\sum_{k=1}^{\infty}\left(a_k\cos\frac{k\pi x}{l}+b_k\sin\frac{k\pi x}{l}\right),\tag{1.73}$$

where a_k and b_k are the coefficients, satisfying

$$a_k=\frac{1}{l}\int_{-l}^{l}f(x)\cos\frac{k\pi x}{l}\,\mathrm{d}x,\ \ k=0,1,\ldots;$$

and

$$b_k=\frac{1}{l}\int_{-l}^{l}f(x)\sin\frac{k\pi x}{l}\,\mathrm{d}x,\ \ k=1,2,\ldots,$$

respectively.

If $f(x)$ is an odd function, the coefficient $a_k = 0$ vanishes, while the coefficient b_k is simplified by

$$\begin{aligned} b_k &= \frac{1}{l}\int_{-l}^{0} f(x)\sin\frac{k\pi x}{l}\,\mathrm{d}x + \frac{1}{l}\int_{0}^{l} f(x)\sin\frac{k\pi x}{l}\,\mathrm{d}x \\ &= -\frac{1}{l}\int_{0}^{l} f(-s)\sin\frac{k\pi s}{l}\,\mathrm{d}s + \frac{1}{l}\int_{0}^{l} f(x)\sin\frac{k\pi x}{l}\,\mathrm{d}x \\ &= \frac{2}{l}\int_{0}^{l} f(x)\sin\frac{k\pi x}{l}\,\mathrm{d}x. \end{aligned}$$

The Fourier series then becomes a sine series expressed by

$$f(x) \sim \sum_{k=1}^{\infty} b_k \sin\frac{k\pi x}{l}, \tag{1.74}$$

which is now defined within the half period $(0, l)$.

Similarly, if $f(x)$ is an even function, we end up with a cosine series, i.e.

$$f(x) \sim \frac{a_0}{2} + \sum_{k=1}^{\infty} a_k \cos\frac{k\pi x}{l}, \tag{1.75}$$

where

$$a_k = \frac{2}{l}\int_{0}^{l} f(x)\cos\frac{k\pi x}{l}\,\mathrm{d}x,\ \ k = 0, 1, \ldots.$$

About second-order linear ordinary differential equation with constant coefficients

A second-order linear and homogeneous ODE with constant coefficients can be generally expressed by

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + 2a\frac{\mathrm{d}y}{\mathrm{d}x} + by = 0, \tag{1.76}$$

where x is the independent variable; y is the dependent variable; $a, b \in \mathbb{R}$ are constant coefficients.

For a second-order linear and homogeneous ODE, one should always find two mutually independent solutions, say $y_1 = f(x)$ and $y_2 = g(x)$, to it. The fundamental solution system for the ODE is thus formulated, i.e. any solution to this ODE should be expressed as their linear combination: $y = \alpha y_1 + \beta y_2$, where α and β are to be determined from the initial–boundary conditions.

When the coefficients take constant values as in Eq. (1.76), its solution is fully related to the roots of its associated algebraic equation

$$x^2 + 2ax + b = 0. \tag{1.77}$$

When $a^2 - b > 0$, Eq. (1.77) yields two real roots. Then the general solution to Eq. (1.76) is given by

$$y = \alpha \mathrm{e}^{(-a+\sqrt{a^2-b})x} + \beta \mathrm{e}^{(-a-\sqrt{a^2-b})x}.$$

This corresponds to case 1 in the main text.

When $a^2 - b = 0$, Eq. (1.77) yields two repeated real roots. Then the general solution to Eq. (1.76) is given by

$$y = (\alpha + \beta x)\mathrm{e}^{-ax}.$$

This corresponds to case 2 in the main text.

When $a^2 - b < 0$, Eq. (1.77) yields no real roots, but two mutually conjugate complex roots. Then the general solution to Eq. (1.76) is given by

$$y = \mathrm{e}^{-ax}\left(\alpha \cos\left(\sqrt{b - a^2}x\right) + \beta \sin\left(\sqrt{b - a^2}x\right)\right).$$

This corresponds to case 3 in the main text.

1.4 Wave Equation in Higher Dimensions

In this section, our discussion is extended for multidimensional cases. First a PDE problem describing small and transverse vibration of a membrane is derived. It is followed by a brief interpretation over the physical implications revealed by the solutions for the obtained PDE problems.

1.4.1 Small and Transverse Vibration of a Membrane

Now we formulate the behaviour of a membrane as suggested by Fig. 1.9. Suppose in its flattened state, the membrane coincides with the x–y plane. The membrane undergoes small and transverse vibration, and we seek for a partial differential equation to describe this phenomenon. Similar as in the (spatially) one-dimensional case, we begin with three physically reasonable presumptions.

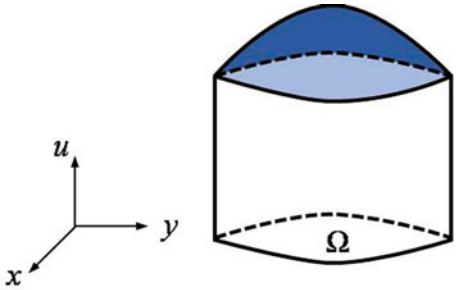


Fig. 1.9 Illustration of a vibrating membrane

1. **The membrane's thickness is far shorter than its overall size**. Each point on the membrane is displaced only transversely, where the displacement field, denoted by $u(x, y; t)$ with t being the temporal variable, stays perpendicular to the x–y plane.
2. **The membrane experiences small vibration**. Mathematically, this is formulated by $|u_x|, |u_y| \ll 1$. Practically, we let high-order infinitesimally small quantities, such as $|u_x|^2$, $|u_x|\,|u_y|$ and $|u_y|^2$, vanish.
3. **The reacting force due to the elastic deformation of the membrane is purely tensional**. It should be noted that, to appropriately analyse the "internal force" of a membrane, the concept of *stress* is needed. This is because for a membrane piece taken from the whole, it feels the interacting force from the neighbouring parts surrounding it. Therefore, if one wishes to define the internal force applied on this membrane piece, one also needs to specify which of its adjacent membrane parts is referred to. This is done by introducing, at the point of interest, an infinitesimally small fictitious cut, whose unit normal vector is denoted by, say, $\boldsymbol{\nu}$. Then the force at this point due to the membrane piece across this cut can be defined. Apparently, the forces with respect to differently oriented cuts should not be fully independent. This issue is resolved by introducing a second-order tensor, or simply a three-by-three matrix $\boldsymbol{\sigma}$, known as the stress tensor, and the internal force across the fictitious cut of unit normal $\boldsymbol{\nu}$ is measured by $\boldsymbol{\sigma}\boldsymbol{\nu}\mathrm{d}s$, where $\mathrm{d}s$ is the length of this cut. One may refer to further conceptualisation of stress in general textbooks on solid mechanics (e.g. see [13]).
   But for the case of membrane, extra requirements are imposed. The internal forces (across any virtual cuts) should all be parallel to the local tangent plane. Hence, the internal force across a cut with unit normal $\boldsymbol{\nu}$ can be decomposed into two mutually orthogonal components: one is parallel with $\boldsymbol{\nu}$ which is termed as the *normal force*, and the other is perpendicular to $\boldsymbol{\nu}$ but parallel with the local tangent plane which is termed as the *shear force*. For a membrane that is in a tensional state, the shear force component should vanish, and the force across this fictitious cut (along $\boldsymbol{\nu}$) is expressed by $T\boldsymbol{\nu}$, where the quantity $T > 0$ is termed as the *surface tension* of the membrane. Moreover, we further assume that the surface tension T here is constant in time and space. In fact, this issue can be justified for the case of small vibration, similar as in Sect. 1.1, and the proof can be found elsewhere (e.g. [12]).

Table 1.3 Physical quantities introduced for modelling the behaviour of a membrane that undergoes small and transverse vibration

Symbol	Physical meaning	Dimension
t	Time	s
x, y	Space	m
$u(x, y; t)$	Transverse displacement	m
$F(x, y; t)$	External load	N/m^2
T	Surface tension	N/m
ρ	Mass density	kg/m^2

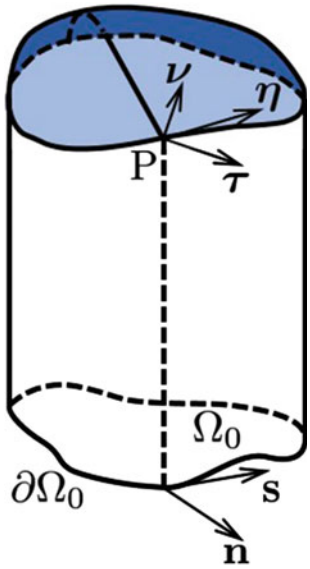


Fig. 1.10 Key vectors characterising a membrane piece arbitrarily taken from the whole

In Table 1.3 summarises the physical quantities employed for modelling membrane vibration.

Here we use Ω to denote the (two-dimensional) domain of the membrane projected onto x-y plane. Since the membrane only experiences transverse vibration, this projected region Ω should stay unchanged during vibration. Our target is to derive a partial differential equation for the transverse displacement field $u(x, y; t)$, where $(x, y) \in \Omega$.

Similar as in the case for modelling string vibration, an arbitrary piece is taken from the membrane. Suppose this membrane piece is projected onto the (two-dimensional) domain of Ω_0 in x–y plane, as shown in Fig. 1.10. For this membrane piece, the momentum along the transverse direction should be conserved within an arbitrary time interval $[t_1, t_2]$, i.e. the change in momentum equals the impulse due to all transverse force components applied on it.

For the change of momentum, it is formulated by

$$\iint_{\Omega_0} \rho \left[u_t|_{t=t_2} - u_t|_{t=t_1} \right] \mathrm{d}x\mathrm{d}y = \int_{t_1}^{t_2} \iint_{\Omega_0} \rho u_{tt} \, \mathrm{d}x\mathrm{d}y\mathrm{d}t, \tag{1.78}$$

where the identity is derived using the Newton–Lebnitz formula with respect to t.

The impulse applied on the membrane piece has two sources: (a) the external load F and (b) the tensional force from the rest parts of the membrane exerted through the boundary of Ω_0, which is termed as $\partial\Omega_0$. The impulse due to the external load is simply formulated by

$$\int_{t_1}^{t_2} \iint_{\Omega_0} F(x, y, t) \mathrm{d}x\mathrm{d}y\mathrm{d}t. \tag{1.79}$$

Now the key to modelling lies on how to calculate the impulse caused by the tensional force due to other parts of the membrane. This entails the introduction of a set of useful unit vectors, as shown in Fig. 1.10. For clarity, bold Greek letters are employed here to denote unit vectors in three-dimensional space $\mathbb{R}^3$. For a point P sitting on the boundary of the membrane piece, as shown by Fig. 1.10, $\boldsymbol{\nu}$ is employed to denote the (unit) vector that is perpendicular to $\partial\Omega_0$ at P. Without loss of generalities, we let the third entry of $\boldsymbol{\nu}$ be positive.

The second key unit vector denoted by $\boldsymbol{\eta}$ is the vector that is tangent to the boundary of the membrane piece at P.

The third key unit vector, denoted by $\boldsymbol{\tau}$, is the vector that is orthogonal both to $\boldsymbol{\nu}$ and $\boldsymbol{\eta}$ at P, and the tensional force due to the rest membrane pieces takes place along direction $\boldsymbol{\tau}$. In fact, the traction (per unit boundary length) is measured by $T\boldsymbol{\tau}$, with T recalled to be the surface tension of the membrane.

Mathematically, as suggested by Fig. 1.10, the aforementioned key unit vectors can be interrelated by

$$\boldsymbol{\tau} = \boldsymbol{\eta} \times \boldsymbol{\nu}, \tag{1.80}$$

where "$\times$" denotes the cross product of two vectors.

Then we express these key three-dimensional unit vectors through the displacement field u at P. The unit normal $\boldsymbol{\tau}$ is expressed first. Note that the membrane is effectively a surface in three-dimensional space measured in x, y and z. Then the membrane profile can be represented (implicitly) by an equation of $z - u(x, y) = 0$. The unit normal vector $\boldsymbol{\nu}$ is thus formulated by

$$\boldsymbol{\nu} = \frac{1}{\sqrt{1 + u_x^2 + u_y^2}} (-u_x, -u_y, 1) \approx (-u_x, -u_y, 1), \tag{1.81}$$

where $|u_x^2| \approx |u_y|^2 \approx 0$ as assumed. To conform with the configuration shown in Fig. 1.10, Eq. (1.81) is set such that the third entry of $\boldsymbol{\nu}$ stays positive.

Now we express the tangent vector $\boldsymbol{\eta}$. For its expression, we need to use two key unit vectors defined in x–y plane, as also shown in Fig. 1.10. Here to distinguish them from the aforementioned three-dimensional key unit vectors, bold English letters are employed to denote these two-dimensional vectors in x-y plane. For the point P shown in Fig. 1.10, it is projected on to x-y plane at $(x, y) \in \partial\Omega_0$. From it, we define, with regard to the boundary $\partial\Omega_0$, its (two-dimensional) tangent vector $\mathbf{s} = (s_1, s_2)$ and its (two-dimensional) normal vector $\mathbf{n} = (n_1, n_2)$. The vector $\mathbf{s}$ is taken in the following sense. When moving along direction $\mathbf{s}$, the domain of interest Ω_0 always lies on the left side. And for the normal vector $\mathbf{n}$, it always points outward Ω_0. Hence, these two-dimensional vectors are linked with each other by

$$n_1 = s_2, \quad n_2 = -s_1. \tag{1.82}$$

Now we look to expressing the tangent vector $\boldsymbol{\eta}$ shown in Fig. 1.10. Its projection onto x-y plane should coincide with the two-dimensional tangent vector $\mathbf{s}$, and its third entry should effectively be equal to the partial derivative of u along the direction of $\mathbf{s}$. In this sense, we have

$$\boldsymbol{\eta} \approx \left(s_1, s_2, u_x s_1 + u_y s_2\right). \tag{1.83}$$

Incorporating Eqs. (1.81) and (1.83) into (1.80) expresses the (three-dimensional) unit vector $\boldsymbol{\tau}$ by

$$\boldsymbol{\tau} \approx (s_2, -s_1, u_x s_2 - u_y s_1) = (n_1, n_2, u_x n_1 + u_y n_2), \tag{1.84}$$

where Eq. (1.82) has been used for obtaining the second identity. Note that $\boldsymbol{\tau}$ by Eq. (1.84) quantifies the direction of the internal force applied to Ω_0 at point P.

Therefore, for an infinitesimally short boundary section from $\partial\Omega_0$, say $\mathrm{d}s$, the force due to the adjacent part of the membrane equals $T\boldsymbol{\tau}\mathrm{d}s$, and the transverse impulse due to surface tension comes from its third component, i.e. $T(u_x n_1 + u_y n_2)\mathrm{d}s$. As a result, the impulse due to the rest membrane pieces within $[t_1, t_2]$ should be calculated by

$$\int_{t_1}^{t_2} \int_{\partial\Omega_0} T(u_x n_1 + u_y n_2)\,\mathrm{d}\Gamma\mathrm{d}t = \int_{t_1}^{t_2} \iint_{\Omega_0} T(u_{xx} + u_{yy})\,\mathrm{d}x\mathrm{d}y\mathrm{d}t, \tag{1.85}$$

where Green's formula has been used for its derivation. Note that Green's formula plays an extremely important role in developing PDE models and solvers. It has various appearances in this book, and they are summarised in the prerequisite part concluding the present section.

Combining Eqs. (1.78)–(1.79) with (1.85), conservation of momentum along the vertical direction reads

$$\int_{t_1}^{t_2} \iint_{\Omega_0} \rho u_{tt} \, \mathrm{d}x\mathrm{d}y\mathrm{d}t = \int_{t_1}^{t_2} \iint_{\Omega_0} [T(u_{xx} + u_{yy}) + F(x, y, t)] \, \mathrm{d}x\mathrm{d}y\mathrm{d}t. \tag{1.86}$$

Given the arbitrariness in the choice of Ω_0, t_1 and t_2, the integrands in Eq. (1.86) should be equated, i.e.

$$\rho u_{tt} - T\left(u_{xx} + u_{yy}\right) = F(x, y, t).$$

Similar as in the (spatially) one-dimensional case examined in Sect. 1.1, we introduce $a^2 = \frac{T}{\rho}$ and the external force per mass defined by $f = \frac{F}{\rho}$. The governing equation for membrane vibration is finally written by

$$\frac{\partial^2 u}{\partial t^2} - a^2 \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = f(x, y, t). \tag{1.87}$$

Eq. (1.87) is termed as the *two-dimensional wave equation*, or the *equation for membrane vibration* in this book.

As a natural extension of the wave equation to three dimensions, we write

$$u_{tt} - a^2 \left(u_{xx} + u_{yy} + u_{zz}\right) = f(x, y, z; t), \tag{1.88}$$

which is called the *three-dimensional wave equation*. Equation (1.88) is expected to describe the physical phenomena which has a fundamental feature of wave propagation. For example, the propagation of electric–magnetic wave can be formulate by Eq. (1.88) under certain circumstances [8], and this topic will be considered in Sec. 4.1.

1.4.2 Definite Problems

Similar as in the case of string vibration, extra conditions are needed to fully identify a physical process of membrane vibration. For initial conditions, the membrane profile and the velocity distribution at $t = 0$ should be specified, that is,

$$u|_{t=0} = \phi(x, y), \qquad u_t|_{t=0} = \psi(x, y). \tag{1.89}$$

When the membrane of interest is infinitely large in size, i.e. $(x, y) \in \mathbb{R}^2$, only initial conditions are needed, and the corresponding PDE problem is known as a Cauchy problem.

When the membrane is of finite size, boundary conditions are also needed, and the corresponding PDE problem becomes an initial–boundary value problem. In analogies with the one-dimensional case, three types of boundary conditions may be imposed.

The first type, or Dirichlet boundary condition, is imposed by controlling the displacement field on the boundary $\partial\Omega$, that is,

$$u|_{\partial\Omega} = g(x, y, t). \tag{1.90}$$

Note that the choice of x and y in Eq. (1.90) is not fully arbitrary. The locus of (x, y) should fall on the domain boundary $\partial\Omega$, and so on for the rest two cases.

The second type, or Neumann boundary condition, is imposed through controlling the force on the membrane, that is,

$$T \left.\frac{\partial u}{\partial n}\right|_{\partial\Omega} = g(x, y, t), \tag{1.91}$$

where $\frac{\partial u}{\partial n}$ denotes the derivative of u along the unit outer normal $\mathbf{n}$ to the domain boundary.

Combining the aforementioned two types of boundary conditions gives the third type, or Robin boundary condition, which is formulated by

$$\left.\left(\sigma u + T\frac{\partial u}{\partial n}\right)\right|_{\partial\Omega} = g(x, y, t). \tag{1.92}$$

Eq. (1.92) is usually formulated through a force agent attached on the boundary, e.g. a spring.

1.4.3 Solutions for Cauchy Problems

The Cauchy problems governed by both the two-dimensional and three-dimensional wave equation actually yield analytic solutions. Interestingly, the solution for the three-dimensional case is logically available first.

To this end, we first refer to the Cauchy problem governed by the three-dimensional wave equation, i.e.

$$\begin{cases} u_{tt} - a^2\left(u_{xx} + u_{yy} + u_{zz}\right) = 0, \ (x, y, z) \in \mathbb{R}^3, \ t > 0; \\ u|_{t=0} = \phi(x, y, z), \quad u_t|_{t=0} = \psi(x, y, z). \end{cases} \tag{1.93}$$

The solution for problem (1.93) can be derived using the *method of averages* in spheres, whose underlying idea is summarised as follows. A piece of information initially at position $\tilde{\mathbf{r}} = (x_0, y_0, z_0)^{\mathrm{T}}$ should be transmitted away isotropically at a constant speed of a. Hence, at any point $\mathbf{r} = (x, y, z)^{\mathrm{T}}$ and time t, the function value

is expected to be equally affected by initial conditions taken at a distance at away from $\mathbf{r}$. In other words, it is the initial values taken on the surface of a sphere centred at $\mathbf{r}$ and of radius at, denoted by $\partial\Omega_{at}(\mathbf{r})$ here, that determine $u(x,t)$. Thus upon averaging over $\partial\Omega_{at}(\mathbf{r})$, the number of the resulting independent variables is greatly reduced, and analytical solutions become available then. Here we simply omit the detailed derivations, which can be found elsewhere (e.g. [12]), and we simply write down the solution for problem (1.93) by

$$u(\mathbf{r};t) = \frac{\partial}{\partial t}\left(\frac{1}{4\pi a^2 t}\iint\limits_{\partial\mathcal{O}_{at}(\mathbf{r})} \phi(\tilde{\mathbf{r}})\,\mathrm{d}S_{\tilde{\mathbf{r}}}\right) + \frac{1}{4\pi a^2 t}\iint\limits_{\partial\mathcal{O}_{at}(\mathbf{r})} \psi(\tilde{\mathbf{r}})\,\mathrm{d}S_{\tilde{\mathbf{r}}}, \tag{1.94}$$

where the integration is defined in regard to the infinitesimal area of $\mathrm{d}S_{\tilde{\mathbf{r}}}$.

Albert its complicated outlook, Eq. (1.94) charts a clear physical picture. To better rationalise the wave propagation behaviour described by Eq. (1.94), we introduce the concept of *wave front*. Given a spatial position $\tilde{\mathbf{r}}$, its associated wave front (at time t) contains all the spatial points, to which the initial conditions at $\tilde{\mathbf{r}}$ are transmitted for the first time. Take the one-dimensional case as an example. D'Alembert's formula (1.27) suggests that at time t, the information initially at $x = x_0$ reaches no farther than the two points at $x_0 - at$ and $x_0 + at$. Thus, the corresponding wave front contains two points: $\{x_0 - at, x_0 + at\}$. Examined with Fig. 1.5(c), the wave front just contains the boundary points of the domain of influence of $x = x_0$ at t. As for wave propagation in three-dimensional space formulated by Eq. (1.94), the wave front at time t due to a point source, say, at (x_0, y_0, z_0) is just the spherical surface given by

$$\left\{(x,y,z)|(x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2 = a^2t^2\right\}. \tag{1.95}$$

The concept of wave front can also be generalised, from cases with pointwise initial conditions to cases where initial conditions are continuously defined in a finite domain. In this case, the wave front contains all the spatial points, to which the initial function values defined in the finite region are transmitted for the first time.

Another key difference lying in wave propagation in three-dimensional space against the one-dimensional case can be spotted through a comparison between Eqs. (1.27) and (1.94). In three-dimensional space, the initial condition at $\tilde{\mathbf{r}} = (x_0, y_0, z_0)$, as suggested by Eq. (1.94), only affects the values of u on its wave front, not the values of u defined in the region enclosed by the wave front. In contrast to the one-dimensional cases, as long as $\psi(\alpha)$ in Eq. (1.27) is non-vanishing, the initial condition at point $x = x_0$ affects all the values of u in the whole domain enclosed by the wave front, i.e. the interval $[x_0 - at, x_0 + at]$. The physical implications indicated by such dimensional differences may be perceived from a fictitious scenario of "sonic waves", whose propagation is supposed to satisfy the wave equation. In this scenario, when a sound is made in three-dimensional space, it is heard after certain time, but no more afterwards, because the spherical surface, as given by Eq. (1.95), has passed by. However, if we are confined in one-dimensional space, we have to

keep hearing the sound after it is heard at the first place, because once included, the observation point stays inside the interval of influence of the sound source.

The idea is generalisable to studying the effects due to initial conditions defined in a bounded region. Its domain of influence at time t now becomes a "spherical shell". As time evolves, both its inner and outer radii grow. Finally at a certain time, one no longer detects the influence caused by the initial conditions (in the considered region). In other words, there are no (constantly) successive effects for wave propagation in three-dimensional space. The physical phenomena implied by the solutions to the Cauchy problems governed by the higher-dimensional wave equation can be further conceptualised by a broader idea elucidated by *Huygens' principle* (e.g. see [2]).

Finally, we consider the solution for the Cauchy problem governed by the two-dimensional wave equation, e.g.

$$\begin{cases} u_{tt} - a^2\left(u_{xx} + u_{yy}\right) = 0, \ (x, y) \in \mathbb{R}^2, \ t > 0; \\ u|_{t=0} = \phi(x, y), \quad u_t|_{t=0} = \psi(x, y). \end{cases} \tag{1.96}$$

The solution to problem (1.96) can be derived using the *method of descent*. Its core idea is to envisage the solution as a function $\tilde{u}$ which is also of z, i.e. $u = \tilde{u}(x, y, z; t)$. Since $\tilde{u}$ is actually independent of z, then $\tilde{u}_{zz} = 0$. Hence, $\tilde{u}$ should satisfy the three-dimensional wave equation too. Then $\tilde{u}$ can be expressed based on the three-dimensional result given by Eq. (1.94). But the actual solution u is derived by projecting $\tilde{u}$ onto x-y plane. Without presenting the derivation details, we write down the solution to problem (1.96) as

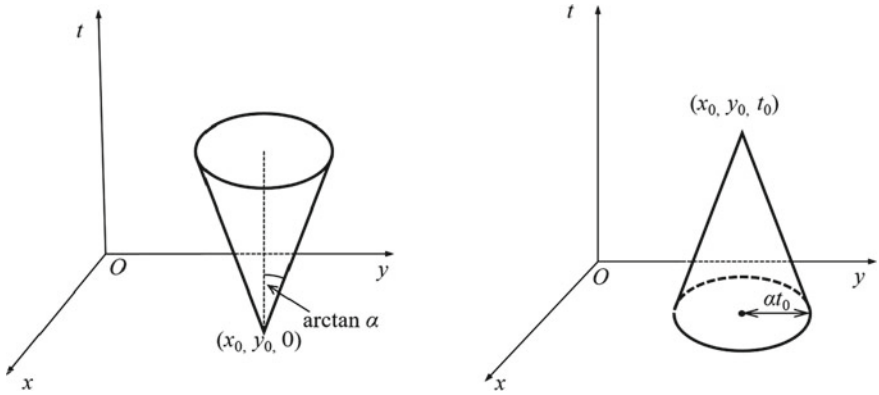
$$\begin{aligned} u(x, y; t) = & \frac{1}{2\pi a}\frac{\partial}{\partial t}\iint\limits_{\mathcal{O}_{at}(x,y)} \frac{\phi(\xi, \eta)\,\mathrm{d}\xi\mathrm{d}\eta}{\sqrt{a^2t^2 - (x-\xi)^2 - (y-\eta)^2}} \\ & + \frac{1}{2\pi a}\iint\limits_{\mathcal{O}_{at}(x,y)} \frac{\psi(\xi, \eta)\,\mathrm{d}\xi\mathrm{d}\eta}{\sqrt{a^2t^2 - (x-\xi)^2 - (y-\eta)^2}}, \end{aligned} \tag{1.97}$$

where $\mathcal{O}_{at}(x, y)$ denote the (two-dimensional) circular region centred at (x, y) and of radius at.

With reference to Eq. (1.97), the corresponding wave front of point (x_0, y_0) should be the circular boundary centred at (x_0, y_0) and of radius at. But since the integration in Eq. (1.97) is conducted within the full region enclosed by the wave front, the corresponding domain of influence for point (x_0, y_0) is the full region of

$$\{(x, y)|(x - x_0)^2 + (y - y_0)^2 \le a^2t^2\}.$$

Viewed in x–y–t space, as shown in Fig. 1.11a, the points belonging to this set form a cone, known as a *characteristic cone*, and the values of u at all points that fall inside the cone should be affected by the initial value at (x_0, y_0). Besides, one may also introduce the domain of determinacy for a spatial point (x_0, y_0) at time t_0, as suggested by the cone in Fig. 1.11b.



(a) Domain of influence (b) Domain of dependence

Fig. 1.11 Characteristics behaviour observed from the solution (1.97) for the Cauchy problem governed by the two-dimensional wave equation

Compared with the three-dimensional case, a distinctive feature shown by wave propagation confined in two-dimensional space is that, it has a successive effect, that is, one will keep hearing the sound from a source after it reaches one's ears at the first place. Of course, there exist no exactly two-dimensional waves in our actual three-dimensional world. But if the initial conditions are translationally invariant along a line, the wave propagation along any planes perpendicular to the line should be identical, and one may "see" wave propagation in two-dimensional space on each plane. A natural phenomenon mimicking this effect is thundering. Implied by lightening, thunder is generated by an initially line source in three-dimensional space. But we hear it rumbling for a while, rather than simply hearing a single sound. The concept of successive effect just provides a rationale to such rumbling phenomena of thundering.

Prerequisite knowledge

Expressing a surface in three-dimensional space

Given a surface in three-dimensional space, it can be represented in two ways. One is to explicitly express its coordinate $\mathbf{r} = (x, y, z)^{\mathrm{T}}$ as functions of two free variables, say, u and v. For instance, any point on the surface of a unit sphere can be described by

$$x = \cos\theta \sin\varphi,\ y = \sin\theta \sin\varphi, z = \cos\varphi,$$

where $\theta \in [0, 2\pi)$ and $\varphi \in [0, \pi]$ are the two free variables.

Alternatively, a surface can also be implicitly represented by an equation satisfied by the coordinates of all points on it. For example, the surface of a unit spherical can also be expressed by $x^2 + y^2 + z^2 = 1$.

Table 1.4 Expressing a surface in $\mathbb{R}^3$—a brief summary

	Explicit	Implicit
Expressions	$\mathbf{r} = \begin{cases} x = x(u, v) \\ y = y(u, v) \\ z = z(u, v) \end{cases}$	$f(x, y, z) = 0$
Normal vector	$\frac{\partial \mathbf{r}}{\partial u} \times \frac{\partial \mathbf{r}}{\partial v}$	∇f
Validity condition	$\left\lvert \frac{\partial \mathbf{r}}{\partial u} \times \frac{\partial \mathbf{r}}{\partial v} \right\rvert \neq 0$	$\lvert \nabla f \rvert \neq 0$

Figure 1.4 summarises the expressions for a three-dimensional surface and the key vectors on it, as well as their validity conditions, in both explicit and implicit cases.

Green's formula

Green's formula plays an essential role in analysing problems involving partial differential equations. Here various types of "Green's formula" appearing in different textbooks are summarised. We start with expressing *Green's formula* (irrespective of the dimensionality) by

$$\int_{\Omega} \frac{\partial f(\mathbf{r})}{\partial r_i} \, \mathrm{d}\mathbf{r} = \int_{\partial\Omega} f(\mathbf{r}) n_i \, \mathrm{d}\Gamma, \tag{1.98}$$

where $\mathbf{r}$ is a vector that can be either two dimensional or three dimensional; r_i represents its ith entry; Ω is a closed domain with $\partial\Omega$ its boundary; $\mathrm{d}\Gamma$ is an infinitesimal length/area on $\partial\Omega$; n_i is the ith entry of the unit outer normal vector at a boundary point. Equation (1.98) can be considered as a higher-dimensional extension of the (one-dimensional) Newton–Lebniz formula, which is also known as the fundamental theorem of calculus.

If one replaces f in Eq. (1.98) by the product of two functions, say, $f = g \cdot h$, rearranging the results gives

$$\int_{\Omega} g \frac{\partial h}{\partial r_i} \, \mathrm{d}\mathbf{r} = \int_{\partial\Omega} g \cdot h n_i \, \mathrm{d}\Gamma - \int_{\Omega} h \frac{\partial g}{\partial r_i} \, \mathrm{d}\mathbf{r}, \tag{1.99}$$

which is the higher-dimensional counterpart of the formula of integration by parts.

In two-dimensional scenarios, Eq. (1.98) bears

$$\iint_{\Omega} \left(\frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y} \right) \mathrm{d}x\mathrm{d}y = \int_{\partial\Omega} (Q n_1 - P n_2) \, \mathrm{d}s,$$

where $\mathrm{d}s$ measures an infinitesimally short arc-length on $\partial\Omega$. Note that for a two-dimensional domain, its boundary normal vector $\mathbf{n}$ and the local tangent $\mathbf{s}$ are inter-

related. Being defined in the sense as in Fig. 1.10, **n** and **s** should satisfy Eq. (1.82), i.e. $s_1 = -n_2, s_2 = n_1$. Then with the use of $\mathrm{d}x = s_1 \mathrm{d}s$, $\mathrm{d}y = s_2 \mathrm{d}s$, the formula above can be re-expressed by

$$\int_{\partial\Omega} P\mathrm{d}x + Q\mathrm{d}y = \int_{\Omega} \left(\frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y} \right) \mathrm{d}x\mathrm{d}y. \tag{1.100}$$

which is the "Green's formula" appearing in most calculus textbooks.

As for three-dimensional situations, Eq. (1.98) bears

$$\iiint_{\Omega} \left(\frac{\partial P}{\partial x} + \frac{\partial Q}{\partial y} + \frac{\partial R}{\partial z} \right) \mathrm{d}x\mathrm{d}y\mathrm{d}z = \iint_{\partial\Omega} (Pn_1 + Qn_2 + Rn_3)\ \mathrm{d}S, \tag{1.101}$$

where $\mathrm{d}S$ measures the infinitesimally small boundary area. It is recalled that $n_1 \mathrm{d}S$ quantifies the infinitesimal area projected onto y–z plane and so on. Thus, Eq. (1.101) can be further rewritten by

$$\iiint_{\Omega} \left(\frac{\partial P}{\partial x} + \frac{\partial Q}{\partial y} + \frac{\partial R}{\partial z} \right) \mathrm{d}x\mathrm{d}y\mathrm{d}z = \iint_{\partial\Omega} P\mathrm{d}y\mathrm{d}z + Q\mathrm{d}x\mathrm{d}z + R\mathrm{d}x\mathrm{d}y, \tag{1.102}$$

which is the "Gauss's theorem" appearing in a large number of calculus textbooks.

1.5 Solution Properties

In this section, properties of solutions for PDE problems governed by the wave equation will be discussed. Our aim is to further explore the linkage between the physical phenomena of vibration and its mathematical representation. On the physics side, we will examine membrane vibration in the perspective of energy conservation. On the mathematics side, we tend to discuss some key properties of solutions for problems governed by the wave equation in higher dimensions.

To this end, we consider the following two-dimensional initial–boundary value problem, which is given by

$$\begin{cases} u_{tt} - a^2(u_{xx} + u_{yy}) = f(x, y; t), \ (x, y) \in \Omega, \ t > 0; \\ u|_{t=0} = \phi(x, y), \ u_t|_{t=0} = \psi(x, y); \\ u|_{\partial\Omega} = h(x, y, t). \end{cases} \tag{1.103}$$

Here the involved physical quantities are represented in a same fashion as in Sect. 1.4, i.e. f represents the load per mass vertically applied on the membrane surface; $a^2 = \frac{T}{\rho}$, where T is the surface tension expanding the membrane and ρ is the mass density.

1.5.1 The Energy of a Vibrating Membrane

We start from a physical viewpoint by formulating the energy of a membrane undergoing small and transverse vibration. The total energy contained in a vibrating membrane, i.e. the *mechanical energy*, comprises of two parts: the *kinetic energy* and the *elastic energy*.

The kinetic energy can be expressed by

$$\mathcal{T} = \frac{1}{2} \iint_{\Omega} \rho u_t^2 \mathrm{d}x\mathrm{d}y, \tag{1.104}$$

where the integrand is a function of both space and time, and it is termed as the *kinetic energy density*.

The system elastic energy can be expressed by

$$\mathcal{U} = \frac{1}{2} \iint_{\Omega} T(u_x^2 + u_y^2)\mathrm{d}x\mathrm{d}y, \tag{1.105}$$

where the integrand is termed as the *elastic energy density*. Note that the expressions for the energy density quantities defined by Eqs. (1.104) and (1.105) are quite typical. They are written in a form of "$\frac{1}{2} \times$ a material constant $\times$ (gradient of a field variable)^2". Such a way of expressing energy densities can be seen elsewhere. For instance, the elastic energy per length of a thin rod (within its elastic limit) is calculated by $\frac{ES}{2}u_x^2$, where E is Young's modulus; S is its cross-sectional area; u measures the longitudinal displacement field. Moreover, the potential energy density of an electrostatic system is formulated by $\frac{\epsilon_0}{2}|\nabla U|^2$, where ϵ_0 is the electric permittivity and U is a field quantity measuring the electric potential.

Therefore, the energy of a membrane undergoing small and transverse vibration is formulated by

$$\mathcal{E} = \frac{1}{2} \iint_{\Omega} \left[\rho u_t^2 + T(u_x^2 + u_y^2)\right] \mathrm{d}x\mathrm{d}y. \tag{1.106}$$

Then we consider the rate of change in the total energy. Note that upon integration with respect to the spatial variables x and y, $\mathcal{E}$ defined by Eq. (1.106) is a function only of time. Thus differentiating Eq. (1.106) with respect to t gives

$$\dot{\mathcal{E}} = \iint_{\Omega} \left[\rho u_t u_{tt} + T(u_x u_{xt} + u_y u_{yt})\right] \mathrm{d}x\mathrm{d}y, \tag{1.107}$$

when $\dot{\mathcal{E}}$ measures the rate of change in the total energy.

As from Green's formula (1.99)

$$\iint_{\Omega} (u_x u_{xt} + u_y u_{yt})\,\mathrm{d}x\mathrm{d}y = \int_{\partial\Omega} u_t \frac{\partial u}{\partial n}\,\mathrm{d}s - \iint_{\Omega} u_t (u_{xx} + u_{yy})\,\mathrm{d}x\mathrm{d}y,$$

where "$\frac{\partial}{\partial n}$" denotes differentiation along the outer normal direction **n** on the boundary; ds measures the length of an infinitesimally small section from the boundary. Inserting the above identity into Eq. (1.107) results in

$$\dot{\mathcal{E}} = \iint_{\Omega} \rho u_t \left[u_{tt} - a^2(u_{xx} + u_{yy})\right]\mathrm{d}x\mathrm{d}y + \int_{\partial\Omega} u_t T \frac{\partial u}{\partial n}\,\mathrm{d}s,$$

where the fact that $a^2 = \frac{T}{\rho}$ has been referred to. On using the governing PDE of problem (1.103), the rate of change in the total energy can be further expressed by

$$\dot{\mathcal{E}} = \iint_{\Omega} \rho u_t f\,\mathrm{d}x\mathrm{d}y + \int_{\partial\Omega} u_t T \frac{\partial u}{\partial n}\,\mathrm{d}s. \tag{1.108}$$

As from the modelling procedure detailed in Sec. 1.4.1, the double integral in Eq. (1.108) measures the power output by the surface force (per weight) f. Moreover, as the quantity $T\frac{\partial u}{\partial n}\mathrm{d}s$ measures the instantaneous force applied on the membrane boundary, the boundary integral in Eq. (1.108) formulates the power output by the external load through the membrane boundary. Therefore, the physical perspective of Eq. (1.108) is clear: the rate of change in the mechanical energy of a membrane system equals the power output by all the external loads. In other words, the system mechanical energy is automatically conserved during the vibrating process described by the two-dimensional wave equation.

1.5.2 Solution Uniqueness of Problems for the Wave Equation

Three issues about solutions for PDE problems are of general interest. They are

- *existence*, whether there exists a solution to a PDE problem;
- *uniqueness*, upon existence, whether the solution is unique;
- *stability*, how sensitive is the solution with a perturbation to initial and/or boundary data.

Apart from the mathematical perspective, analysing the above-listed properties has engineering significance too. This is because analytical solutions for general PDE problems are not always available in practice. Thus, computer simulations are often used to find their approximated *numerical solutions*. Then solution existence

validates the implemented numerical solvers. And solution uniqueness ensures that one ends up with approximating a same solution using different schemes. Besides, theoretically stable solutions ensure that the (inevitable) numerical errors, either caused by the measurement of the input data or brought by the digital approximation ubiquitous in computer simulations, do not cause unacceptable deviations from the true solutions. Analysing other properties of solutions for PDE problems is also practically meaningful. In this book, we will mainly emphasise the solution properties of problems governed by linear PDEs in the aforementioned three aspects.

First, we consider the solution existence of problems governed by the wave equation for multidimensional cases. As discussed in this chapter, we have managed to derive, under certain circumstances, analytical solutions both for the Cauchy problem in Sect. 1.2 (for one-dimension situations), Sect. 1.4 (for higher-dimensional situations) and the initial–boundary value problems in Sect. 1.3. Deriving its analytical solutions is of course the most straight forward way to demonstrate the solution existence of a PDE problem. Nonetheless, this is often not the case. For many PDE problems, analytical solutions are not available, but their solution existence can still be proved somehow. This often entails the usage of advanced mathematical tools and techniques, which will not be covered by this book.

In theory, there may be more than one solution for a PDE problem. Then the issue of solution uniqueness should be looked into. In this subsection, we are mainly focused on demonstrating solution uniqueness for the initial–boundary value problem governed by the two-dimensional wave equation, as formulated by Eq. (1.103). Note that if $u_1(x, y; t)$ and $u_2(x, y; t)$ are both solutions for problem (1.103), then we introduce $v(x, y; t) = u_1 - u_2$, which should satisfy

$$\begin{cases} v_{tt} - a^2(v_{xx} + v_{yy}) = 0, \ (x, y) \in \Omega, \ t > 0; \\ v|_{t=0} = 0, \ v_t|_{t=0} = 0; \\ v|_{\partial\Omega} = 0. \end{cases} \tag{1.109}$$

Here we make use of the fact that the superposition of linear problems is still linear. In this viewpoint, proving solution uniqueness for problem (1.103) is equivalent to showing that problem (1.109) only bears a trivial solution, i.e. $v \equiv 0$. In fact, this offers a routine for demonstrating solution uniqueness for general linear PDE problem, that is, to show that the corresponding homogeneous problem (with both the equation and the initial and/or boundary conditions being homogeneous) only yields a trivial solution.

For its proof, we note that problem (1.109) is still an initial–boundary value problem for the two-dimensional wave equation. It actually corresponds to the situation of a freely vibrating membrane with its boundary fixed. In this scenario, there is no work done by the external loads either on the membrane surface, or through the boundary. Checked with Eq. (1.108), the mechanical energy of the system should stay constant, i.e.

$$\dot{\mathcal{E}} = 0.$$

Thus as time evolves, the system energy stays the same as the initial value. It can be read from problem (1.108) that the initial mechanical energy is zero too. Therefore, at any time t,

$$\mathcal{E} = \frac{1}{2}\int_{\Omega}\left[\rho v_t^2 + T(v_x^2 + v_y^2)\right]\mathrm{d}x\mathrm{d}y = 0. \tag{1.110}$$

Note that all the terms appearing in the integrand of Eq. (1.110) are non-negative. In order to make Eq. (1.110) hold, $v_t = v_x = v_y = 0$, suggesting that v is independent of both time and space, i.e. v is a constant-valued function. Since $v|_{t=0} = 0$, then $v \equiv 0$, indicating that Eq. (1.109) only yields a trivial solution. Hence, the solution uniqueness for problem (1.103) is demonstrated.

The key idea underlying the proof above is to write down the corresponding homogeneous problems first and then to show that the density of the total energy is invariant both in time and space. The idea sees its generalisation in other cases, for instance, when the governing equation is one dimensional or three dimensional in space, or when other types of boundary conditions are involved. Note that the expressions for the total energy may vary then, and more examples can be found in Exercise 1.21.

Finally, we briefly mention the solution stability for problem (1.103). Suppose that numerical errors are brought in during evaluation for initial–boundary conditions, or parameters in problem (1.103), induced either through measurement or numerical approximations. Then we actually solve a problem for $\tilde{u}$ given by

$$\begin{cases} \tilde{u}_{tt} - a^2(\tilde{u}_{xx} + \tilde{u}_{yy}) = f + \Delta f, \ (x, y) \in \Omega, \ t > 0; \\ \tilde{u}|_{t=0} = \phi + \Delta\phi \quad \tilde{u}_t|_{t=0} = \psi + \Delta\psi; \\ \tilde{u}|_{\partial\Omega} = h + \Delta h, \end{cases} \tag{1.111}$$

where Δf, $\Delta\phi$, $\Delta\psi$ and Δh measure the deviations in the applied force on the membrane surface, the initial displacements, the initial velocities and boundary displacements, respectively. We expect as such deviations tend to 0, the error in solution, given by $u - \tilde{u}$, tends to zero at a high rate. This offers a non-rigorous description over the solution stability of the wave equation. For a more rigorous argument and the proof, one may extend the energy expression (1.108) for an energy inequality, which will not be covered in the present book. But one may refer to other materials for further studies [7].

Exercise

1. A thin heterogeneous rod of cylindrical shape undergoes small and longitudinal vibration caused by external loads applied at its ends. Let $u(x, t)$ denote the longitudinal displacement away from its equilibrium position corresponding to point x at time t. Assume that the density distribution of the rod satisfies $\rho(x)(\sim\mathrm{kg/m}^3)$; the distribution of Young's modulus satisfies $E(x)$, and the tension resulting from deformation produced satisfies Hookean law.

(a) Show that $u(x, t)$ satisfies the following equation

$$\frac{\partial}{\partial t}\left(\rho(x)\frac{\partial u}{\partial t}\right) = \frac{\partial}{\partial x}\left(E(x)\frac{\partial u}{\partial x}\right).$$

(b) Write down the boundary conditions corresponding to the following three scenarios: (1) the end of the rod is fixed; (2) the end of the rod is free of external loads; (3) the end point is attached to a spring whose elastic coefficient equals k_1.

2. Consider a conical pivot which vibrates along the direction orthogonal to the cone bottom. Show that the governing equation is given by

$$E\frac{\partial}{\partial x}\left[\left(\frac{x}{h}\right)^2\frac{\partial u}{\partial x}\right] = \rho\left(\frac{x}{h}\right)^2\frac{\partial^2 u}{\partial t^2},$$

where h is the height of the cone and E is Young's modulus of the material.

3. Determine the order of the following partial differential equations. Also determine whether the PDEs are linear or not. If it is the case, determine whether the PDE is homogeneous. Here u represents the unknown functions; x, y and t are independent variables; f and μ are given functions; ν and a are coefficients.

(a) *Burgers' equation*:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2}.$$

(b) The heat equation:

$$\frac{\partial u}{\partial t} - a^2\frac{\partial^2 u}{\partial x^2} = f(x, t).$$

(c) *Bi-harmonic equation*:

$$\frac{\partial^4 u}{\partial x^4} + 2\frac{\partial^4 u}{\partial x^2\partial y^2} + \frac{\partial^4 u}{\partial y^4} = 0.$$

(d) The governing equation for the electrostatic potential in an inhomogeneous region:

$$\frac{\partial}{\partial x}\left(\frac{1}{\mu(x, y)}\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{1}{\mu(x, y)}\frac{\partial u}{\partial y}\right) = 0.$$

4. Solve the Cauchy problem governed by the wave equation given by

$$\begin{cases} u_{tt} - a^2 u_{xx} = 0, \ (x, t) \in \mathbb{R} \times \mathbb{R}^+; \\ u|_{t=0} = 0, \quad u_t|_{t=0} = \dfrac{1}{1 + x^2}. \end{cases}$$

5. Consider the following equation:

$$\frac{x^2}{a^2}\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x}\left[x^2\frac{\partial u}{\partial x}\right]$$

(a) Prove that its general solution can be written as

$$u(x,t) = \frac{F(x-at)+G(x+at)}{x},$$

where $F(\cdot)$ and $G(\cdot)$ are arbitrary unary functions that are twice differentiable.

(b) If the equation also satisfies the following initial conditions:

$$u|_{t=0} = \phi(x), \quad \left.\frac{\partial u}{\partial t}\right|_{t=0} = \psi(x),$$

derive the expression for the solution for the resulting Cauchy problem.

6. With reference to the method detailed in Sect. 1.2.3, solve the *Goursat* problem for the wave equation:

$$\begin{cases} u_{tt} - a^2 u_{xx} = 0, \ (x,t) \in \mathbb{R}\times\mathbb{R}^+; \\ u|_{x-at=0} = \phi(x), \quad u|_{x+at=0} = \psi(x), \end{cases}$$

where $\phi(0) = \psi(0)$.

7. Consider the Cauchy problem where a string is set still initially, i.e.

$$\begin{cases} u_{tt} - u_{xx} = 0, \ (x,t) \in \mathbb{R}\times\mathbb{R}^+; \\ u|_{t=0} = \phi(x), \quad u_t|_{t=0} = 0. \end{cases}$$

Suppose that the initial profile of the string is given by

$$\phi(x) = \begin{cases} 3-x, & x \in [0,3]; \\ 3+x, & x \in [-3,0]; \\ 0, & |x| > 3. \end{cases}$$

(a) Draw the string profile at time $t = 1$ and 2.

(b) At what time do the leftward and rightward waves stop interfering with each other?

8. Solve

$$\begin{cases} u_{tt} - a^2 u_{xx} = 0, \ (x,t) \in \mathbb{R}^+ \times \mathbb{R}^+; \\ u|_{t=0} = \phi(x), \quad u_t|_{t=0} = 0; \\ (u_x - k u_t)|_{x=0} = 0, \end{cases}$$

where k is a positive constant.

9. Given a string which is semi-infinitely long with its end fixed at the origin, solve the corresponding PDE problem formulated by

$$\begin{cases} u_{tt} - a^2 u_{xx} = 0, \ (x,t) \in \mathbb{R}^+ \times \mathbb{R}^+; \\ u|_{t=0} = \phi(x), \ u_t|_{t=0} = \psi(x); \\ u|_{x=0} = 0. \end{cases}$$

10. Verify the Duhamel's principle for the Cauchy problem governed by the wave equation, that is, Eq. (1.41) is the solution for problem (1.39).
11. Solve the Cauchy problem for the wave equation formulated by

$$\begin{cases} \dfrac{\partial^2 u}{\partial t^2} - \dfrac{\partial^2 u}{\partial x^2} = t \cos x, \\ u|_{t=0} = 0, \quad u_t|_{t=0} = 0. \end{cases}$$

12. Consider the initial–boundary value problem for the wave equation:

$$\begin{cases} u_{tt} - a^2 u_{xx} = f(x,t), \ (x,t) \in (0,l) \times \mathbb{R}^+; \\ u|_{t=0} = \phi(x), \quad u_t|_{t=0} = \psi(x); \\ \text{Boundary conditions.} \end{cases}$$

Reformulate the problem such that the boundary conditions become homogeneous:

(a) $u_x|_{x=0} = \mu_1(t), \ u_x|_{x=l} = \mu_2(t)$;
(b) $u|_{x=0} = \mu_1(t), \ (u + u_x)|_{x=l} = \mu_2(t)$.

13. Use the method of separation of variables to solve the following problems:

(a) $$\begin{cases} u_{tt} - a^2 u_{xx} = 0, \ x \in (0,l), \ t > 0; \\ u|_{t=0} = \sin \dfrac{3\pi x}{l}, \quad u_t|_{t=0} = x(l-x); \\ u|_{x=0} = u|_{x=l} = 0. \end{cases}$$

(b) $$\begin{cases} u_{tt} - a^2 u_{xx} = 0, \ x \in (0,1), \ t > 0; \\ u|_{t=0} = 0, \quad u_t|_{t=0} = x; \\ u|_{x=0} = 0, \quad u_x|_{x=1} = 0. \end{cases}$$

14. Use the method of separation of variables to solve the initial–boundary value problem given by

$$\begin{cases} u_{tt} - a^2 u_{xx} = g, \ 0 < x < l, \ t > 0; \\ u|_{t=0} = 0, \ u_t|_{t=0} = 0; \\ u|_{x=0} = u|_{x=l} = 0, \end{cases}$$

where g is constant.

15. Use the method of separation of variables to solve the initial–boundary value problem given by

$$\begin{cases} u_{tt} + 2bu_t - a^2 u_{xx} = 0, \ x \in (0, 1), \ t > 0; \\ u|_{t=0} = x(2 - x), \quad u_t|_{t=0} = 0; \\ u|_{x=0} = u_x|_{x=1} = 0, \end{cases}$$

where b is constant and satisfies $a > b > 0$.

16. Based on Eq. (1.94), write down the solution for the following Cauchy problems for the three-dimensional wave equation:

(a) $\begin{cases} u_{tt} - a^2(u_{xx} + u_{yy} + u_{zz}) = 0, \ (x, y, z) \in \mathbb{R}^3, \ t > 0; \\ u|_{t=0} = 0, \quad u_t|_{t=0} = xy + z^2 \end{cases}$

(b) $\begin{cases} u_{tt} - a^2(u_{xx} + u_{yy} + u_{zz}) = 0, \ (x, y, z) \in \mathbb{R}^3, \ t > 0; \\ u|_{t=0} = 2x^2 z + y^3, \quad u_t|_{t=0} = 0. \end{cases}$

17. The Cauchy problem for the three-dimensional inhomogeneous wave equation is given by

$$\begin{cases} u_{tt} - a^2(u_{xx} + u_{yy} + u_{zz}) = f(x, y, z; t), \ (x, y, z) \in \mathbb{R}^3, \ t > 0; \\ u|_{t=0} = 0, \quad u_t|_{t=0} = 0. \end{cases}$$

Write down the corresponding Duhamel's principle.

18. Solve the Cauchy problem given by

$$\begin{cases} u_{tt} = u_{xx} + u_{yy} + u_{zz} + 4(t - z), \ (x, y, z) \in \mathbb{R}^3, \ t > 0; \\ u|_{t=0} = 0, \quad u_t|_{t=0} = 0. \end{cases}$$

19. Show that the solution for the following initial–boundary value problem, if existing, must be unique

$$\begin{cases} u_{tt} - a^2(u_{xx} + u_{yy}) = f(x, y; t), \ (x, y) \in \Omega, \ t > 0; \\ u|_{t=0} = \phi(x, y), \ u_t|_{t=0} = \psi(x, y); \\ \left.\dfrac{\partial u}{\partial n}\right|_{\partial\Omega} = h(x, y, t). \end{cases}$$

20. For a vibrating string, if there is frictional force which is proportional to the vibrating velocity, the transverse displacement u satisfies

$$u_{tt} = a^2 u_{xx} - \mu u_t,$$

where the constant $\mu > 0$ is the coefficient of friction.

(a) Express the system energy, and show that the system energy decreases as vibration proceeds.
(b) Demonstrate that the solution for the initial–boundary value problem given by

$$\begin{cases} u_{tt} = a^2 u_{xx} - \mu u_t + f, \ 0 < x < l, \ t > 0; \\ u|_{t=0} = \phi(x), \ u_t|_{t=0} = \psi(x); \\ u|_{x=0} = u|_{x=l} = 0 \end{cases}$$

is unique.

21. Consider the following initial–boundary value problem

$$\begin{cases} u_{tt} - a^2(u_{xx} + u_{yy}) = 0, \ (x, y) \in \Omega, \ t > 0; \\ u|_{t=0} = \phi(x, y), \quad u_t|_{t=0} = \psi(x, y); \\ \left.\left(T\dfrac{\partial u}{\partial n} + \sigma u\right)\right|_{\partial\Omega} = 0, \end{cases}$$

imposed with Robin boundary condition, where $\sigma > 0$ is constant and $a^2 = T/\rho$. The energy of the resulting system should be formulated by

$$\mathcal{E}(t) = \frac{1}{2}\iint\limits_{\Omega}\left[\rho u_t^2 + T(u_x^2 + u_y^2)\right]\mathrm{d}x\mathrm{d}y + \frac{1}{2}\int\limits_{\partial\Omega}\sigma u^2 \mathrm{d}s.$$

(a) Consider the physical implications of the energy integral above.
(b) Show that $\mathcal{E}(t)$ stays constant in time and space and thus demonstrate the uniqueness of solutions for the above problem.

Chapter 2
The Heat Equation

In this chapter, we consider formulating the physical phenomena of heat conduction. We start with the derivation of the governing equation, the heat equation. This is followed by the introduction of the method of integral transform, a method typically used to solve PDE problems defined in infinitely large domains. We will also revisit the method of separation of variables, motivated by the need to find solutions for the initial–boundary value problems for the heat equation. Along this direction, the concept of the Sturm–Liouville differential equation system is then presented. In the end of this chapter, we discuss the maximum principle for the heat equation which underlies the diffusive feature of heat conduction. From a mathematical viewpoint, the maximum principle is presented to investigate the properties of solutions for problems governed by the heat equation. The contents in this chapter are summarised in the knowledge map as charted in Fig. 2.1.

2.1 Modelling Heat Conduction

2.1.1 Derivation of the Heat Equation

We begin by considering how temperature evolves within a three-dimensional domain denoted by $\Omega \in \mathbb{R}^3$. To this end, we introduce $u(x, y, z; t)$ to denote the temperature around the spatial point (x, y, z) at time t, and our aim is to derive a partial differential equation for $u(x, y, z; t)$.

For modelling, a number of physical laws should be specified. The first one is *Fourier's law of thermal/heat conduction*, which is used to calculate the amount of heat flowing across an infinitesimally small piece of surface, which is of area $\mathrm{d}S$ and perpendicular to its outer normal vector $\mathbf{n}$. It says that the amount of heat

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Y. Zhu, *Equations and Analytical Tools in Mathematical Physics*,
https://doi.org/10.1007/978-981-16-5441-1_2

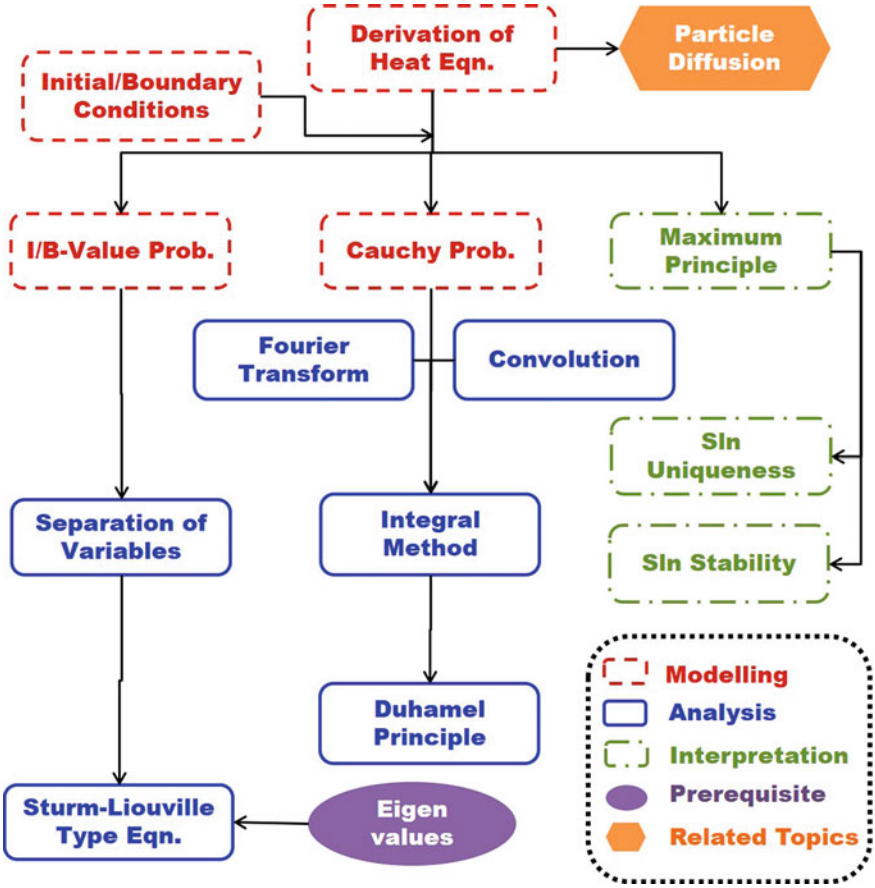

Fig. 2.1 Knowledge map—heat equation

passing through the surface piece during a short period dt, which is denoted by dQ, is formulated by

$$\mathrm{d}Q = -k\frac{\partial u}{\partial n}\mathrm{d}S\mathrm{d}t, \tag{2.1}$$

where $k(x, y, z)$ is a coefficient measuring the *thermal conductivity* of the medium. Note that the negative sign in Eq. (2.1) implies that heat flow always takes place from high-temperature regions to low-temperature regions. Note that Fourier's law of heat conduction is summarised from experimental observation.

To further rationalise Eq. (2.1), one may envisage heat transfer as a "fluid" flowing in space, and the "momentum" or the flow intensity can be measured by a field (vector-valued) quantity of *heat flux*, denoted by **J**, which is in unit joule per area per second. Note that the most "efficient" way to dissipate heat by nature is to "guide" the heat

flow along the direction with the steepest descent in temperature u. The heat flux is thus formulated by

$$\mathbf{J} = -k(x, y, z)\nabla u. \tag{2.2}$$

For a given infinitesimally small area $\mathrm{d}S$, the rate in the amount of heat passing through it should be calculated by

$$\frac{\mathrm{d}Q}{\mathrm{d}t} = \mathbf{J} \cdot \mathbf{n}\mathrm{d}S = -k\frac{\partial u}{\partial n}\mathrm{d}S,$$

which coincides with Eq. (2.1).

Note that Eq. (2.2) is defined under the presumption where the medium is *isotropic* for heat transfer, that is, there is no preferred direction for heat conduction. Mathematically, an isotropic medium for heat transfer corresponds to the case where the thermal conductivity k is scalar. If the medium is anisotropic for heat transfer, the thermal conductivity should be represented by a second-order tensor, which can be simply treated as a matrix (for details, see Exercise 2.3). When the thermal conductivity is uniform in space, the medium is *homogeneous* for heat transfer.

The second physical law for our use is the *law of heat capacity*. It says that the heat units needed for altering the temperature of an object are proportional to its mass, and the temperature difference, i.e.

$$\mathrm{d}Q = c\rho\mathrm{d}x\mathrm{d}y\mathrm{d}z\mathrm{d}u, \tag{2.3}$$

where the proportionality c is the (mass) heat capacity, and ρ is the material mass density.

The last piece of physical law needed stems from the first law of thermodynamics, or simply the conservation of thermal energy. It says that, in the absence of work done to a system, the change in system thermal energy equals the (signed) heat units generated by internal heat sources/sinks, less the net (signed) heat units transferred away from the system. Here we introduce a scalar quantity of $F(x, y, z; t)$ to measure the rate in heat generation/absorption per volume.

In Table 2.1, summarise the physical quantities needed for modelling thermal conduction.

To derive a PDE for u, we consider an arbitrary domain Ω during a time interval (t_1, t_2). As from the law of heat capacity, the heat units required to bring about a temperature change from $u|_{t=t_1}$ to $u|_{t=t_2}$ is formulated by

$$\Delta Q = \iiint_{\Omega} c\rho\, u|_{t_1}^{t_2}\, \mathrm{d}x\mathrm{d}y\mathrm{d}z = \int_{t_1}^{t_2} \iiint_{\Omega} c\rho\frac{\partial u}{\partial t}\, \mathrm{d}x\mathrm{d}y\mathrm{d}z\mathrm{d}t, \tag{2.4}$$

where the second identity is from the fundamental theorem of calculus.

Table 2.1 Physical quantities used for modelling heat conduction

Notation	Physical meaning	Dimension
x, y, z	Spatial variable	Meter (m)
t	Temporal variable	Second (s)
$u(x, y, z; t)$	Temperature	Kelvin (K)
$\mathbf{d}Q$	Heat transferred	Joule (J)
$\mathbf{J}$	Heat flux	J/(m^2 s)
c	Heat capacity	J/(kg K)
ρ	Mass density	kg/m^3
ΔU	Internal energy	J
F	Heat source/sink	J/(m^3 s)

According to Fourier's law of heat transfer, the net heat units flowing out of the system boundary $\partial\Omega$ (along the outer normal direction $\mathbf{n}$) is calculated by

$$\begin{aligned}\Delta Q &= \int_{t_1}^{t_2} \oiint_{\partial\Omega} -k\frac{\partial u}{\partial n}\,\mathrm{d}S\mathrm{d}t \\ &= -\int_{t_1}^{t_2} \iiint_{\Omega} k\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial x^y}+\frac{\partial^2 u}{\partial z^2}\right)\mathrm{d}x\mathrm{d}y\mathrm{d}z\mathrm{d}t,\end{aligned} \tag{2.5}$$

where "$\oiint$" implies that the integration is carried out over the full surface enclosing the domain Ω, and Green's formula, as given by Eq. (1.101), is also used to derive the second identity.

As the total thermal energy is conserved, the heat units needed for the temperature change over $[t_1, t_2]$ should be equal to the (net) heat units generated by sources/sinks less that flowing away through the system boundary, that is,

$$\begin{aligned}&\int_{t_1}^{t_2} \iiint_{\Omega} c\rho\frac{\partial u}{\partial t}\,\mathrm{d}x\mathrm{d}y\mathrm{d}z\mathrm{d}t \\ &= \int_{t_1}^{t_2} \iiint_{\Omega} F\,\mathrm{d}x\mathrm{d}y\mathrm{d}z\mathrm{d}t + \int_{t_1}^{t_2} \iiint_{\Omega} k\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right)\mathrm{d}x\mathrm{d}y\mathrm{d}z\mathrm{d}t.\end{aligned} \tag{2.6}$$

Given the arbitrariness in the choice of t_1, t_2 and Ω, the integrands in Eq. (2.6) should be equated, and a PDE for u is finally derived to be

$$\rho c\frac{\partial u}{\partial t} - k\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right) = F(x, y, z; t). \tag{2.7}$$

Similar as in the case for the wave equation, we introduce

$$a^2 = \frac{k}{\rho c}, \quad f = \frac{F}{\rho c},$$

and Eq. (2.7) finally becomes

$$u_t - a^2(u_{xx} + u_{yy} + u_{zz}) = f(x, y, z; t). \tag{2.8}$$

Eq. (2.8) is called the (three-dimensional) *heat equation*.

Accordingly, we write down the (one-dimensional) heat equation by

$$u_t - a^2 u_{xx} = f(x; t), \tag{2.9}$$

and the (two-dimensional) heat equation by

$$u_t - a^2(u_{xx} + u_{yy}) = f(x, y; t). \tag{2.10}$$

2.1.2 Initial and Boundary Conditions

Initial and boundary conditions are also needed to complement the heat equation. When the domain of definition is the whole space of $\mathbb{R}^n$, the resulting PDE problem is known as a Cauchy problem. In this scenario, we simply need one initial condition, usually formulated through the initial temperature distribution, i.e.

$$u|_{t=0} = \phi(x, y, z). \tag{2.11}$$

This is in contrast with the case for the wave equation, where two pieces of initial conditions are necessary. A mathematical rationale to this is that the highest temporal derivative in the heat equation is of first order. Thus, one piece of information suffices to identify the physical process of interest.

When the domain of definition is bounded, boundary conditions are also necessary to define a problem for the heat equation. Similar as in the case for the wave equation, three types of boundary conditions can be imposed.

If the temperature distribution on the boundary is known, we have

$$u|_{\partial\Omega} = h(x, y, z, t), \tag{2.12}$$

which is the Dirichlet boundary condition. In particular, the homogeneous case with $h = 0$ corresponds to the situation where the temperature is uniform and stays invariant on the boundary. For instance, on an ice–water interface, the temperature is kept as the melting temperature.

If one manages to measure the heat flux across the domain boundary, then with reference to Fourier's law of heat conduction, we write

$$-k\frac{\partial u}{\partial n}\bigg|_{\partial\Omega} = h(x, y, z, t), \tag{2.13}$$

which is the Neumann boundary condition. In particular, the homogeneous case with $h = 0$ corresponds to the situation where the domain becomes *heat-insulated*.

A more practical situation is when the system of interest is surrounded by another medium. Then probably we do not know the exact temperature on the system boundary, but the environmental temperature. To set up the corresponding boundary condition, one should refer to *Newton's law of heat conduction*, i.e. the rate of heat units flowing across the interface separating the two media is proportional to the temperature difference across it. Mathematically, it is given by

$$\mathrm{d}Q = k_0(u - u_0)\mathrm{d}S\mathrm{d}t. \tag{2.14}$$

where k_0 is determined by the properties of the interface; u_0 is the environmental temperature. Combining Eq. (2.14) with Fourier's law of heat conduction (2.1) gives

$$\left(k\frac{\partial u}{\partial n} + k_0 u\right)\bigg|_{\partial\Omega} = k_0 u_0.$$

Rearranging the above identity expresses the corresponding Robin boundary condition by

$$\left(\frac{\partial u}{\partial n} + \sigma u\right)\bigg|_{\partial\Omega} = h(x, y, z, t). \tag{2.15}$$

2.1.3 Physical Analogies

In the end of this section, other physical processes that can be formulated through the heat equation are discussed. To this end, we consider the *diffusion* phenomena widely observed in nature, e.g. chemical elements spreading in air or water, point defects diffusing in crystalline materials. Although these phenomena arise with various physical backgrounds, the mathematical formulations of the underlying driving mechanisms see analogies. In order to maximise the "efficiency" of diffusion by nature, the transportation of the diffusing substances should take place along the direction in line with the negative spatial gradient of the substance concentration. In comparison with Fourier's law of heat conduction, we can introduce again the concept of substance flux denoted by $\mathbf{J}$, i.e.

$$\mathbf{J} = -D(x, y, z)\nabla c(x, y, z; t), \tag{2.16}$$

where c (mol per volume) represents the concentration distribution of the diffusing substances; D is called the *diffusivity* determined by the medium where diffusion takes place.

Within a bounded region Ω, the change in the substance units should be equal to the number of elements diffusing into it, added/subtracted by those generated/absorbed by internal sources/sinks, e.g. due to chemical reactions. The governing differential equation is thus established to be

$$\frac{\partial c}{\partial t} - \left(\frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(D\frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(D\frac{\partial c}{\partial z}\right)\right) = f(x, y, z). \tag{2.17}$$

Eq. (2.17) should also be coupled with certain initial and boundary conditions, which can be imposed in analogy with that discussed in Sect. 2.1.2. In particular, when the diffusivity D assumes constant values, Eq. (2.17) becomes the heat equation (2.7) with $D = a^2$.

To rationalise such a wide coverage over physical phenomena shown by the heat equation, one may refer to its underlying mechanism from a more microscopic viewpoint. The movement of individual particles/atoms is considered random, and their behaviour is usually treated as the *Brownian motion*. It says that a particle/atom randomly walks around a mean position in a probabilistic manner following certain normal distributions. Then the collective behaviour of such particles should be formulated by Eq. (2.17), and the diffusivity D is actually related to the variance of the associated normal distribution. To establish a more systematic linkage between the macroscopic diffusion behaviour and its underlying (microscopic) Brownian motion, one may refer to the topic of stochastic differential equation (e.g. [6]).

On the macroscopic level, however, the common feature shared by various physical processes that can be described by the heat equation is quite clear: the heat/substance transfer takes place along the direction in coincidence with the negative spatial gradient of the temperature/concentration of the elements.

2.2 Method of Integral Transform

In this section, we introduce the method of integral transform, an approach typically used for solving linear PDE problems defined in $\mathbb{R}^n$ or the half space. As an example, the Cauchy problem for the one-dimensional heat equation is considered:

$$\begin{cases} u_t - a^2 u_{xx} = f(x, t), \ \ (x, t) \in \mathbb{R} \times \mathbb{R}^+; \\ u|_{t=0} = \phi(x). \end{cases} \tag{2.18}$$

2.2.1 Convolution and Fourier Transform

In order to carry on with discussion over the method of integral transform, two types of related mathematical operations, convolution and Fourier transform, should be introduced in advance.

2.2.1.1 Convolution

Given two unary functions both of which are defined in the whole space of $\mathbb{R}$, their convolution, denoted by $f * g$, or $f * g(x)$, is defined to be

$$f * g = \int_{-\infty}^{\infty} f(x-t)g(t)\mathrm{d}t. \tag{2.19}$$

As Eq. (2.19) is defined through integration with respect to t, the convolution operation outputs another unary function (of x).

Example. Suppose

$$f(x) = \begin{cases} 1, & |x| \le 1; \\ 0, & |x| > 1, \end{cases} \quad g(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}.$$

Calculate $f * g$.

Solution. As the function f is defined piecewisely, $f(x-t)$ is nonzero only when $t-1 \le x \le t+1$, or equivalently when $x-1 \le t \le x+1$. Thus, incorporating the expressions of f and g into Eq. (2.19) gives

$$f * g = \frac{1}{\sqrt{2\pi}} \int_{x-1}^{x+1} e^{-\frac{t^2}{2}} \mathrm{d}t.$$

Note that $g(t)$ is actually the probability density function of the standard normal distribution. Thus, $f * g = P(x+1) - P(x-1)$, where $P(x)$ is the corresponding probability distribution function of the standard normal distribution. It is observed that upon convolution, $f * g$ becomes nonzero everywhere.

From this example, several characterising features of the convolution operation may be perceived. First, through its definition (2.18), one should quickly verify that $f * g = g * f$. Second, although $f(x)$ may not be continuous as shown by the example, its convolution with a continuous function $g(x)$ becomes a continuous function. In other words, the convolution operation outputs a function that is as smooth as the input function which is smoother. In fact, the convolution operation redefines a function,

e.g. the input function f, by getting its function values averaged in a weighted manner, and the weight is identified by the other input function $g(x)$.

The operation of convolution can be generalised to higher-dimensional cases. Suppose that $f(\mathbf{r})$ and $g(\mathbf{r})$ are functions both defined in $\mathbb{R}^n$. Their convolution is thus defined to be

$$f * g(\mathbf{r}) = \int_{\mathbb{R}^n} f(\mathbf{r} - \mathbf{s}) g(\mathbf{s}) \mathrm{d}\mathbf{s}. \tag{2.20}$$

It can be readily verified that the convolution operation in higher dimensions maintains all the properties as shown in the one-dimensional case.

2.2.1.2 Fourier Transform

For a given function $y = f(x)$ that is integrable over the whole space of $\mathbb{R}$, its *Fourier transform*, denoted by $\mathcal{F}[f]$ or $\tilde{f}$ in this book, is defined by

$$\mathcal{F}[f] = \int_{-\infty}^{\infty} f(x) e^{-\mathrm{i}x\xi} \, \mathrm{d}x = \tilde{f}(\xi), \tag{2.21}$$

where i is the imaginary unit with $\mathrm{i}^2 = -1$.

Equation (2.21) transforms a function (of x) to another function (of ξ). Note that the square brackets in Eq. (2.21) are adopted so as to indicate that the input argument of $\mathcal{F}$ is a function.

Actually, Fourier transform can be viewed as a limiting case of Fourier series, and their linkage is illustrated in the subsection about the prerequisite knowledge concluding this section. It can also be read from the prerequisite subsection that Fourier transform (2.21) can be reversed by

$$\mathcal{F}^{-1}[\tilde{f}] = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{f}(\xi) e^{\mathrm{i}x\xi} \mathrm{d}\xi = f(x), \tag{2.22}$$

which is known as the *inverse Fourier transform*.

In the following list several properties of Fourier transform that are quite useful for implementing the method of integral transform.

1. **Linearity**. If α and β are two complex numbers, and $f(x)$ and $g(x)$ are two integrable functions, then

$$\mathcal{F}[\alpha f + \beta g] = \alpha \mathcal{F}[f] + \beta \mathcal{F}[g]. \tag{2.23}$$

2. **Differentiation**

$$\mathcal{F}[f'] = \mathrm{i}\xi \mathcal{F}[f], \tag{2.24}$$

where f' denotes the first derivative of f. For its proof, knowledge on functions with complex input arguments is needed. Here one may "naively" treat the imaginary unit i as a simple real constant (although this is not always the case for calculating integrals with complex arguments). Thus we write

$$\mathcal{F}[f'] = f(x)\mathrm{e}^{-\mathrm{i}x\xi}\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} f(x)\,\mathrm{d}\mathrm{e}^{-\mathrm{i}x\xi} = \mathrm{i}\xi\int_{-\infty}^{\infty} f(x)\mathrm{e}^{-\mathrm{i}x\xi}\,\mathrm{d}x = \mathrm{i}\xi\mathcal{F}[f].$$

3. **In conjunction with convolution**. Upon Fourier transform, the convolution of two functions equals the product of the Fourier transforms of the two individual functions, i.e.

$$\mathcal{F}[f * g] = \mathcal{F}[f]\cdot\mathcal{F}[g]. \tag{2.25}$$

For its proof, we can replace the input of Eq. (2.21) by (2.19) and let $s = x - t$. Then we have

$$\begin{aligned}\mathcal{F}[f * g] &= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \mathrm{e}^{-\mathrm{i}x\xi} f(x-t)g(t)\mathrm{d}t\mathrm{d}x = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \mathrm{e}^{-\mathrm{i}(s+t)\xi} f(s)g(t)\mathrm{d}t\mathrm{d}s \\ &= \int_{-\infty}^{+\infty} \mathrm{e}^{-\mathrm{i}s\xi} f(s)\mathrm{d}s \cdot \int_{-\infty}^{+\infty} \mathrm{e}^{-\mathrm{i}t\xi} g(t)\mathrm{d}t = \mathcal{F}[f]\cdot\mathcal{F}[g].\end{aligned}$$

Fourier transform can be similarly defined for high-dimensional cases. To this end, we define

$$\mathcal{F}[f] = \int_{\mathbb{R}^n} f(\mathbf{r})\mathrm{e}^{-\mathrm{i}\mathbf{r}\cdot\boldsymbol{\xi}}\,\mathrm{d}\mathbf{r} = \tilde{f}(\boldsymbol{\xi}), \tag{2.26}$$

where $\mathbf{r}\cdot\boldsymbol{\xi}$ denotes the inner product of two n-dimensional vectors. The corresponding inverse Fourier transform is given by

$$\mathcal{F}^{-1}[\tilde{f}] = \frac{1}{(2\pi)^n}\int_{\mathbb{R}^n} \tilde{f}(\boldsymbol{\xi})e^{\mathrm{i}\mathbf{r}\cdot\boldsymbol{\xi}}\mathrm{d}\xi = f(\mathbf{r}). \tag{2.27}$$

The (inverse) Fourier transforms of certain functions are listed in Table 2.2.

Note that the aforementioned three properties also see their generalisations in higher dimensions. In particular, the second property formulated through Eq. (2.24) should be generalised to the case with partial differentiation, i.e.

$$\mathcal{F}\left[\frac{\partial f}{\partial r_i}\right] = \mathrm{i}\xi_i\mathcal{F}[f] \tag{2.28}$$

hold for all indices $i = 1, \ldots, n$.

Fourier transform (2.21) is defined by means of *integral transform*, which takes a general form of

$$\mathcal{T}\left[f\right](\xi) = \int_{\mathcal{A}} f(x)K(x;\xi)\,\mathrm{d}x, \tag{2.29}$$

where $K(x;\xi)$ is a (possibly complex) function known as the *kernel* function; $\mathcal{A}$ represents the domain of integration. For Fourier transform, $K(x;\xi) = \mathrm{e}^{-\mathrm{i}x\xi}$ and $\mathcal{A} = \mathbb{R}$.

The general form given by Eq. (2.29) serves to be the backbone of the method of integral transform, as it has several attractive features which can help reduce the complexity of a linear PDE. For instance, as from the second property mentioned above, Fourier transform turns the differentiation operation into a function product. Hence, one may use Fourier transform to turn a linear PDE into an ODE, and this will be discussed in greater detail in the next subsection.

As another important type of integral transform, *Laplace transform* is defined by

$$\mathcal{H}\left[f\right](\xi) = \int_{0}^{\infty} f(x)\mathrm{e}^{-\mathrm{i}x\xi}\,\mathrm{d}x. \tag{2.30}$$

A comparison between Eqs. (2.29) and (2.30) suggests that $K(x;\xi) = \mathrm{e}^{-\mathrm{i}x\xi}$ and $\mathcal{A} = \mathbb{R}^+$ for Laplace transform.

Laplace transform exhibits many attractive features that are similar as that of Fourier transform, partly because they share a same kernel function $K(x;\xi) = \mathrm{e}^{-\mathrm{i}x\xi}$. Laplace transform is widely used for solving linear PDE problems defined in the half space $\mathbb{R}^+$. But the associated method of integral transform involves intensive use of operations over functions with complex input arguments. Hence, further discussion on Laplace equation is not included in this book.

2.2.2 Solution for Cauchy Problems

Now we consider the situation where the governing equation is homogeneous, and the Cauchy problem of our interest becomes

$$\begin{cases} u_t - a^2 u_{xx} = 0, \ (x,t) \in \mathbb{R} \times \mathbb{R}^+; \\ u|_{t=0} = \phi(x). \end{cases} \tag{2.31}$$

For its solution, the method of integral transform can be implemented as follows.

First, we apply Fourier transform with respect to x on the governing equation of problem (2.31), leading to

$$\mathcal{F}[u_t] - a^2\mathcal{F}[u_{xx}] = 0, \tag{2.32}$$

where the linearity property of Fourier transform, which is indicated by Eq. (2.23), can be used.

Then with the differentiation rule for Fourier transform given by Eq. (2.24), Eq. (2.32) is rewritten by

$$\mathcal{F}[u_t] + a^2\xi^2\mathcal{F}[u] = 0.$$

As Fourier transform is applied only with respect to the spatial variable x, $\mathcal{F}[u_t] = \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}[u]$. Thus, we obtain

$$\frac{\mathrm{d}\mathcal{F}[u]}{\mathrm{d}t} + a^2\xi^2\mathcal{F}[u] = 0. \tag{2.33}$$

Fourier transform is also applied to the initial condition of problem (2.32), giving rise to

$$\mathcal{F}[u]|_{t=0} = \mathcal{F}[\phi](\xi). \tag{2.34}$$

Upon Fourier transform, the homogeneous heat equation is transformed into an ordinary differential equation (for $\mathcal{F}[u]$) in t, with Eq. (2.34) as its initial condition. And the variable ξ introduced by Fourier transform now simply serves as a parameter. Solving this ODE problem gives

$$\mathcal{F}[u] = \mathcal{F}[\phi](\xi) \cdot e^{-a^2\xi^2 t}. \tag{2.35}$$

Note that the right side of Eq. (2.35) is a product. We refer to the third property of Fourier transform mentioned above, which is given by Eq. (2.25). Suppose that the solution u can be expressed in a convolution form, say, $u = \phi * h$. If one manages to find the inverse Fourier transform of the second factor of Eq. (2.35), i.e.

$$\mathcal{F}^{-1}[e^{-a^2\xi^2 t}] = h(x, t), \tag{2.36}$$

one can use Eq. (2.25) to rewrite (2.35) by

$$\mathcal{F}[u] = \mathcal{F}[\phi * h] = \mathcal{F}[\phi]\mathcal{F}[h]. \tag{2.37}$$

Naturally, the solution $u(x, t)$ is calculated by

$$u(x, t) = \phi * h = \int_{-\infty}^{\infty} \phi(s)h(x - s, t)\mathrm{d}s, \tag{2.38}$$

where the definition of convolution by Eq. (2.19) has been used.

Therefore, in order to fully calculate $u(x, t)$, the expression for $h(x, t)$ defined by Eq. (2.36) is desired. Note that calculating the inverse Fourier transform of a function is generally not a trivial task, because it often involves evaluation of integrals with respect to arguments assuming complex values. Thus, detailed procedure for calculating $h(x, t)$ is not discussed here. But one may refer to Table 2.2 to write

$$h(x,t) = \mathcal{F}^{-1}[e^{-a^2\xi^2 t}] = \frac{1}{2a\sqrt{\pi t}} e^{-\frac{x^2}{4a^2 t}},$$

which is just the probability density function corresponding to the normal distribution with zero expectation and variance $2a^2 t$. Incorporating the expression for h into Eq. (2.38) finally expresses the solution for problem (2.31), that is,

$$u(x,t) = \frac{1}{2a\sqrt{\pi t}} \int_{-\infty}^{\infty} \phi(s) \mathrm{e}^{-\frac{(x-s)^2}{4a^2 t}} \mathrm{d}s. \tag{2.39}$$

To verify that Eq. (2.39) is actually the solution for problem (2.31), the following two issues should be taken into consideration.

First, we must ensure that $u(x,t)$ by Eq. (2.39) is well defined for all $x \in \mathbb{R}, t > 0$. In other words, the integral given by Eq. (2.39) needs to be uniformly convergent for any $(x,t) \in \mathbb{R} \times \mathbb{R}^+$. This is actually the case, provided that the function $\phi(x)$ is bounded. Mathematically, if $|\phi(x)| \leq M < +\infty$, then

$$|u(x,t)| \leq M \cdot \frac{1}{2a\sqrt{\pi t}} \int_{-\infty}^{\infty} \mathrm{e}^{-\frac{(x-s)^2}{4a^2 t}} \mathrm{d}s = M.$$

As the output of Eq. (2.39) is uniformly bounded by a finite number M, the integral appearing in Eq. (2.39) is thus uniformly convergent for all $(x,t) \in \mathbb{R} \times \mathbb{R}^+$, i.e. $u(x,t)$ by Eq. (2.39) is well defined.

Second, one needs to verify that $u(x,t)$ of Eq. (2.39) satisfies problem (2.31). Two steps are taken. Firstly, since the integral given by Eq. (2.39) is uniformly convergent in the domain of definition, the sequence of applying integration and differentiation on it is interchangeable. Then, it can be readily checked that Eq. (2.39) satisfies the homogeneous (spatially one-dimensional) heat equation. Secondly, one is also required to check Eq. (2.39) with the initial condition. It is worth nothing that one cannot simply let $t = 0$ in Eq. (2.39), as t serves to be a factor in the denominator. Checking of the initial condition should be carried out through a limiting process, i.e.

$$\lim_{t \to 0^+} u(x,t) = \phi(x),$$

and its proof is omitted here.

Through the derivations for the solution expression (2.39), one may perceive how the method of integral transform works. Upon proper integral transform, the governing PDE can be transformed into a parameterised ODE, e.g. with Eq. (2.33). The solution for the resulting ODE problem is likely expressed in the form of a product, e.g. Eq. (2.35). If the inverse integral transforms of the functions (constituting the product) are both expressible, the solution to the original linear PDE problem should be expressed in a convolution form.

The method of integral transform is generalisable for solving Cauchy problems for the high-dimensional heat equation, e.g.

$$\begin{cases} u_t - a^2(u_{xx} + u_{yy} + u_{zz}) = 0, \ (x, y, z) \in \mathbb{R}^3, t > 0; \\ u|_{t=0} = \phi(x, y, z). \end{cases} \tag{2.40}$$

Without presenting derivation details, the expression of the solution for problem (2.40) is given by

$$u(x, y, z; t) = \frac{1}{(2a\sqrt{\pi t})^3} \iiint\limits_{\mathbb{R}^3} \phi(s_1, s_2, s_3) \mathrm{e}^{-\frac{(x-s_1)^2+(y-s_2)^2+(z-s_3)^2}{4a^2 t}} \mathrm{d}s_1 \mathrm{d}s_2 \mathrm{d}s_3. \tag{2.41}$$

2.2.3 Solution Properties

To reveal the solution properties of Cauchy problem (2.31), we set the initial condition to be

$$\phi(x) = \begin{cases} 1, & 0 < x < 1; \\ 0, & \text{elsewhere}. \end{cases}$$

It says that initially the whole space of $\mathbb{R}$ is divided into two regions. The interval $(0, 1)$ corresponds to an initially high-temperature region.

Inserting this initial condition into Eq. (2.39) indicates that the successive temperature distribution should evolve as

$$u(x, t) = \frac{1}{2a\sqrt{\pi t}} \int_0^1 \mathrm{e}^{-\frac{(x-s)^2}{4a^2 t}} \mathrm{d}s. \tag{2.42}$$

Letting $a = 0.2$ in Eq. (2.42), the temperature profiles at various time slots are shown in Fig. 2.2. It can be observed that the temperature in the initially high-temperature region $[0, 1]$ keeps dropping, as it transmits heat elsewhere. As time evolves, the temperature of the whole region tends to uniformly zero. This is because the excessive but finite amount of heat initially maintained in the interval $[0, 1]$ is not sufficient to bring about considerable temperature change in an infinitely large domain.

Then, we examine the domain of influence of the initial condition for the heat equation. It is known from the discussion in Sect. 1.4.3 that, for physical processes described by the wave equation, the information (carried by the unknown function u) propagates at a finite speed, which can be captured by introducing the concept of wave fronts, i.e. for an initial point source, at any time t, there always exists a position, beyond which the initial point source cast no influence in the function value

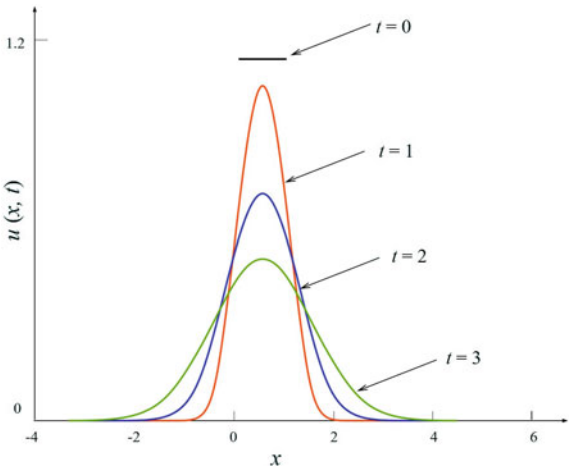

Fig. 2.2 Evolution of the temperature distribution suggested by Eq. (2.42) with $a = 0.2$

of u. As for the case with the heat equation, we see from Eq. (2.42) that $u(x, t) > 0$ for any $t > 0$ and any $x \in \mathbb{R}$. This implies that the initial temperature at one point affects the temperature distribution throughout the whole space at any time. In other words, the speed of heat transfer formulated through the heat equation is unlimited.

Apparently, the speed of heat transfer is limited in practice. The reason behind is that Fourier's law of heat conduction offers a first-order approximation to the actual situation, and inclusion of higher-order correction terms in it should "limit" the speed of heat conduction. Despite such a conceptually unphysical feature, the heat equation still offers a reasonable approximation to the actual situation with a sufficiently high degree of accuracy for engineering applications. Take Eq. (2.42) as an example. Although $u(x, t)$ is nonzero as $x \to \infty$, the amount of temperature rise is exponentially small. Hence, the function values of $u(x, t)$ vanish numerically.

Note that such trade-off between modelling accuracies and solution analyticity is ubiquitously seen when PDEs are applied to analyse real-world problems.

The condition that validates Eq. (2.39) is that the initial condition $\phi(x)$ is integrable in $\mathbb{R}$. But as suggested by Eq. (2.42), this means the initially stored amount of heat that can be used to bring about a considerable temperature change throughout the whole space is finite. As a result, the solution by Eq. (2.39) should always tend to a state of being uniformly zero. Actually, it can be shown that as $t \to \infty$,

$$|u(x, t)| \leq Ct^{-\frac{1}{2}}, \tag{2.43}$$

where $C > 0$ is a coefficient whose upper bound is fully determined by ϕ. Equation (2.43) identifies the asymptotic behaviour of the system described by problem (2.31) as $t \to \infty$. It suggests that the (maximum) system temperature drops to 0, roughly at a rate of $t^{-\frac{1}{2}}$, as $t \to \infty$.

2.2.4 Inhomogeneous Governing Equations

Finally, we consider the case where the governing equation becomes inhomogeneous, i.e.

$$\begin{cases} u_t - a^2 u_{xx} = f(x,t), \ \ (x,t) \in \mathbb{R} \times \mathbb{R}^+; \\ u|_{t=0} = 0. \end{cases} \tag{2.44}$$

In this case, the corresponding Duhamel's principle for the Cauchy problem governed by the inhomogeneous heat equation reads as follows.

Duhamel's principle. The solution for problem (2.44) can be expressed by

$$u(x,t) = \int_0^t W(x,t;\tau)\mathrm{d}\tau, \tag{2.45}$$

where the parameterised function $W(x,t;\tau)$ satisfies

$$\begin{cases} W_t - a^2 W_{xx} = 0, \ \ x \in \mathbb{R}, \ t > \tau; \\ W|_{t=\tau} = f(x,\tau). \qquad \square \end{cases} \tag{2.46}$$

With reference to Eq. (2.39), problem (2.46) can be solved by

$$W(x,t;\tau) = \frac{1}{2a\sqrt{\pi(t-\tau)}} \int_{-\infty}^{+\infty} f(s,\tau)\mathrm{e}^{-\frac{(x-s)^2}{4a^2(t-\tau)}}\mathrm{d}s. \tag{2.47}$$

Inserting it into Eq. (2.45), we express the solution for problem (2.44) by

$$u(x,t) = \frac{1}{2a\sqrt{\pi}} \int_0^t \int_{-\infty}^{+\infty} \frac{f(s,\tau)}{t-\tau} e^{-\frac{(x-s)^2}{4a^2(t-\tau)}}\,\mathrm{d}s\mathrm{d}\tau. \tag{2.48}$$

Prerequisite knowledge

Relating Fourier transform to Fourier series

Fourier transform (2.21) can be understood from a viewpoint of Fourier series. Given a function $f(x)$ which is periodic in $(-l, l)$, its Fourier series is written by

$$f(x) = \frac{a_0}{2} + \sum_{k=1}^{\infty} a_k \cos\frac{k\pi x}{l} + b_k \sin\frac{k\pi x}{l}, \tag{2.49}$$

where

$$a_k = \frac{1}{l}\int_{-l}^{l} f(s)\cos\frac{k\pi s}{l}\mathrm{d}s,\ k = 0, 1, \ldots; \tag{2.50a}$$

$$b_k = \frac{1}{l}\int_{-l}^{l} f(s)\sin\frac{k\pi s}{l}\mathrm{d}s,\ k = 1, 2, \ldots. \tag{2.50b}$$

Incorporating Eq. (2.50) into (2.49), we have

$$\begin{aligned} f(x) &\sim \frac{a_0}{2} + \frac{1}{l}\sum_{k=1}^{\infty}\int_{-l}^{l} f(s)\left(\cos\frac{k\pi s}{l}\cos\frac{k\pi x}{l} + \sin\frac{k\pi s}{l}\sin\frac{k\pi x}{l}\right)\mathrm{d}s \\ &\sim \frac{1}{2l}\int_{-l}^{l} f(s)\mathrm{d}s + \sum_{k=1}^{\infty}\int_{-l}^{l} f(s)\cos\frac{k\pi(s-x)}{l}\mathrm{d}s. \end{aligned} \tag{2.51}$$

Now we consider the case as $l \to \infty$. Note that $\int_{-l}^{l} f(s)\mathrm{d}s$ is a finite number. Then as $l \to \infty$, the first term in Eq. (2.51) should tend to 0. Now let $\frac{k\pi}{l} = \xi_k$ and $\frac{\pi}{l} = \Delta\xi$ (with $\Delta\xi \to 0$). Equation (2.51) is thus rewritten by

$$f(x) \sim \lim_{\Delta\xi\to 0}\frac{\Delta\xi}{\pi}\sum_{k=1}^{\infty}\int_{-\infty}^{+\infty} f(s)\cos\left[\xi_k(s-x)\right]\mathrm{d}s. \tag{2.52}$$

The right side of Eq. (2.52) is expressed by means of a (Riemman) summation of infinitely many terms, which can be approximated by an integral. To be more precise, the semi-infinitely long interval of $\xi \in (0, \infty)$ can be divided into infinitely many intervals of length $\Delta\xi$. In the kth interval, $f(\xi_k)$ is chosen to represent the function value within it. Hence, the summation is approximated by an integral through

$$\begin{aligned} f(x) &= \frac{1}{\pi}\int_{0}^{+\infty}\int_{-\infty}^{+\infty} f(s)\cos\left[\xi(s-x)\right]\mathrm{d}s\mathrm{d}\xi \\ &= \frac{1}{2\pi}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} f(s)\cos\left[\xi(s-x)\right]\mathrm{d}s\mathrm{d}\xi, \end{aligned}$$

where the last identity holds since $\cos\left[\xi(s-x)\right]$ is mirror-symmetric about $\xi = 0$.

Moreover, since $\sin[\xi(x-s)]$ is an odd function in ξ, its integration over $\xi \in (-\infty, +\infty)$ vanishes. Thus, the above identity is further re-written by

$$\begin{aligned} f(x) &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(s) \left(\cos\xi\,(s-x) - \mathrm{i}\sin\xi\,(s-x)\right) \mathrm{d}s\mathrm{d}\xi \\ &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{e}^{\mathrm{i}\xi x} \int_{-\infty}^{+\infty} f(s)\mathrm{e}^{-\mathrm{i}\xi s}\,\mathrm{d}s\mathrm{d}\xi. \end{aligned} \tag{2.53}$$

Now we let

$$\tilde{f}(\xi) = \int_{-\infty}^{+\infty} f(s)\mathrm{e}^{-\mathrm{i}\xi s}\,\mathrm{d}s.$$

A comparison between this expression of $\tilde{f}(\xi)$ and Eq. (2.21) suggests that $\tilde{f}(\xi)$ is just the Fourier transform of $f(x)$. Incorporating this expression for $\tilde{f}(\xi)$ into Eq. (2.53), we obtain

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{e}^{\mathrm{i}\xi x}\tilde{f}(\xi)\mathrm{d}\xi,$$

which effectively transforms $\tilde{f}(\xi)$ back to $f(x)$. This is just the definition for the inverse Fourier transform given by Eq. (2.22).

In Table 2.2 list the Fourier transforms of a number of widely used functions.

Table 2.2 Note that $\delta(\cdot)$ denotes the Dirac-δ function. For its rigorous definition, one may refer to an advanced textbook on PDEs, e.g. see Sect. 2.2.1 of Ref. [7]

$f(x)$	$\mathcal{F}[f](\xi)$
1	$\delta(\xi)$
$e^{-a\lvert x\rvert}, a > 0$	$\frac{2a}{a^2+\xi^2}$
$\cos(ax)$	$\pi\left[\delta(\xi-a)+\delta(\xi+a)\right]$
$\sin(ax)$	$\mathrm{i}\pi\left[\delta(\xi-a)+\delta(\xi+a)\right]$
$\frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{x^2}{2\sigma^2}}$	$e^{-\frac{\xi^2\sigma^2}{2}}$
$\frac{1}{x^2+a^2}, a \in \mathbb{R}\ \{0\}$	$-\frac{\pi}{a}e^{a\lvert\xi\rvert}$
$\delta(x)$	1

2.3 A Revisit to the Method of Separation of Variables

In this section, we extend the discussion on the method of separation of variables from Sect. 1.3. Here we are focused on solving an initial–boundary value problem for the heat equation given by

$$\begin{cases} u_t - a^2 u_{xx} = f(x,t), \ (x,t) \in (0,l) \times \mathbb{R}^+; \\ u|_{t=0} = \phi(x); \\ u|_{x=0} = \mu_1(t), \quad \left(\dfrac{\partial u}{\partial x} + hu\right)\Big|_{x=l} = \mu_2(t). \end{cases} \tag{2.54}$$

Apart from the governing equation, another key difference between the present one and problem (1.46) in Sect. 1.3 is from the boundary conditions. Here the situation with both Dirichlet and Robin boundary conditions is examined.

As in the case investigated in Sect. 1.3, it is expected to take three steps to solve problem (2.54). First, treatments of making the boundary conditions homogeneous should be taken. Since the procedure is quite similar as in Exercise 1.12, more details over this issue are omitted here. Then, the case with a homogeneous governing equation is examined with the use of the method of separation of variables. Finally, the corresponding Duhamel's principle is presented to resolve the problem where the governing equation becomes inhomogeneous. In the end of this section, we will introduce the concept of Sturm–Liouville system, which is quite useful for implementing the method separation of variables in more complicated situations.

2.3.1 An Example with the Heat Equation

Hence, we start with an initial–boundary value problem given by

$$\begin{cases} u_t - a^2 u_{xx} = 0, \ (x,t) \in (0,l) \times \mathbb{R}^+; \\ u|_{t=0} = \phi(x); \\ u|_{x=0} = 0, \quad \left(\dfrac{\partial u}{\partial x} + hu\right)\Big|_{x=l} = 0. \end{cases} \tag{2.55}$$

As a routine operation for applying the method of separation of variables, we look for solutions taking the form of

$$u(x,t) = X(x)T(t). \tag{2.56}$$

Inserting it into the heat equation, we have

$$\frac{T'}{a^2T} = \frac{X''}{X} = -\lambda,$$

where λ is a constant to be determined. Thus, a pair of ODEs are established to be

$$T' + a^2\lambda T = 0; \tag{2.57a}$$

$$X'' + \lambda X = 0. \tag{2.57b}$$

Combining Eq. (2.57b) with the homogeneous boundary conditions gives an eigenvalue problem of

$$\begin{cases} X'' + \lambda X = 0, \ x \in (0, l); \\ X|_{x=0} = 0, \ \left(X' + hX\right)\Big|_{x=l} = 0. \end{cases} \tag{2.58}$$

The expression for $X(x)$, as discussed in Sect. 1.3, depends on the sign of λ. It can be readily verified that when $\lambda < 0$, problem (2.58) only yields trivial solutions, i.e. $X \equiv 0$.

When $\lambda = 0$, the general solution to ODE (2.57b) is $X(x) = A + Bx$, with A and B two constants to be determined. Then inserting the boundary conditions into it, we end up with only trivial solutions, i.e. $A = B = 0$, too, given that $h > 0$.

As for $\lambda > 0$, the general solution to ODE (2.57b) becomes

$$X(x) = A\cos\sqrt{\lambda}x + B\sin\sqrt{\lambda}x.$$

Letting $x = 0$ and using the boundary condition at $x = 0$ give $A = 0$. Inserting the other boundary condition into the general solution, we derive

$$B\left(\sqrt{\lambda}\cos\sqrt{\lambda}l + h\sin\sqrt{\lambda}l\right) = 0. \tag{2.59}$$

In order to get a non-trivial solution, the term in the brackets of Eq. (2.59) should vanish. This establishes an equation for the eigenvalue λ:

$$\tan\sqrt{\lambda}l = -\frac{\sqrt{\lambda}}{h}. \tag{2.60}$$

One may further introduce $z = \sqrt{\lambda}$ to slightly simplify Eq. (2.60) to be

$$\tan zl = -\frac{z}{h}. \tag{2.61}$$

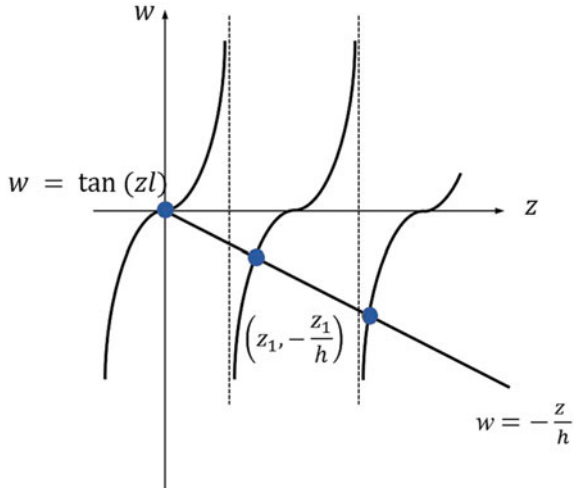

Fig. 2.3 A diagram indicating the solution properties of the transcendental equation (2.61)

Equation (2.61) is a transcendental equation for z, and it is difficult to analytically solve it. But an examination over the properties of the solutions for Eq. (2.61) should shed light on finding its approximate solutions via computer simulations, or simply its numerical solutions. To this end, a diagram is drawn as shown in Fig. 2.3. In the diagram, the solutions to Eq. (2.61) should correspond to the intersecting points of two sets of curves given by $w = \tan zl$ and $w = -z/h$, respectively.

Observation can be made in the following aspects:

- For $z > 0$, there are infinitely many intersecting points between the two sets of curves. If we use z_k, $k = 1, 2, \ldots$, to denote the z-value of the kth intersecting point, $z = z_1, z_2, \ldots$ all solve Eq. (2.61).
- In each period of $w = \tan zl$ with $z > 0$, there exists and only exists one z_k, i.e.

$$\left(k - \frac{1}{2}\right)\frac{\pi}{l} \le z_k \le \frac{k\pi}{l}. \tag{2.62}$$

- As k becomes large, z_k is expected to asymptote $\frac{(2k-1)\pi}{2l}$.

Albeit analytically intractable, z_k should be numerically computed, and its features outlined above should speed up the procedure of approximating z_k via computer simulation. For instance, once we know the bounds for z_k by Eq. (2.62), we can identify the range within which z_k is computed for.

Suppose that z_k are now available. Then, the eigenvalues of problems (2.60) can be calculated by $\lambda_k = z_k^2$, $k = 1, 2, \ldots$. And the corresponding eigenfunctions are also derived to be

$$X_k(x) = \sin\sqrt{\lambda_k}x, \quad k = 1, 2, \ldots. \tag{2.63}$$

The ODE for the temporal function $T(t)$ is solved in turn. On using $\lambda = \lambda_k$, Eq. (2.57a) becomes

$$T_k' + a^2 \lambda_k T_k = 0. \tag{2.64}$$

Its general solution is given by $T_k(t) = A_k e^{-a^2 \lambda_k t}$, where A_k are the coefficients to be determined.

The solution for problem (2.55) is thus expressed by means of a series given by

$$u(x, t) = \sum_{k=1}^{\infty} T_k(t) X_k(x) \sim \sum_{k=1}^{\infty} A_k e^{-a^2 \lambda_k t} \sin \sqrt{\lambda_k} x. \tag{2.65}$$

The validity of Eq. (2.65) relies on the fact that the series is uniformly convergent for $x \in (0, l)$ and $t > 0$, and its proof is omitted here.

To determine the coefficients A_k, we insert Eq. (2.65) into the initial condition of problem (2.55), and obtain

$$\phi(x) = \sum_{k=1}^{\infty} A_k \sin \sqrt{\lambda_k} x. \tag{2.66}$$

One thing that makes the present case essentially different from that in Sect. 1.3 is the periods of the eigenfunctions defined by Eq. (2.63) are no longer half-integer times the size of the spatial domain l. As a result, the method based on Fourier series, as in Sect. 1.3, does not work here. Such an essential difference is caused by the presence of Robin boundary condition in problem (2.65).

Here we need to employ the concept of function orthogonality, whose key issues have already been summarised in Table 1.2.

To this end, we multiply Eq. (2.66) by $\sin \sqrt{\lambda_j} x$ and integrate the results over the interval $(0, l)$ to derive

$$\int_0^l \phi(x) \sin \sqrt{\lambda_j} x \mathrm{d}x = \sum_{k=1, k \neq j}^{\infty} A_k \int_0^l \sin \sqrt{\lambda_k} x \sin \sqrt{\lambda_j} x \, \mathrm{d}x + A_j \int_0^l \sin^2 \sqrt{\lambda_j} x \, \mathrm{d}x, \tag{2.67}$$

where the orders of integration and summation are interchanged, given the uniform convergence of the series defined by Eq. (2.66).

If one manages to verify that, for $k \neq j$,

$$\int_0^l \sin \sqrt{\lambda_k} x \sin \sqrt{\lambda_j} x \, \mathrm{d}x = 0 \tag{2.68}$$

always holds, then the summation on the right side of Eq. (2.67) should vanish. The jth coefficient A_j is naturally calculated by

$$A_j = \frac{1}{M_j} \int_0^l \phi(x) \sin \sqrt{\lambda_j} x \mathrm{d}x, \tag{2.69}$$

where M_j is termed as the modulus of the eigenfunction X_j, given by

$$M_j = \int_0^l \sin^2 \sqrt{\lambda_j} x \, \mathrm{d}x. \tag{2.70}$$

Now we seek to prove Eq. (2.68), that is, $\{X_k(x) = \sin \sqrt{\lambda_k} x, k = 1, 2, \ldots\}$ are mutually orthogonal for $x \in [0, l]$.

For any two given eigenfunctions, say, $X_k(x)$ and $X_j(x)$ with $k \neq j$, we refer to Eq. (2.58) and write

$$X_k'' + \lambda_k X_k = 0, \qquad X_j'' + \lambda_j X_j = 0.$$

Multiplying the first identity by $X_j(x)$ and integrating the results over $x \in (0, l)$, we have

$$\begin{aligned} 0 &= \int_0^l (X_j X_k'' + \lambda_k X_k X_j) \mathrm{d}x \\ &= X_j(l) X_k'(l) - X_j(0) X_k'(0) - \int_0^l X_j' X_k' \, \mathrm{d}x + \lambda_k \int_0^l X_k X_j \, \mathrm{d}x, \end{aligned}$$

where integration by part is used to derive the second identity. Similar treatments can be applied to the equation for X_j, and we should derive

$$X_j'(l) X_k(l) - X_j'(0) X_k(0) - \int_0^l X_j' X_k' \, \mathrm{d}x + \lambda_j \int_0^l X_k X_j \, \mathrm{d}x = 0$$

Subtracting the two identities results in

$$(\lambda_k - \lambda_j) \int_0^l X_k X_j \, \mathrm{d}x = (X_k(l) X_j'(l) - X_j(l) X_k'(l)) + \Big(X_j(0) X_k'(0) - X_k(0) X_j'(0) \Big). \tag{2.71}$$

On one hand, $X_j(0) = 0$ and $X_k(0) = 0$, as from the homogeneous Dirichlet boundary condition at $x = 0$. Consequently, the terms in the second brackets on the right side of Eq. (2.71) vanish. On the other hand, Robin boundary condition of problem (2.58) leads to

$$X_k(l)X_j'(l) = -hX_k(l)X_j(l) = X_j(l)X_k'(l),$$

implying that the terms in the first brackets on the right side of Eq. (2.71) also vanish. Then, we obtain

$$(\lambda_k - \lambda_j)\int_0^l X_k X_j \,\mathrm{d}x = 0.$$

When $k \neq j$, it is already shown through Fig. 2.3 that $\lambda_k \neq \lambda_j$. Thus dividing the identity above by $(\lambda_k - \lambda_j)$ finally proves Eq. (2.68). The formula for the coefficient A_j calculated based on Eq. (2.69) is thus validated.

For evaluating the modulus M_k given by Eq. (2.70) (by replacing j by k), we write

$$\begin{aligned} M_k &= \int_0^l \sin^2\sqrt{\lambda_k}x\mathrm{d}x = \frac{1}{2}\int_0^l 1 - \cos(2\sqrt{\lambda_k}x)\,\mathrm{d}x \\ &= \frac{l}{2} - \frac{\sin(2\sqrt{\lambda_k}l)}{4\sqrt{\lambda_k}} = \frac{l}{2} - \frac{1}{4\sqrt{\lambda_k}}\cdot\frac{2\tan\sqrt{\lambda_k}l}{1+\tan^2\sqrt{\lambda_k}l} \\ &= \frac{l}{2} + \frac{h}{2(h^2+\lambda_k)}, \end{aligned} \tag{2.72}$$

where Eq. (2.60), i.e. $\tan\sqrt{\lambda_k}l = -\sqrt{\lambda_k}/h$, has been used.

Therefore, the solution for problem (2.55) is finally expressed in a series form given by

$$u(x,t) = \sum_{k=1}^{\infty} A_k e^{-a^2\lambda_k t}\sin\sqrt{\lambda_k}x, \tag{2.73}$$

where

$$A_k = \frac{1}{M_k}\int_0^l \phi(x)\sin\sqrt{\lambda_k}x\mathrm{d}x \tag{2.74}$$

with the modulus M_k determined by Eq. (2.72)

With Eq. (2.73), we are enabled to predict the long-term behaviour of the physical phenomenon described by problem (2.55). It is not surprising to read from Eq. (2.73) that $u \to 0$ as $t \to \infty$. This is because on one hand, zero temperature is maintained at the boundary of $x = 0$, and on the other hand, the medium stays in contact with a zero-temperature environment at $x = l$. As a result, the system temperature keeps rising/decreasing towards zero, as heat gets transmitted inward/outward the system until $u \equiv 0$.

Moreover, as $\lambda_1 < \lambda_2 < \cdots$, we have

$$|u(x,t)| \leq Ce^{-a^2\lambda_1 t},$$

as $t \to +\infty$, indicating that the system temperature tends to 0 at an exponential rate. This is faster than the case revealed by Eq. (2.48) for Cauchy problems defined within the whole space. It suggests that the presence of a cold object at the system boundary should be more effective in cooling down the system, if compared with the situation with infinitely large domain where heat dissipates naturally.

2.3.2 Sturm–Liouville System

With reference to the example for the heat equation here, as well as the initial–boundary value problem for the wave equation studied in Sect. 1.3, a general procedure for implementing the method of separation of variables can be summarised as follows.

1. Assume a variable-separated form (2.55), and the governing PDE (2.56) is then decomposed into several ODEs as given by (2.57a) and (2.57b).
2. Incorporate the spatial ODE with the homogeneous boundary conditions, and calculate the corresponding eigenvalues and eigenfunctions.
3. Solve the temporal equation (2.64) with the calculated eigenvalues.
4. Express the solution in a series form (2.65), and determine the involved coefficient [through Eq. (2.74)] using the properties of orthogonal functions [formulated by Eq. (2.68)].

A pivotal step when applying the method of separation of variables lies in the manipulation of the eigenvalues and the eigenfunctions. Interestingly, for the eigenfunctions obtained either with purely Dirichlet boundary conditions as in Sect. 1.3 or with Robin boundary conditions involved as it is here, they both form a set of orthogonal functions. This is in fact not a coincidence, but a property shared by eigenfunctions calculated from a Sturm–Liouville system.

Inner product

Before explaining the behaviour of a Sturm–Liouville system, we formally introduce the generalised concept of *inner product* of functions. For any two real functions, say, $f(x)$ and $g(x)$ belonging to a space consisting of certain functions, their inner product over the interval $x \in (a, b)$ with the *weighting function* $w(x) > 0$ is defined by

$$\langle f, g \rangle = \int_a^b f(x) g(x) w(x) \, \mathrm{d}x. \tag{2.75}$$

Note that the positive definiteness of the weighting function $w(x)$ over the interval $x \in (a, b)$ is crucial. When $\langle f, g \rangle = 0$, the two functions are said to be *orthogonal* about the inner product (2.75).

Sturm–Liouville equation

To this end, we consider a second-order linear ODE for the unknown $y = y(x)$, given by

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(k(x)\frac{\mathrm{d}y}{\mathrm{d}x}\right) - q(x)y(x) + \lambda\rho(x)y(x) = 0,\ x \in (a, b), \tag{2.76}$$

where the given functions satisfy $k(x) > 0, q(x) \geq 0, \rho(x) > 0$ for all $x \in (a, b)$; λ is a parameter actually representing the eigenvalue of the resulting ODE problem. Here Eq. (2.76) (with the sign requirement on the known functions satisfied) is termed as a *Sturm–Liouville equation*. A first glance at Sturm–Liouville equation (2.76) suggests that it identifies a family of second-order linear and homogeneous ODEs (parameterised by λ).

For a Sturm–Liouville equation, as defined by Eq. (2.76), it is naturally associated with an inner product defined by Eq. (2.75), where the weighting function $w(x)$ is now specified to be $\rho(x)$ from Eq. (2.76), i.e.

$$\langle f, g\rangle = \int_a^b \rho(x)f(x)g(x)\,\mathrm{d}x. \tag{2.77}$$

Boundary conditions

In order to define an ODE problem, boundary conditions at $x = a$ and $x = b$ may be needed. But whether a boundary condition should be imposed, e.g. at $x = a$, is actually determined by the value of $k(x)$ there.

If $k(a) = 0$, then no boundary conditions need to be declared, but we just require the function value be finite there, i.e.

$$|y(a)| < \infty, \qquad \text{when } k(a) = 0, \tag{2.78}$$

which is known as a *natural boundary condition*. In order to rationalise natural boundary conditions, we interpret Eq. (2.76) as a spring system, where $k(x)$ measures the spring stiffness at x. When $k(x) = 0$, the spring loses its stiffness, and any imposed load should induce an infinite displacement. Thus the most "natural" way to identify the behaviour at the boundary with $k = 0$ is to leave it as it is.

In contrast, if $k(a) > 0$, for example, then a boundary condition should be imposed at $x = a$, i.e.

$$\left[\sigma y(x) + hy'(x)\right]\Big|_{x=a} = 0, \qquad \text{when } k(a) > 0. \tag{2.79}$$

Note that Eq. (2.79) is expressed with Robin boundary condition, where Dirichlet and Neumann boundary conditions are also in consideration as its spatial cases. Similar situation also applies for the boundary at $x = b$.

Sturm–Liouville system

A Sturm–Liouville equation (2.76), along with boundary conditions (2.78) or (2.79), defines a *Sturm–Liouville system*.

Checking with its definition, the ODE problem (2.58) is effectively a Sturm–Liouville system. The governing ODE of problem (2.58), as compared with Eq. (2.76), is a Sturm–Liouville equation, where $k = 1 > 0$, $q = 0$, and $\rho = 1 > 0$. Besides, with $k = 1 > 0$ at both boundaries of $x = 0$ and $x = l$, boundary conditions are necessary at both ends in order to determine the corresponding eigenvalue problem. Then an inner product, as from Eq. (2.77) with $\rho(x) = 1$, can be introduced as

$$\langle f\,,\ g\rangle = \int_0^l f(x)g(x)\,\mathrm{d}x.$$

Example 2.1 Show that

$$x\frac{\mathrm{d}^2y}{\mathrm{d}x^2} + \frac{\mathrm{d}y}{\mathrm{d}x} + \left(\lambda x - \frac{1}{x}\right)y = 0, \quad x \in (0, 1), \tag{2.80}$$

is a Sturm–Liouville equation, and write down the inner product associated with it. Indicate what types of boundary conditions should be given at the two ends.

Solution. Expanding the first term of Sturm–Liouville equation (2.76) gives

$$k(x)\frac{\mathrm{d}^2y}{\mathrm{d}x^2} + k'(x)\frac{\mathrm{d}y}{\mathrm{d}x} - q(x)y(x) + \lambda\rho(x)y(x) = 0. \tag{2.81}$$

It implies that for a second-order linear and homogeneous ODE, if the derivative of the coefficient of its second derivative term coincides with the coefficient for its first derivative term, the ODE can be reformulated in the form of Eq. (2.81). This is just the case for Eq. (2.80). Hence, $k(x) = x$, Eq. (2.80) can be reformulated by

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(x\frac{\mathrm{d}y}{\mathrm{d}x}\right) - \frac{y}{x} + \lambda xy = 0, \quad x \in (0, 1). \tag{2.82}$$

A comparison with Eq. (2.76) and checking with the signs give

$$k(x) = x > 0, \quad q(x) = \frac{1}{x} > 0, \quad \rho(x) = x,$$

for $x \in (0, 1)$. A further comparison with Eq. (2.77) introduces its associated inner product given by

$$\langle f\,,\ g\rangle = \int_0^1 xf(x)g(x)\,\mathrm{d}x.$$

As for the system boundary conditions, we simply require y to be bounded at $x = 0$, because $k(x)$ vanishes there. At the other end, $k(1) = 1 > 0$. Hence, a boundary condition, as given by Eq. (2.79), should be imposed there. □

Example 2.2 Reformulate

$$y'' + xy' + \lambda y = 0, \quad x \in (-1, 1) \tag{2.83}$$

in the form of Sturm–Liouville equation (2.76). Write down the boundary conditions it should complement, as well as the inner product induced by it.

Solution. This time, the derivative coefficient for y'' is no longer equal to the coefficient for y'. Thus as it appears, Eq. (2.83) cannot be transformed to the form given by Sturm–Liouville equation (2.76). Now we multiply Eq. (2.83) by a function $\mu(x)$, and obtain

$$\mu(x)y'' + x\mu(x)y' + \lambda\mu(x)y = 0, \quad x \in (-1, 1). \tag{2.84}$$

If we require

$$\frac{\mathrm{d}\mu}{\mathrm{d}x} = x\mu(x), \tag{2.85}$$

Eq. (2.84) should be converted in coincidence with Eq. (2.76). Equation (2.85) is effectively an ODE which can be explicitly solved with

$$\mu(x) = \mathrm{e}^{\frac{x^2}{2}} \tag{2.86}$$

being one of its solutions.

With Eq. (2.86), Eq. (2.84) can be expressed in the form of Sturm–Liouville equation, i.e.

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\mathrm{e}^{\frac{x^2}{2}}\frac{\mathrm{d}y}{\mathrm{d}x}\right) + \lambda\mathrm{e}^{\frac{x^2}{2}}y = 0, \tag{2.87}$$

indicating that $k(x) = \mathrm{e}^{\frac{x^2}{2}}$, $q(x) = 0$ and $\rho(x) = \mathrm{e}^{\frac{x^2}{2}}$ as compared with Eq. (2.76).

As $k(x) > 0$ at both ends, two boundary conditions should be imposed for Eq. (2.87), and the inner product induced by Eq. (2.87) is

$$\langle f, g\rangle = \int_{-1}^{1} \mathrm{e}^{\frac{x^2}{2}} f(x)g(x)\,\mathrm{d}x. \quad \square$$

Conclusions from a Sturm–Liouville system The reason that a Sturm–Liouville system arises our interest is that it exhibits several attractive features summarised as follows.

1. **Existence of non-negative eigenvalues**. For a Sturm–Liouville system, there exist infinitely many non-negative eigenvalues, say,

$$0 \leq \lambda_1 < \lambda_2 < \cdots .$$

For each $\lambda = \lambda_k$, the Sturm–Liouville system yields a non-trivial solution, denoted by $y = y_k(x)$, which is the eigenfunction corresponding to the eigenvalue λ_k.

2. **Orthogonality**. When $k \neq m$, the corresponding eigenfunctions y_k and y_m are orthogonal about the inner product defined by Eq. (2.77), i.e.

$$\int_a^b \rho(x) y_k(x) y_m(x)\, \mathrm{d}x = 0. \tag{2.88}$$

3. **Completeness**. For any continuous function $f(x)$ with $x \in (a, b)$, which satisfies the corresponding boundary conditions, it can always be expressed as a linear combination of the (infinitely many) eigenfunctions, i.e.

$$f(x) = \sum_{k=1}^{\infty} A_k y_k(x), \tag{2.89}$$

where the coefficient A_k is given by

$$A_k = \frac{\int_a^b \rho(x) f(x) y_k(x)\, \mathrm{d}x}{\int_a^b \rho(x) (y_k(x))^2\, \mathrm{d}x}. \tag{2.90}$$

In summary, a Sturm–Liouville system should result in a set of non-positive eigenvalues, and further their corresponding eigenfunctions. These eigenfunctions naturally form a *complete set of orthogonal functions*, and the corresponding series, as define by Eq. (2.89), is termed as a *general orthogonal series*.

Most of the properties outlined above are not difficult to verify. Here we particularly present the proof for Eq. (2.88).

To this end, we suppose that λ_k and λ_m are two eigenvalues of the Sturm–Liouville system governed by Eq. (2.76), and $y_k(x)$ and $y_m(x)$ are their corresponding eigenfunctions, respectively, i.e.

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(k(x)\frac{\mathrm{d}y_k}{\mathrm{d}x}\right) - q(x) y_k(x) + \lambda_k \rho(x) y_k(x) = 0; \tag{2.91a}$$

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(k(x)\frac{\mathrm{d}y_m}{\mathrm{d}x}\right) - q(x) y_m(x) + \lambda_m \rho(x) y_m(x) = 0, \tag{2.91b}$$

for $x \in (a, b)$. Here without loss of generalities, a natural boundary condition is imposed on the left boundary, i.e. $k(a) = 0$. On the right boundary, $k(b) > 0$, and a boundary condition of

$$\left[\sigma y(x) + h y'(x)\right]\Big|_{x=b} = 0 \tag{2.92}$$

is imposed.

Now Eq. (2.91a) is multiplied by $y_m(x)$, and the result is then integrated over (a, b), i.e.

$$\begin{aligned} 0 &= \int_a^b y_m(x) \left(\frac{\mathrm{d}}{\mathrm{d}x} \left(k(x) \frac{\mathrm{d}y_k}{\mathrm{d}x} \right) - q(x) y_k(x) + \lambda_k \rho(x) y_k(x) \right) \mathrm{d}x \\ &= k(b) y_m(b) \left. \frac{\mathrm{d}y_k}{\mathrm{d}x} \right|_{x=b} - k(a) y_m(a) \left. \frac{\mathrm{d}y_k}{\mathrm{d}x} \right|_{x=a} \\ &\quad - \int_a^b \left(k(x) \frac{\mathrm{d}y_m}{\mathrm{d}x} \frac{\mathrm{d}y_k}{\mathrm{d}x} + q(x) y_k(x) y_m(x) \right) \mathrm{d}x + \lambda_k \int_a^b \rho(x) y_k(x) y_m(x) \, \mathrm{d}x, \end{aligned} \tag{2.93}$$

where integration by parts is used and two boundary terms are then generated. With $k(a) = 0$, the second term on the right side of Eq. (2.93) vanishes. On using boundary condition (2.92), Eq. (2.93) is finally rewritten by

$$\left. \frac{\sigma k y_m y_k}{h} \right|_{x=b} + \int_a^b \left(k(x) \frac{\mathrm{d}y_m}{\mathrm{d}x} \frac{\mathrm{d}y_k}{\mathrm{d}x} + q(x) y_k y_m \right) \mathrm{d}x = \lambda_k \int_a^b \rho(x) y_k(x) y_m(x) \, \mathrm{d}x. \tag{2.94}$$

On the other hand, one may multiply $y_k(x)$ by Eq. (2.91b) and integrate the result over (a, b) again. Repeating the same procedure as above, we obtain

$$\left. \frac{\sigma k y_m y_k}{h} \right|_{x=b} + \int_a^b \left(k(x) \frac{\mathrm{d}y_m}{\mathrm{d}x} \frac{\mathrm{d}y_k}{\mathrm{d}x} + q(x) y_k y_m \right) \mathrm{d}x = \lambda_m \int_a^b \rho(x) y_k(x) y_m(x) \, \mathrm{d}x. \tag{2.95}$$

Subtracting Eq. (2.94) by (2.95) gives

$$(\lambda_k - \lambda_m) \int_a^b \rho(x) y_k(x) y_m(x) \, \mathrm{d}x = 0. \tag{2.96}$$

With $\lambda_k \neq \lambda_m$, Eq. (2.88) is thus justified.

An example The above statements on Sturm–Liouville system and its properties are quite general. Now they are checked with the problem (2.58) presented in Sect. 2.3.1.

As discussed above problem (2.58) effectively identifies a Sturm–Liouville system. Thus, the following conclusions should hold.

1. As indicated by Fig. 2.3, there exist infinitely many positive eigenvalues $\{\lambda_k\}_{k=1}^{\infty}$, and their corresponding eigenfunctions are given by $X_k(x)$ defined by Eq. (2.63).
2. Letting $\rho(x) = 1$ in Eq. (2.88) (and replacing y_k and y_m by X_k and X_m, respectively) leads to Eq. (2.68), which just ensures that the eigenfunctions $\{X_k\}_{k=1}^{\infty}$ defined by Eq. (2.63) are mutually orthogonal.
3. As from Eq. (2.66), the initial condition $\phi(x)$ can be expressed as a general orthogonal series. The coefficients A_k are calculated as a quotient of inner products given by Eq. (2.74), which is a natural result of Eq. (2.89) with $\rho = 1$, $y_k = X_k$.

In fact, these properties summarised from Sturm–Liouville system form a theoretical basis for analysing the behaviour of the eigenfunctions that are needed for implementing the method of separation of variables. More of their applications can be found in Chaps. 5 and 6 of this book.

Mathematical analogies with orthogonal vectors in $\mathbb{R}^n$

In Sect. 1.3, a brief discussion on generalising the concept of orthogonality from Euclidean space to functional space has been made. Actually, a more comprehensive comparison between the two topics can be drawn, and the key issues are summarised in Table 2.3.

First of all, a linear transformation between $\mathbb{R}^n$ is represented through an n-by-n matrix. Comparatively, a linear differential operator $\mathcal{L}$, as defined in Sect. 1.1.3, represents a linear operation transforming a function (in a functional space, say, $\mathcal{H}$) to another.

For instance, one may define a linear differential operator by

$$\mathcal{L}[y(x)] = \frac{\mathrm{d}}{\mathrm{d}x}\left(k(x)\frac{\mathrm{d}y}{\mathrm{d}x}\right) - q(x)y(x). \tag{2.97}$$

With Eq. (2.97), Sturm–Liouville equation (2.76) can be simply re-written by

$$\mathcal{L}[y(x)] + \lambda\rho(x)y(x) = 0. \tag{2.98}$$

Table 2.3 A comparison between the properties induced by symmetric matrices and Sturm–Liouville system

	Euclidean space $\mathbb{R}^n$	Functional space $\mathcal{H}$
Elements	$\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$	$y(x), w(x) \in \mathcal{H}$
Linear operator	n-by-n matrix A	Differential operator $\mathcal{L}$
Symmetry in operation	$(\mathbf{v}, A\mathbf{u}) = (A\mathbf{v}, \mathbf{u})$	$\int_a^b w(x)\mathcal{L}[y(x)]\,\mathrm{d}x = \int_a^b y(x)\mathcal{L}[w(x)]\,\mathrm{d}x$
Eigenvalue problem	$A\mathbf{v} = \lambda\mathbf{v}$	$\mathcal{L}[y(x)] + \lambda\rho(x)y(x) = 0$
Eigenvector/function	Orthogonal, complete	Orthogonal, complete

Given an n-by-n matrix A, an eigenvalue problem should be introduced as $A\mathbf{u} = \lambda\mathbf{u}$. From this viewpoint, Eq. (2.98) also defines an eigenvalue problem induced by the linear operator $\mathcal{L}$. In particular, when the matrix A is symmetric and positively defined, it has n positive eigenvalues, and n corresponding eigenvectors, say, $\mathbf{v}^1, \mathbf{v}^2, \ldots, \mathbf{v}^n$. Moreover, the eigenvectors form an orthogonal basis, i.e. $(\mathbf{v}^j, \mathbf{v}^k) = 0$. Besides, for any ($n$-dimensional) vector $\mathbf{u}$, it can be calculated by a linear combination of these orthogonal basis, i.e. $\mathbf{u} = \sum_{k=1}^{n} a_k \mathbf{v}^k$, where $a_k = \frac{(\mathbf{u}, \mathbf{v}^k)}{(\mathbf{v}^k, \mathbf{v}^k)}$, as already summarised in Table 1.2.

From a comparative viewpoint, if a linear operator $\mathcal{L}$ is "positively defined" and "symmetric", the mentioned findings from linear algebra should see their counterparts for ODE eigenvalue problem induced by $\mathcal{L}[\cdot]$. As for Sturm–Liouville equation (2.76), the condition $k(x) > 0$ somehow indicates that the linear differential operator $\mathcal{L}[\cdot]$ is "positively defined".

Then we try to demonstrate the symmetry shown by the linear differential operator $\mathcal{L}[\cdot]$. Again, we refer to the properties of a symmetric matrix A. When A is symmetric, it satisfies

$$(\mathbf{v}, A\mathbf{u}) = (A\mathbf{v}, \mathbf{u}),$$

for any $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$. As discussed in Sect. 1.3, the concept of inner product on functional spaces is induced by an integral of the function product. Thus, one may say a linear operator is symmetric, if

$$\int_a^b w(x)\mathcal{L}[y(x)]\,\mathrm{d}x = \int_a^b y(x)\mathcal{L}[w(x)]\,\mathrm{d}x. \tag{2.99}$$

hold for any $y(x)$ and $w(x)$ belonging to the functional space $\mathcal{H}$. Note that a differential equation problem with a "symmetric" linear operator and the associated boundary conditions is called a *self-adjoint* problem. It can be verified that, with the use of integration by parts, Eq. (2.99) (for any $y(x), w(x) \in \mathcal{H}$) holds for the linear operator $\mathcal{L}[\cdot]$ defined by Eq. (2.97) (see Exercise 2.13 for details).

Two issues are noted with reference to a self-adjoint problem. First, the elements in the functional space $\mathcal{H}$ should conform to the boundary conditions imposed. In other words, $\mathcal{H}$ only contains functions that satisfy the imposed (homogeneous) boundary conditions. Second, Eq. (2.99) must hold for any pairs of functions in $\mathcal{H}$, not some of them.

2.3.3 Inhomogeneous Governing Equations

Based on the results compiled in Sect. 2.3.1, we carry on with studying the cases where the governing PDEs are inhomogeneous. To this end, we consider the initial–boundary value problem given by

$$\begin{cases} u_t - a^2 u_{xx} = f, \ (x,t) \in (0,l) \times \mathbb{R}^+; \\ u|_{t=0} = 0; \\ u|_{x=0} = 0, \quad \left(\dfrac{\partial u}{\partial x} + hu\right)\Big|_{x=l} = 0. \end{cases} \tag{2.100}$$

To this end, we introduce the corresponding Duhamel's principle.

Duhamel's principle. If $W(x,t;\tau)$ is a function of x and t, parameterised by τ, and it satisfies

$$\begin{cases} W_t - a^2 W_{xx} = 0, \ x \in (0,l), \ t > \tau; \\ W|_{t=\tau} = f(x,\tau); \\ W|_{x=0} = 0, \quad \left(\dfrac{\partial W}{\partial x} + hW\right)\Big|_{x=l} = 0, \end{cases} \tag{2.101}$$

then

$$u(x,t) = \int_0^t W(x,t;\tau)\mathrm{d}\tau \tag{2.102}$$

is a solution for problem (2.100). □

2.4 Solution Properties

In this section, the properties of solutions for initial–boundary value problems governed by the heat equation, such as uniqueness and stability, will be discussed, and the corresponding maximum principle will be introduced. The discussion will be focused on spatially one-dimensional problems, but the results should be generalised for analysing high-dimensional cases.

2.4.1 Maximum Principle

Consider a heat-conduction process within a bounded region in the absence of internal heat sources/sinks. Intuitively, the overall highest temperature point should happen only at one of the following two occasions: (a) the initially highest temperature position, because the temperature there should drop afterwards as heat is transferred away; (b) at a boundary point where external heat may flow into the system, and the on-site temperature is maintained at a high level. Mathematically, the time and position when and where the highest/lowest temperature takes place can be identified by the following maximum principle.

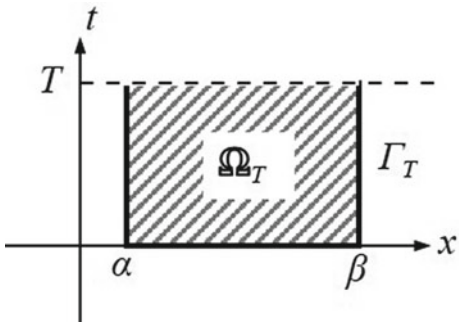

Fig. 2.4 The domain Ω_T employed to introduce the maximum principle for the heat equation

The *maximum principle*, or sometimes called the maximum–minimum value principle, for the heat equation can be stated as follows.

Suppose that $u(x, t)$ is a continuous function defined in a time–space domain $\Omega_T = \{\alpha \le x \le \beta, 0 \le t \le T\}$, as shown in Fig. 2.4, and it satisfies the heat equation

$$\frac{\partial u}{\partial t} - a^2 \frac{\partial^2 u}{\partial x^2} = 0. \tag{2.103}$$

If we further introduce Γ_T to collectively denote the two sides ($x = \alpha$, $x = \beta$) and the bottom line of Ω_T (as highlighted by the thick segments in Fig. 2.4), then the extreme values of u in Ω_T are the same as its extreme values on Γ_T. Mathematically, we write

$$\max_{\Omega_T} u(x, t) = \max_{\Gamma_T} u(x, t), \ \min_{\Omega_T} u(x, t) = \min_{\Gamma_T} u(x, t). \tag{2.104}$$

Here we simply mention the key idea underlying the proof of this maximum principle. First, if one manages to validate the first half of Eq. (2.104), i.e. the maximisation part, then the minimisation part should be validated readily. This is because if we replace $u(x, t)$ by $-u(x, t)$ in the theorem, $-u(x, t)$ still satisfies the heat equation, but the maximum value [of $-u(x, t)$] corresponds to the minimum value [of $u(x, t)$]. Therefore, we only seek to validate the first part of Eq. (2.104). This is also the reason why the term "maximum principle" also covers the cases for minimisation.

In fact, if $u(x, t)$ attains its maximum in the region of $\Omega_T \backslash \Gamma_T$, it must be one of the following two cases. Maximisation takes place either in the interior of Ω_T or at the boundary $t = T$. They should be examined separately.

If the maximisation of $u(x, t)$ takes place in the interior region of Ω_T, say, $(x^*, t^*) \in \Omega_T \backslash (\Gamma_T \cup \{t = T\})$, then the derivatives of u at (x^*, t^*) should "generally" satisfy

$$\left.\frac{\partial u}{\partial t}\right|_{(x^*,t^*)} \ge 0, \ \left.\frac{\partial u}{\partial x}\right|_{(x^*,t^*)} = 0, \ \left.\frac{\partial^2 u}{\partial x^2}\right|_{(x^*,t^*)} < 0. \tag{2.105}$$

The reason we employ the term "generally" here is because under certain circumstances, $u_{xx}|_{(x^*,t^*)} = 0$ may still hold for a local maximum point at (x^*, t^*). But this is

a far rarer occasion if compared with the case where $u_{xx}|_{(x^*,t^*)} < 0$. In the prerequisite knowledge subsection concluding this section, we give a comprehensive summary over the interrelationship between a point where maximisation takes place and the values/signs of the function derivatives evaluated at it.

With Eq. (2.105), one naturally concludes $(u_t - a^2 u_{xx})\big|_{(x^*,t^*)} > 0$, which contradicts the heat equation (2.103). Therefore, $u(x, t)$ should "generally" not be maximised at an interior point of Ω_T. A more rigorous proof over this issue should also cover the case with $u_{xx}|_{(x^*,t^*)} = 0$, and the detail is not discussed here.

On the other hand, when $u(x, t)$ is maximised at $x = x^*$ on the boundary where $t = T$. Also from the prerequisite knowledge subsection, $u_t|_{(x^*,T)} \geq 0$. Now as $u_{xx}|_{(x^*,T)} < 0$ still holds "generally", the heat equation is violated again. Therefore, u cannot be maximised on the boundary $t = T$ either.

The maximum principle here actually reveals the key diffusive feature of those phenomena governed by the heat equation. As heat being conducted, the spatial/temporal difference in temperature gets gradually smeared out, and a spatially uniform state (in the absence of external sources/sinks) is the final destination. Therefore, extreme values should not appear in a middle stage of the evolution towards that destination.

When there are internal heat sources, i.e. $u_t - a^2 u_{xx} = f$ with $f \geq 0$. From a physical viewpoint, the temperature may be maximised at a heat source, while the lowest temperature should still be observed on Γ_T, i.e. the second half of Eq. (2.104) still holds. Conversely when only internal heat sinks are at present, i.e. $f \leq 0$, the maximum case of Eq. (2.104) should still hold.

2.4.2 Solution Uniqueness

Equipped with the maximum principle above, we now discuss the solution uniqueness for problem (2.54). Again, we start with the situation where Dirichlet boundary conditions are imposed at both ends. Similar as the linear cases for the wave equation, we only need to show that the fully homogeneous problem given by

$$\begin{cases} u_t - a^2 u_{xx} = 0, \ (x, t) \in (a, b) \times \mathbb{R}^+; \\ u|_{t=0} = 0; \\ u|_{x=a} = 0, \quad u|_{x=b} = 0 \end{cases} \tag{2.106}$$

simply yields a trivial solution, i.e. $u \equiv 0$.

The proof is rather straight forward. As from the maximum principle, we know that

$$\max_{\Omega_T} u(x, t) = \max_{\Gamma_T} u(x, t) = 0.$$

Similarly, $\min_{\Omega_T} u(x, t) = \min_{\Gamma_T} u(x, t) = 0$. As a result, $u \equiv 0$. □

Now we consider the solution uniqueness for problem (2.54), where Robin boundary condition is imposed at one end. This time, the fully homogeneous problem of our interest is

$$\begin{cases} u_t - a^2 u_{xx} = 0, \ (x,t) \in (a,b) \times \mathbb{R}^+; \\ u|_{t=0} = 0; \\ u|_{x=a} = 0, \quad \left(\dfrac{\partial u}{\partial x} + hu\right)\Big|_{x=b} = 0, \quad h > 0, \end{cases} \tag{2.107}$$

and we will show that problem (2.107) only yields a trivial solution.

For its proof, we look at the maximum value of u first, and we are going to show that $\max_{\Omega_T} u = 0$. From the maximum principle, $\max_{\Omega_T}, u = \max_{\Gamma_T} u$. If $\max_{\Gamma_T} u$ is achieved initially ($t = 0$) or on the left boundary ($x = a$), we naturally conclude with $\max_{\Omega_T} u = 0$.

If the maximum value (which should be then positive) is attained on the right boundary $x = b$, say at $t = t^*$, then we assume $u|_{x=b,t=t^*} = \bar{u} > 0$. Since maximisation now takes place on the boundary, we also have $u_x|_{x=b,t=t^*} \geq 0$, as from the prerequisite subsection. Combining these results, we reach $(u_x + hu)|_{x=b,t=t^*} > 0$, which contradicts Robin boundary condition imposed at $x = b$ in problem (2.107). Hence, $u \leq 0$ holds for all $t > 0$ at $x = b$.

On the other hand, one can similarly show that $\min_{\Omega_T} u = 0$, i.e. $u \geq 0$. Thus, $u \equiv 0$, and the solution uniqueness is demonstrated. □

2.4.3 Stability

Finally, we consider the issue of solution stability concerning the heat equation. When small perturbations against the actual values (e.g. introduced through measurement) occur in initial/boundary conditions, an interesting question is how much the computed solution deviates from the actual solution. To examine the issue of solution stability, we here introduce two functions, $u^1(x,t)$ and $u^2(x,t)$, or collectively denoted by $u^{1,2}(x,t)$. Suppose that they satisfy

$$\begin{cases} u_t^{1,2} - a^2 u_{xx}^{1,2} = 0, \ (x,t) \in (a,b) \times \mathbb{R}^+; \\ u^{1,2}|_{t=0} = \phi^{1,2}; \\ u^{1,2}|_{x=a} = \mu_1^{1,2}(t), \quad u^{1,2}|_{x=b} = \mu_2^{1,2}(t), \end{cases} \tag{2.108}$$

respectively.

Here one may treat $u^1(x,t)$ as the actual temperature profile under the true initial and boundary conditions (formulated through ϕ^1, μ_1^1, μ_2^1). And ϕ^2, μ_1^2, μ_2^2 are the corresponding measured initial and boundary conditions, and $u^2(x,t)$ is the solution under these conditions.

Suppose that the largest deviation due to the measurements against the initial and boundary conditions is measured by ϵ. Then

$$\max\left\{\max_{a\le x\le b}|\phi^1-\phi^2|,\ \max_{t>0}|\mu_1^1-\mu_1^2|,\ \max_{t>0}|\mu_2^1-\mu_2^2|\right\}<\epsilon. \tag{2.109}$$

What we expect to estimate is the error of the temperature profile within the whole domain of Ω_T, which is formulated through $v=u^1-u^2$. Using Eq. (2.108), v should satisfy

$$\begin{cases} v_t-a^2v_{xx}=0,\ \ (x,t)\in(a,b)\times\mathbb{R}^+;\\ v|_{t=0}=\phi^1-\phi^2;\\ v|_{x=a}=\mu_1^1(t)-\mu_1^2(t),\quad v|_{x=b}=\mu_2^1(t)-\mu_2^2(t)\end{cases} \tag{2.110}$$

From the maximum principle

$$\max_{\Omega_T}=|u^1-u^2|=\max_{\Omega_T}|v(x,t)|=\max_{\Gamma_T}|v(x,t)|\le\epsilon$$

indicating that for an initial–boundary value problem for the heat equation, the derivation of the computed temperature from the actual case is no greater than the deviation caused by the measurements against the initial and boundary conditions.

Prerequisite knowledge

Finding the maxima of a function

Given a function, say $f(\mathbf{r})$, which is twice differentiable in a bounded domain $\Omega\subset\mathbb{R}^n$, $f(\mathbf{r}^*)$ is said to be a (local) maximum of $f(\mathbf{r})$, if $f(\mathbf{r})\le f(\mathbf{r}^*)$ for all $\mathbf{r}$ falling in a small neighbourhood of $\mathbf{r}^*$ inside Ω.

To facilitate our search for function maxima, the following two terms are mentioned in advance. The gradient of $f(\mathbf{r})$, denoted by ∇f, is an n-dimensional vector containing all the first partial derivatives of f, i.e.

$$\nabla f=\left(\frac{\partial f}{\partial r_1},\dots,\frac{\partial f}{\partial r_n}\right)^{\mathrm{T}}.$$

The Hessian matrix associated with f, denoted by $\mathbf{H}$ or $\nabla\otimes\nabla f$, is an n-by-n matrix sequentially containing all the second derivatives of f, i.e.

$$\mathbf{H}=\nabla\otimes\nabla f=\begin{pmatrix}\frac{\partial^2 f}{\partial r_1^2} & \frac{\partial^2 f}{\partial r_1\partial r_2} & \cdots & \frac{\partial^2 f}{\partial r_1\partial r_n}\\ \frac{\partial^2 f}{\partial r_1\partial r_2} & \frac{\partial^2 f}{\partial r_2^2} & \cdots & \frac{\partial^2 f}{\partial r_2\partial r_n}\\ \vdots & \cdots & \cdots & \vdots\\ \frac{\partial^2 f}{\partial r_1\partial r_n} & \frac{\partial^2 f}{\partial r_2\partial r_n} & \cdots & \frac{\partial^2 f}{\partial r_n^2}\end{pmatrix}.$$

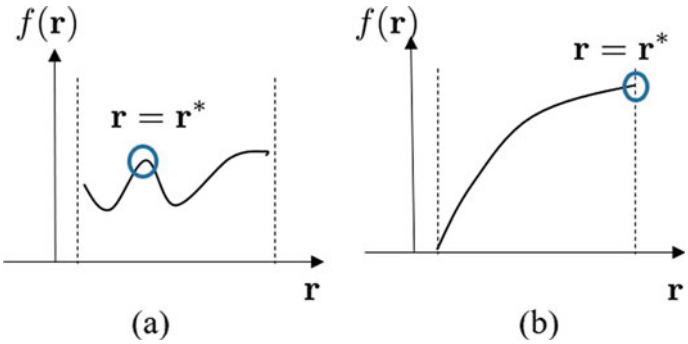

Fig. 2.5 Given a bounded region, a function may be maximised **a** at an interior point; **b** at a boundary point

Given a bounded region Ω, a function defined on it may be maximised either in its "interior" or on the boundary, as shown in Fig. 2.5. The two cases should be examined separately.

We start with the case where the function f is maximised in the interior of Ω. A sufficient condition to ensure that $f(\mathbf{r})$ is (locally) maximised at $\mathbf{r}^*$ is that (a) all its first derivatives at $\mathbf{r}^*$ vanish, i.e.

$$\nabla f|_{\mathbf{r}=\mathbf{r}^*} = \mathbf{0}, \text{ or } \left.\frac{\partial f}{\partial r_i}\right|_{\mathbf{r}=\mathbf{r}^*} = 0, \text{ for } i = 1, \ldots, n,$$

and (b) the Hessian matrix is negative definite at $\mathbf{r}^*$, i.e. for any $\mathbf{v} \in \mathbb{R}^n \backslash \{\mathbf{0}\}$,

$$\mathbf{v}^{\mathrm{T}}\, \mathbf{H}|_{\mathbf{r}=\mathbf{r}^*}\, \mathbf{v} < 0.$$

Conversely, if $f(\mathbf{r})$ gets maximised at $\mathbf{r} = \mathbf{r}^*$, then (a) $\nabla f|_{\mathbf{r}=\mathbf{r}^*} = \mathbf{0}$ and (b) the Hessian matrix is simply semi-negative definite, i.e. for any $\mathbf{v} \in \mathbb{R}^n\, \{\mathbf{0}\}, \mathbf{v}^{\mathrm{T}}\, \mathbf{H}|_{\mathbf{r}=\mathbf{r}^*}\, \mathbf{v} \leq 0$.

The sufficient and necessary conditions above are distinguished by the degree of the negative definiteness in $\mathbf{H}$ at $\mathbf{r}^*$. This subtle difference can be perceived from the Taylor series of f near $\mathbf{r} = \mathbf{r}^*$, i.e.

$$f(\mathbf{r}) \sim f(\mathbf{r}^*) + (\mathbf{r} - \mathbf{r}^*)^{\mathrm{T}}\, \nabla f|_{\mathbf{r}^*} + \frac{1}{2}(\mathbf{r} - \mathbf{r}^*)^{\mathrm{T}}\, \mathbf{H}|_{\mathbf{r}^*}\, (\mathbf{r} - \mathbf{r}^*) + \mathcal{O}(|\mathbf{r} - \mathbf{r}^*|^3), \tag{2.111}$$

where $\mathcal{O}(|\mathbf{r} - \mathbf{r}^*|^3)$ stands for terms taking an order of magnitude the same as $|\mathbf{r} - \mathbf{r}^*|^3$.

Equation (2.111) suggests that the values of $f(\mathbf{r})$ in a small neighbourhood of $\mathbf{r}^*$ can be approximated by a quadratic polynomial in $\mathbf{r}$. If f is maximised at $\mathbf{r}^*$, then $\nabla f|_{\mathbf{r}^*} = \mathbf{0}$ holds definitely. To be precise, when $\nabla f|_{\mathbf{r}^*} \neq \mathbf{0}$, there must exist certain $\mathbf{r}^0$, such that $(\mathbf{r} - \mathbf{r}^*)^{\mathrm{T}}\, \nabla f|_{\mathbf{r}^*} > 0$, e.g. $\mathbf{r}^0 = \mathbf{r}^* + \epsilon\, \nabla f|_{\mathbf{r}^*}$ (with $\epsilon > 0$). When ϵ is

sufficiently small, $f(\mathbf{r}^0)$ can be evaluated through a first-order approximation, such that

$$f(\mathbf{r}^0) \approx f(\mathbf{r}^*) + \epsilon \left|\nabla f(\mathbf{r}^*)\right|^2 + \mathcal{O}(\epsilon^2) > f(\mathbf{r}^*).$$

As a result, f cannot be maximised at $\mathbf{r}^*$ if $\nabla f|_{\mathbf{r}^*} \neq \mathbf{0}$.

Letting $\nabla f|_{\mathbf{r}^*} = \mathbf{0}$ in Eq. (2.111) gives

$$f(\mathbf{r}) \sim f(\mathbf{r}^*) + \frac{1}{2}(\mathbf{r} - \mathbf{r}^*)^{\mathrm{T}}\, \mathbf{H}|_{\mathbf{r}^*}\, (\mathbf{r} - \mathbf{r}^*) + \mathcal{O}(|\mathbf{r} - \mathbf{r}^*|^3). \tag{2.112}$$

When $\mathbf{H}|_{\mathbf{r}^*}$ is negative definite, then the quadratic term in Eq. (2.112) is always negative, indicating that $f(\mathbf{r}) < f(\mathbf{r}^*)$ in a small neighbourhood of $\mathbf{r}^*$. As a result, claiming the negative definiteness of $\mathbf{H}|_{\mathbf{r}^*}$ (along with $\nabla f|_{\mathbf{r}^*} = \mathbf{0}$) suffices to ensure that f is locally maximised at $\mathbf{r}^*$. But when $\mathbf{H}|_{\mathbf{r}^*}$ is simply semi-negative definite, there is still a (big) chance that f gets maximised at $\mathbf{r}^*$, but one needs to analyse the higher-order effects for $(\mathbf{r} - \mathbf{r}^*)$ that diminishes the quadratic term in Eq. (2.112).

If f is maximised at a boundary point $\mathbf{r}^*$, as schematically shown in Fig. 2.5(b), it gives rise to $\left.\frac{\partial f}{\partial m}\right|_{\mathbf{r}^*} \geq 0$, where the derivative represents the partial derivative of f with respect any vector, say, $\mathbf{m}$, which points outward the domain, or mathematically, $\mathbf{m} \cdot \mathbf{n} \geq 0$ with $\mathbf{n}$ the outer normal of the domain boundary at $\mathbf{r}^*$.

The above-summarised properties are employed to interpret the maximum principle detailed in Sect. 2.4.1, where the domain of interest is the (bounded) two-dimensional domain Ω_T in time t and space x. When $u(x; t)$ attains its maximum value at (x^*, t^*) in the interior of Ω_T, the results on its first derivatives read

$$\left.\frac{\partial u}{\partial t}\right|_{t=t^*} = 0, \quad \left.\frac{\partial u}{\partial x}\right|_{x=x^*} = 0. \tag{2.113}$$

To make the corresponding Hessian matrix $\mathbf{H}$ be semi-negative definite at (x^*, t^*), the primary minors of $\mathbf{H}$ should satisfy

$$u_{xx} \leq 0, \quad , u_{tt} \leq 0, \quad u_{tt}u_{xx} - (u_{xt})^2 \geq 0, \tag{2.114}$$

which is a property that can be found in almost any textbooks on linear algebra.

If the maximum value of $u(x, t)$ happens to occur on the $t = T$ boundary of Ω_T, then the requirement on u_t is loosen to be

$$\left.\frac{\partial u}{\partial t}\right|_{t=t^*} \geq 0.$$

Exercise

1. Given a cylindrical thin rod, whose cross-sectional radius is uniformly equal to r, it exchanges heat with its surrounding medium through its side surface, and the heat units flowing out of it follow Newton's law of heat conduction given by

$$\mathrm{d}Q = k_1(u - u_1)\mathrm{d}S\mathrm{d}t,$$

where u_1 is the temperature of the surrounding medium. Assume that the temperature on each cross section is the same, and the density of the rod is ρ; the specific heat is c; the heat conductivity is k.

(a) Derive the equation for the temperature u which only varies along the longitudinal direction.
(b) Suppose the thin rod is also a wire with its electric conductivity being σ, and a steady electric current I goes through it. Show that the (longitudinal) temperature distribution on the wire is governed by

$$c\rho\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2} - \frac{2k_1(u - u_1)}{r} + \frac{1}{\sigma}\cdot\left(\frac{I}{\pi r^2}\right)^2.$$

Tips: The electric resistance R of a cylindrical wire satisfies $R = \frac{l}{\sigma A}$, where l is the length of the wire, A is the cross section of a wire. The thermal power generated by a steady current I then equals $\frac{\mathrm{d}Q}{\mathrm{d}t} = I^2R$.

2. In analogies with the derivation of the heat equation in Sect. 2.1.1, derive the partial differential equation (2.17) describing the (isotropic) diffusion process of particles.
3. The heat conduction within materials may be inhomogeneous and anisotropic. Then the law of heat conduction, given by Eq. (2.2) for the homogeneous and isotropic case, is reformulated by

$$\mathbf{J} = -\mathbf{\Lambda}(x, y, z)\nabla u,$$

where $\mathbf{\Lambda} = \left(\Lambda_{ij}\right)$, $(i, j = 1, 2, 3)$ is a symmetric and positive definite matrix (or more precisely, a second-order tensor). Derive the governing PDE for the temperature u then.
4. Concretes can gradually release heat when mixed with water, known as the *heat of hydration*, which is denoted by H here, and measured in the unit of J/(m^3). The rate of change in the heat of hydration is found proportional to heat units still stored in the concretes. Suppose that the evolution of the heat of hydration is known, and assume that the specific heat of the concrete is c; density is ρ, the thermal conductivity is k. Find the differential equation for u, which represents the temperature of the concretes upon hydration.
5. Objects are all found to radiate heat to its surrounding medium from its surface, and the amount of the radiated heat units satisfies the *Stefan–Boltzmann law* given by,

$$\mathrm{d}Q = \sigma u^4\mathrm{d}S\mathrm{d}t,$$

where u measures the local (absolute) temperature on the surface and σ is a parameter. Here we only consider the thermal radiation between the object and

its surrounding media (in both directions). Write down the boundary condition on the surface where thermal radiation takes place.

6. Solve the Cauchy problem for the (spatially) two-dimensional heat equation with the method of integral transform:

$$\begin{cases} u_t - a^2(u_{xx} + u_{yy}) = 0, \ (x, y; t) \in \mathbb{R} \times \mathbb{R} \times \mathbb{R}^+; \\ u|_{t=0} = \phi(x, y). \end{cases}$$

7. Apply the method of integral transform to solve the Cauchy problem for the wave equation given by

$$\begin{cases} u_{tt} - a^2 u_{xx} = 0, \ (x, t) \in \mathbb{R} \times \mathbb{R}^+; \\ u|_{t=0} = \phi(x), \quad u_t|_{t=0} = \psi(x). \end{cases}$$

   (a) Use Fourier transform to turn the problem above into an ODE problem and determine its solution.
   (b) Check with the table for the inverse Fourier transform to finally express the solution, and compare the result with D'Alembert's formula (1.27).

8. Solve

$$\begin{cases} u_t - a^2 u_{xx} = 0, \ x \in (0, \pi), \ t > 0; \\ u|_{t=0} = \phi(x); \\ u|_{x=0} = u_x|_{x=\pi} = 0 \end{cases}$$

   with the method of separation of variables.

9. Consider the initial–boundary value problem describing (spatially) one-dimensional heat conduction. When the system is insulated to heat transfer at the two ends, the corresponding problem reads

$$\begin{cases} u_t - a^2 u_{xx} = 0, \ x \in (0, l), \ t > 0; \\ u|_{t=0} = \phi(x); \\ u_x|_{x=0} = u_x|_{x=l} = 0. \end{cases}$$

   (a) Solve this initial–boundary value problem using the method of separation of variables.
   (b) Predict the *asymptotic behaviour* of the system, as time t tends to infinity, that is, $\lim_{t\to\infty} u(x, t)$. Interpret this limiting result from a physical viewpoint.

10. Solve the initial–boundary value problem governed by an inhomogeneous heat equation, which is given by

$$\begin{cases} u_t - a^2 u_{xx} = e^{-t} x(l - x), \ x \in (0, l), \ t > 0; \\ u|_{t=0} = 0; \\ u|_{x=0} = u|_{x=l} = 0. \end{cases}$$

11. Use the method of separation of variables to solve

$$\begin{cases} u_t = a^2 u_{xx} - b^2 u, \ x \in (0, l), \ t > 0; \\ u|_{t=0} = 0; \\ u|_{x=0} = 1, \quad (u_x + \sigma u)|_{x=l} = 0, \end{cases}$$

where a, b and σ are all constants.

12. Determine whether the following ODEs can be transformed into Sturm–Liouville equations taking the form of Eq. (2.76). If yes, specify the functions corresponding to $k(x)$, $q(x)$ and $\rho(x)$, as well as the eigenvalue λ. Then state what types of boundary conditions (natural or imposed) should be given on the two ends of their corresponding domains of definitions. Here α serves as a parameter.

    (a) $(1 - x^2)\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} - 2x\frac{\mathrm{d}y}{\mathrm{d}x} - \frac{y}{1-x^2} + \lambda y = 0, x \in (-1, 1)$;
    (b) $\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + \lambda x y = 0, x \in (-1, 1)$;
    (c) $x^2 \frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + x\frac{\mathrm{d}y}{\mathrm{d}x} + (\lambda x^2 - \alpha^2) y = 0, x \in (0, 1)$.

13. Show that the linear operator (2.97) inducing the Sturm–Liouville equation [given by Eq. (2.76)] imposed with proper boundary conditions is self-adjoint.

    (a) Express the functional space $\mathcal{H}$ which contains all the functions satisfying the boundary condition (2.79).
    (b) Use integration by parts (twice) to verify that for any $y(x)$, $w(x) \in \mathcal{H}$, Eq. (2.99) holds for the differential operator $\mathcal{L}$ defined by Eq. (2.97).

14. Verify Duhamel's principle in Sect. 2.3, that is, if $W(x, t; \tau)$ is the solution for problem (2.101), $u(x, t)$ defined by Eq. (2.102) is the solution for problem (2.100).

Chapter 3
Poisson's Equation

In this chapter, discussion is made over topics about modelling, analysis and interpretation related to Poisson's equation, with Laplace's equation as its special case. First, a number of physical phenomena that can be described by Poisson's equation are examined, and their physical analogies are summarised then. To solve PDE problems for Poisson's equation, the concepts of variational principle and Green's function are introduced in turn. In the end of this chapter, the issue of solution uniqueness is looked into in the context of Poisson's equation, and the corresponding (strong) maximum principle is mentioned. The contents in this chapter are summarised in the knowledge map charted by Fig. 3.1.

3.1 Poisson's Equation and Harmonic Equation

3.1.1 Definitions

In this chapter, we examine PDEs taking the following form:

$$\begin{aligned} &\text{two-dimensional:} \quad \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y); \\ &\text{three-dimensional:} \quad \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = f(x, y, z), \end{aligned} \tag{3.1}$$

where u is the unknown function and f is a given function. The equations given by Eq. (3.1) are both called *Poisson's equation*. As a special case when $f = 0$, the resulting homogeneous Poisson's equation is called *Laplace's equation*, or the *harmonic equation*. A function that satisfies Laplace's equation is called a *harmonic function*.

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Y. Zhu, *Equations and Analytical Tools in Mathematical Physics*,
https://doi.org/10.1007/978-981-16-5441-1_3

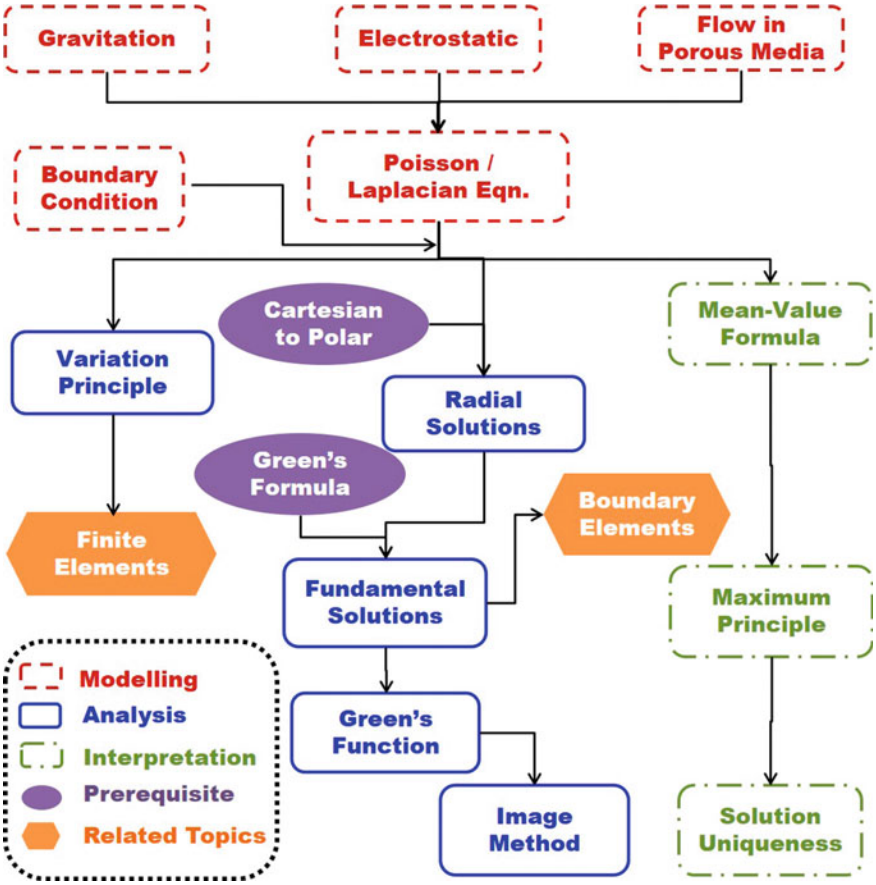

Fig. 3.1 Knowledge map—Poisson's equation

For simplicity, we introduce $\Delta u = f$ to represent both equations in (3.1), where "Δ" is called a *Laplacian operator*. Note that unless specified, Laplacian operator "Δ" is introduced irrespective of the dimensionality of definition. With Laplacian operator, the wave equation defined in multiple dimensions can be summarised by

$$u_{tt} - a^2 \Delta u = f;$$

the heat equation can be summarised by

$$u_t - a^2 \Delta u = f.$$

Through introducing symbols for differential operators, physical phenomena in multidimensional space can be modelled in a unified and concise manner. Other key

linear differential operators that are widely used for modelling are summarised in the prerequisite part of this section.

Since a certain portion of analysis in this chapter is conducted irrespective of the dimensionality of definition, the following notation rules are employed in general. A bold English letter in lower case is utilised to denote a vector (consisting of scalar functions) in $\mathbb{R}^2$ or $\mathbb{R}^3$, and the corresponding Italic letter with a subscript represents one of its entry, e.g. u_1 stands for the first entry of $\mathbf{u}$. Here the bold letter $\mathbf{r}$ is employed to denote specifically a point either in $\mathbb{R}^2$ or in $\mathbb{R}^3$, where $|\mathbf{r}|$ measures the distance from $\mathbf{r}$ to the origin. When the situation of interest is specified to be three-dimensional, $\mathbf{r} = (r_1, r_2, r_3)^{\mathrm{T}} = (x, y, z)^{\mathrm{T}}$. Thus, the three-dimensional Poisson's equation, for instance, can be expressed equivalently by

$$\Delta u = \frac{\partial^2 u}{\partial r_1^2} + \frac{\partial^2 u}{\partial r_2^2} + \frac{\partial^2 u}{\partial r_3^2} = f(\mathbf{r}).$$

In summary, we will be focused on

$$\text{Poisson's equation:} \qquad -\Delta u = f; \tag{3.2a}$$

$$\text{Laplace's/harmonic equation:} \qquad \Delta u = 0 \tag{3.2b}$$

in this chapter. Compared to Eq. (3.1), a negative sign is included on the left-hand side of Eq. (3.2a), so as to comply with the conventional representation for Poisson's equation.

3.1.2 Motivation from Physics

3.1.2.1 Equilibrium/Steady States

In Sect. 1.4, a membrane undergoing small and transverse vibration has been modelled by the two-dimensional wave equation (1.87). When the membrane is in a force-balanced state, then $u_{tt} = 0$. Equation (1.87) thus becomes $-a^2 \Delta u = f$. Dividing a^2 on both sides returns Poisson's equation (3.2a).

For the heat equation (2.8), when $u_t = 0$, the temperature distribution no longer evolves in time and space, indicating that the system reaches a thermally equilibrated state. Letting $u_t = 0$ in Eq. (2.8) returns Poisson's equation (3.2a) again. It is noted that there is still heat conduction in a system which sits in its thermal equilibrium. But the intake and output of heat units balance each other everywhere. In other words, the system reaches a thermally steady state.

From the two examples mentioned above, one may perceive certain key features shared by the physical phenomena that can be formulated through Poisson's equation, that is, the corresponding system is in equilibrium, and the system behaviour is thus time-independent.

3.1.2.2 Gravitation

Given a point mass m located at $\mathbf{r}^* = (x^*, y^*, z^*)$, it exerts a *gravitational field* calculated by

$$\mathbf{g} = -\frac{Gm^*(\mathbf{r} - \mathbf{r}^*)}{|\mathbf{r} - \mathbf{r}^*|^3}, \tag{3.3}$$

where G is the *gravitational constant*; $\mathbf{r}$ are the independent spatial variables marking the position of measurement. Equation (3.3) is just the well known *Newton's law of gravity*.

A point mass m located at $\mathbf{r}$ should feel a *gravitational force*

$$\mathbf{F} = m\mathbf{g} \tag{3.4}$$

from the point mass at $\mathbf{r}^*$.

Now we further introduce a function $\phi(\mathbf{r}; \mathbf{r}^*)$ defined by

$$\phi(\mathbf{r}; \mathbf{r}^*) = -\frac{Gm^*}{|\mathbf{r} - \mathbf{r}^*|}. \tag{3.5}$$

Here $\phi(\mathbf{r}; \mathbf{r}^*)$ has $\mathbf{r}$ as its independent spatial variables, while $\mathbf{r}^*$ are treated as its parameters. Hence when ϕ gets differentiated, the differentiation is meant to be with respect to $\mathbf{r}$. Such a differentiation rule on $\phi(\mathbf{r}; \mathbf{r}^*)$ will be repeatedly employed in the rest of this chapter.

With Eq. (3.5), it is quite straight forward to verify (with reference to Sect. 3.3) that the gravitational field $\mathbf{g}$ given by Eq. (3.3) can be related to $\phi(\mathbf{r}; \mathbf{r}^*)$ by

$$\mathbf{g} = -\nabla\phi. \tag{3.6}$$

Actually the function $\phi(\mathbf{r}; \mathbf{r}^*)$ measures the *gravitational potential* due to the point mass at $\mathbf{r}^*$. It can be verified (with reference to Sect. 3.3) that $\phi(\mathbf{r}; \mathbf{r}^*)$ satisfies Laplace's equation (of $\mathbf{r}$), provided that $\mathbf{r} \neq \mathbf{r}^*$.

The formulation can be extended to examine the gravitational potential due to a continuously distributed mass. For simplicity, we let $G = 1$. This is equivalent to declaring that all physical quantities of unit $\mathrm{m}^3/(\mathrm{kg}\cdot\mathrm{s}^2)$ is actually measured in the unit of G.

Given an object occupying a domain of $\Omega \in \mathbb{R}^3$, its mass density is measured by $\rho(\mathbf{s})$ with $\mathbf{s} \in \Omega$. Then the gravitational potential due to this object should be calculated by

$$\phi(\mathbf{r}) = -\iiint_{\Omega} \frac{\rho(\mathbf{s})\mathrm{d}\mathbf{s}}{|\mathbf{r} - \mathbf{s}|}. \tag{3.7}$$

For deriving Eq. (3.7), one may partition Ω into many infinitesimally small regions, and $\frac{\rho(\mathbf{s})\mathrm{d}\mathbf{s}}{|\mathbf{r}-\mathbf{s}|}$ just approximates the gravitational potential at $\mathbf{r}$ due to the mass

occupying the infinitesimally small region surrounding $\mathbf{s}$. And the overall gravitational effect at $\mathbf{r}$ due to the whole object is formulated through integration over Ω.

Equation (3.7) is well defined for $\mathbf{r} \in \mathbb{R}^3 \backslash \Omega$, and it can be verified that Eq. (3.7) is a harmonic function (of $\mathbf{r}$) outside Ω.

But when $\mathbf{r} \in \Omega$, $\mathbf{s}$ may coincide with $\mathbf{r}$, making the integrand of Eq. (3.7) be ill-defined. The issue can be resolved by taking a physical viewpoint. As we know, a point does not exert gravitational force on itself. Hence when the gravitational effect at $\mathbf{r}$ is formulated, removal of an infinitesimally small neighbourhood of $\mathbf{r}$ from the domain of integration does not change the outcome. Mathematically, this is carried out by means of a limiting process, i.e.

$$\phi(\mathbf{r}) = -\lim_{\epsilon \to 0} \iiint\limits_{\Omega \backslash \mathcal{O}_\epsilon(\mathbf{r})} \frac{\rho(\mathbf{s}) \mathrm{d}\mathbf{s}}{|\mathbf{r} - \mathbf{s}|}, \tag{3.8}$$

where $\mathcal{O}_\epsilon(\mathbf{r})$ denotes a sphere centred at $\mathbf{r}$ and of radius ϵ.

Note that Eq. (3.8) is consistent with (3.7), where $\mathbf{r} \notin \Omega$. Thus, $\phi(\mathbf{r})$ defined by Eq. (3.8) formulates the gravitational potential all over $\mathbb{R}^3$ due to the object. It will be shown in Sect. 3.4 that ϕ defined by Eq. (3.8) satisfies Poisson's equation in the sense of

$$\Delta\phi = \begin{cases} 4\pi\rho(\mathbf{r}), & \mathbf{r} \in \Omega; \\ 0, & \mathbf{r} \in \mathbb{R}^3 \backslash \Omega. \end{cases} \tag{3.9}$$

3.1.2.3 Electrostatics

With a number of electric charges distributed in space, an electric field $\mathbf{E}$ is induced, which is linked with the electric potential u by

$$\mathbf{E} = -\nabla u. \tag{3.10}$$

For a bounded region Ω, as suggested by *Gauss's law*, the net electric flux passing through its boundary $\partial\Omega$, should be proportional to the net charge quantities inside Ω. If $\rho(\mathbf{r})$ describes the density distribution of the electric charges, Gauss's law reads

$$\iint\limits_{\partial\Omega} \mathbf{E} \cdot \mathbf{n} \, \mathrm{d}S = \frac{1}{\epsilon_0} \iiint\limits_{\Omega} \rho(\mathbf{r}) \, \mathrm{d}\mathbf{r}, \tag{3.11}$$

where $\mathbf{n}$ is the unit outer normal vector to $\partial\Omega$; $\mathrm{d}S$ measures an infinitesimally small area taken from the boundary surface; ϵ_0 is the *permittivity* of the medium. On using Green's formula, as detailed in the prerequisite knowledge of Sect. 1.4, the boundary integral in Eq. (3.11) can be written by

$$\iint_{\partial\Omega} \mathbf{E} \cdot \mathbf{n} \, \mathrm{d}S = \iiint_{\Omega} \nabla \cdot \mathbf{E} \, \mathrm{d}\mathbf{r}.$$

As the domain Ω is chosen arbitrarily, we combine the above identity with Eq. (3.11) to obtain

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon}. \tag{3.12}$$

Inserting Eq. (3.12) into (3.10) suggests that, in an electrostatic case, the electric potential u satisfies Poisson's equation, i.e.

$$-\Delta u = \frac{\rho}{\epsilon_0}. \tag{3.13}$$

To calculate the electric potential u, one may refer to the procedure of expressing the gravitational potential field above. From *Coulomb's law*, the electric field due to a unit point charge located at the origin can be expressed by

$$\mathbf{E} = \frac{1}{4\pi\epsilon_0} \cdot \frac{\mathbf{r}}{|\mathbf{r}|^3}. \tag{3.14}$$

Combining Eq. (3.14) with (3.10), it can be checked that the corresponding electric potential function satisfies

$$u = \frac{1}{4\pi\epsilon_0 |\mathbf{r}|}.$$

Then similar as the case of gravitation, the electric potential function due to a charge distribution (of density ρ) should be formulated by an integral of

$$u(\mathbf{r}) = \lim_{\delta \to 0} \frac{1}{4\pi\epsilon_0} \iiint_{\Omega \setminus O_\delta(\mathbf{r})} \frac{\rho(\mathbf{s}) \mathrm{d}\mathbf{s}}{|\mathbf{r} - \mathbf{s}|}. \tag{3.15}$$

Naturally, the electric potential u formulated by Eq. (3.15) should solve Poisson's equation (3.13).

Now the mathematical analogies between the gravitational case and the electrostatic case are worth being mentioned here. On a fundamental basis, the Newton's law of gravity given by Eq. (3.3) shares a same form with the Coulomb's law given by Eq. (3.14) with a tiny difference in their proportionality coefficients. That is partly the reason why they are both associated with Poisson's equation.

Besides, the potential field due to a unit mass/charge is found to play an essential role in the expression for the potential functions in other cases. This is not a coincidence. To further interpret the issue, we consider the special case when $\Omega = \mathbb{R}^3$. Equation (3.15) then takes a convolution form as introduced in Sect. 2.2. To be specific, Eq. (3.15) can be rewritten by

$$u = \frac{\rho}{4\pi\epsilon_0} * \frac{1}{|\mathbf{r}|}, \tag{3.16}$$

where "$*$" stands for the operation of the convolution of two functions as specified by Eq. (2.20). The two functions that consist of the convolution (3.16) are: (a) the right-hand side of Poisson's equation (3.13) (divided by 4π); (b) the potential function due to a unit charge put at the origin, which is fully independent of the external source (introduced through the right-hand side of Poisson's equation). Again, this is not a coincidence. It hints an effective tool for solving linear PDE problems, the concept of fundamental solution. In fact, $1/(4\pi|\mathbf{r}|)$ is a fundamental solution to three-dimensional Poisson's equation. Generally speaking, the solution to a definite linear PDE problem can be expressed by a specific fundamental solution to the governing PDE taking the convolution with the inhomogeneous part of the governing differential equation. The topic will be further examined in Sect. 3.4.

3.1.2.4 Physical Analogies

Based on the derivations for both the gravitational and electrostatic cases above, we now try to summarise the physical analogies underpinning the phenomena that can be formulated through Poisson's equation.

First, a vector-valued field quantity (e.g. the electric field $\mathbf{E}$) is in proportion to a scalar field (e.g. the electric potential u). The proportionality (e.g. the permittivity ϵ_0) fully depends on the materials that occupy the domain of definition, and it is normally evaluated through experimentation. Such a gradient-based relationship is termed as a generalised *constitutive relation*.

Second, the total net flux from the vector-value field over the surface of any closed region should be balanced with some internal sources, as given by Eq. (3.11). With the use of Green's formula, the boundary integral measuring the total net flux over the domain surface can be transformed into a body integral, and thus a divergence-based *conservation relation* is established, as given by Eq. (3.12). Note that one may refer to the prerequisite part of this section for more details about the divergence operator.

Finally, incorporating the divergence-based conservation relation with the gradient-based constitutive relation should give rise to Poisson's equation, as appearing in the derivation of Eq. (3.13).

Actually, such mechanisms are found underlying many physical phenomena. For instance, there exist in nature various geologically *porous media*, where underground liquids are gradually and steadily driven from high-pressured regions to low-pressured regions.

Note that for a porous medium, it is generally not economic and often not necessary to examine the fluidic details through the geometrically complicated pathways. A more effective way is to model the *homogenised velocity field*, denoted by $\mathbf{v}$ here, which is the mean velocity of all the fluids around the point of measurement. Under such treatments, the homogenised velocity becomes a field that is smoothly varying in space.

Experimental studies indicate that the homogenised velocity of the fluids in porous media can be formulated by

$$\mathbf{v} = -\frac{k}{\mu}\nabla p, \tag{3.17}$$

where p is the *hydrostatic pressure* field; k is the *permeability* of the medium; μ is the *viscosity* of the fluids. Equation (3.17) is coined as *Darcy's law*, which identifies a gradient-based constitutive relation.

When the fluids are *incompressible*, the mass density of the fluids stays unchanged with time. Then for any closed region Ω, the total net flux through its surface should vanish, i.e.

$$\iint_{\partial\Omega} \mathbf{v} \cdot \mathbf{n} \mathrm{d}S = 0, \tag{3.18}$$

and a divergence-based conservation law is thus established.

Inserting Eq. (3.17) into (3.18), then we use Green's formula and the arbitrariness in the choice of Ω, and thus find that the hydrostatic pressure field p satisfies Laplace's equation.

In summary, the physical phenomena that can be modelled by Poisson's equation are potentially driven by certain gradient-based constitutive relation, but the system is maintained at its equilibrium/steady state by means of a divergence-based conservation law. Note that such a modelling strategy can be generalised to model more complicated situations in their equilibrium states. From a broader viewpoint, the resulting second-order governing PDEs are all of elliptic type, whose definition will be systematically introduced in Sect. 4.1. More importantly, the methods to be introduced in the rest of this chapter are also applicable, upon modification, to examine the behaviour of more complicated system governed by generalised second-order elliptic PDEs. For more models that give rise to Poisson's equation or other second-order elliptic PDEs, one may refer to advanced textbooks over this subject (e.g. [9]).

3.1.3 Boundary Conditions

As discussed above, Poisson's equation is normally employed to describe a system in equilibrium/steady state, which is independent of time. Usually only boundary conditions are necessary in order to define a problem for Poisson's equation.

When the domain of interest is bounded, as shown in the shaded region Ω in Fig. 3.2, the corresponding PDE problem is called an *interior boundary value problem*.

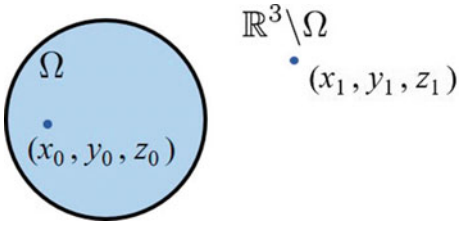

Fig. 3.2 Domains on which an interior or an exterior boundary value problem is defined

Three types of boundary conditions can be imposed on the domain boundary $\partial\Omega$.

$$\text{Dirichlet boundary condition:} \quad u|_{\partial\Omega} = h(\mathbf{r}); \tag{3.19a}$$

$$\text{Neumann boundary condition:} \quad \left.\frac{\partial u}{\partial n}\right|_{\partial\Omega} = h(\mathbf{r}); \tag{3.19b}$$

$$\text{Robin boundary condition:} \quad \left.\left(\frac{\partial u}{\partial n} + \sigma u\right)\right|_{\partial\Omega} = h(\mathbf{r}). \tag{3.19c}$$

For the electrostatic case, Dirichlet boundary condition identifies the electric potential on the boundary, and Neumann boundary condition measures the (steady) electric current across the boundary.

When the domain of interest is unbounded, as in the non-shaded region in Fig. 3.2, the corresponding PDE problem is called an *exterior boundary value problem*. In this scenario, we not only need to specify the boundary conditions on the boundary $\partial\Omega$, but also the function behaviour at infinity. If the function behaviour at infinity is not declared, one may end up with multiple solutions.

As a demonstrative example, suppose that $u(\mathbf{r})$ is a harmonic function outside a unit sphere, i.e. $\mathbb{R}^3 \backslash \{\mathbf{r} | |\mathbf{r}| < 1\}$. On the spherical boundary, we let $u|_{|\mathbf{r}|=1} = 1$. Apparently, $u \equiv 1$ is a harmonic function satisfying the boundary condition. On the other hand, it is shown in the gravitational case that $u = 1/|\mathbf{r}|$ also solves Laplace's equation, and it satisfies the same boundary condition, too. Therefore, when an exterior boundary value problem for Poisson's equation is presented, the function behaviour at infinity should be specified so as to ensure solution uniqueness.

Prerequisite knowledge

Vector calculus operations

Generally speaking, a differential operator identifies a mapping rule between functions by means of differentiation. Apart from Laplacian operator "Δ" given in Sect. 3.1.1, we introduce three other differential operators which are extremely useful for simplifying the representations of PDEs.

The *gradient operator*, usually denoted by "**grad**" or "∇", has been introduced for describing the heat flux of Eq. (2.2). It transforms a differentiable function to a vector consisting of all its first derivatives. In a three-dimensional scenario, for instance,

$$\mathbf{grad}\, u = \nabla u = \left(\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}, \frac{\partial u}{\partial z}\right)^{\mathrm{T}}. \tag{3.20}$$

Note that the demonstrative examples are given for three-dimensional cases here, and one may readily write their two-dimensional counterparts, whenever applicable.

The *divergence operator*, usually denoted by "div" or "$\nabla\cdot$", measures the spatial rate of variation of a vector-valued function, say $\mathbf{u} = (u_1, u_2, u_3)^{\mathrm{T}}$. Mathematically, it is defined by

$$\mathrm{div}\, \mathbf{u} = \nabla \cdot \mathbf{u} = \frac{\partial u_1}{\partial x} + \frac{\partial u_2}{\partial y} + \frac{\partial u_3}{\partial z}. \tag{3.21}$$

The reason for the notation "$\nabla \cdot \mathbf{u}$" is as follows. One may treat the gradient operator "∇" as a vector, and the dot "$\cdot$" simply induces the inner product of two "vectors".

The *curl operator*, usually denoted by "**curl**", "**rot**", or "$\nabla\times$", measures the space rate of rotation of a vector-valued function $\mathbf{u} = (u_1, u_2, u_3)^{\mathrm{T}}$. Mathematically, it is defined by

$$\mathbf{curl}\, \mathbf{u} = \mathbf{rot}\, \mathbf{u} = \nabla \times \mathbf{u} = \left(\frac{\partial u_3}{\partial y} - \frac{\partial u_2}{\partial z}, \frac{\partial u_1}{\partial z} - \frac{\partial u_3}{\partial x}, \frac{\partial u_2}{\partial x} - \frac{\partial u_1}{\partial y}\right)^{\mathrm{T}}, \tag{3.22}$$

where the symbol "$\times$" can be read as the cross product of two vectors. Note that the curl operator only applies in three-dimensional situations.

It can be readily checked that the following results obtained through the composition of different operators hold:

$$\nabla \cdot (\nabla \times \mathbf{u}) = 0, \ \nabla \times (\nabla f) = \mathbf{0} \tag{3.23}$$

and

$$\nabla \cdot (\nabla u) \triangleq \nabla^2 u = \Delta u, \ \nabla \times (\nabla \times \mathbf{u}) = \nabla(\nabla \cdot \mathbf{u}) - \Delta \mathbf{u}, \tag{3.24}$$

where "Δ" operating on a vector-valued function $\mathbf{u}$ stands for applying the Laplacian operator on each entry of $\mathbf{u}$.

3.2 Variational Principle

The *variational principle*, or sometimes termed as the *variational method*, offers an effective tool for analysing PDE problems describing a system in its equilibrium/steady state. It establishes a solid theoretical foundation for the powerful numerical scheme of finite element method.

To this end, we consider a PDE problem established in $\mathbb{R}^2$, which is given by

$$\begin{cases} -\Delta u = f, \ \mathbf{r} \in \Omega; \\ u|_{\partial\Omega} = 0. \end{cases} \tag{3.25}$$

Problem (3.25) describes a membrane in equilibrium with its boundary fixed. From a physical viewpoint, when a system reaches its equilibrium state, a certain energy quantity should be minimised. Otherwise the system should keep on evolving to bring down the energy level of the system. Not surprisingly, the energy quantity for the case of membrane vibration is chosen to be the system potential energy less the work done due to the external load.

For a membrane with its boundary fixed, as discussed in Sect. 1.5, the system potential energy less the external work is formulated by

$$\iint_{\Omega} \left[\frac{T}{2} \left(u_x^2 + u_y^2 \right) - Fu \right] \mathrm{d}x\mathrm{d}y,$$

where T is recalled to be the surface tension of the membrane; F measures the external force per area on the membrane surface. Note that dividing a function by a constant does not make a difference in the corresponding minimisation procedure. Hence, we divide the quantity of the system energy less the external work by the surface tension T, and let $f = \frac{F}{T}$.

The resulting potential energy less the external work (scaled by the surface tension T), denoted by $\mathcal{J}$, thus becomes

$$\mathcal{J}[u] = \iint_{\Omega} \left[\frac{1}{2} \left(u_x^2 + u_y^2 \right) - fu \right] \mathrm{d}\mathbf{x}, \tag{3.26}$$

where the square brackets suggest that the input of $\mathcal{J}[\cdot]$ is a function rather than a variable. Actually, $\mathcal{J}[u]$ is called a *functional*, whose input and output are a function and a number, respectively. The functional defined by Eq. (3.26) has a clear physical meaning. For a membrane with its boundary fixed, it may undertake various displacement states formulated by the function $u(x, y)$, and the functional $\mathcal{J}[u]$ represents the corresponding potential energy less the external work (divided by the surface tension T).

Here only displacement states satisfying fixed boundary conditions are of our interest. To this end, a function set is introduced as

$$V_0 = \{ v(\mathbf{r}) \mid v|_{\partial\Omega} = 0 \}, \tag{3.27}$$

which contains all possible membrane states whose boundaries are fixed. It can be checked that, if $u, v \in V_0$, then $\alpha u + \beta v \in V_0$ for any $\alpha, \beta \in \mathbb{R}$. Therefore, V_0 defined by Eq. (3.27) is not only a set, but actually a linear functional space. For more details

over the concept of linear functional space, one may refer to advanced PDE textbooks on functional analysis (e.g. [7]).

From a physical viewpoint, the displacement field corresponding to the equilibrium state should minimise the (rescaled) quantity of the potential energy less the external among all possible displacement states contained in V_0. Translating this statement in mathematics, we write

$$\mathcal{J}[u] = \min_{v \in V_0} \mathcal{J}[v], \tag{3.28}$$

where u is expected to be the solution for problem (3.25).

This is the physical intuition of the variational principle for Poisson's equation, which is stated as follows.

(a) When Eq. (3.28) holds, the minimiser $u(x, y)$ is the solution for problem (3.25).
(b) If the solution u for problem (3.25) exists, u should minimise the functional $\mathcal{J}$ given by Eq. (3.26) among all functions in V_0, i.e. Eq. (3.28) holds.

Proof The statement (a) is validated first, and the key idea is to transform the minimisation statement about a functional (with respect to its input functions) into a minimisation problem of a function (with respect to its independent variables).

Suppose Eq. (3.28) holds. Then one can quickly reach $u|_{\partial\Omega} = 0$, which is just the boundary condition of problem (3.25).

Now we are focused on showing that the minimiser u of Eq. (3.28) also solves the governing Poisson's equation of problem (3.25). Note that any function v belonging to V_0 defined by Eq. (3.27) can be expressed by

$$v = u + \lambda w, \tag{3.29}$$

where u is the minimiser of Eq. (3.28); λ is a number; $w \in V_0$ is another function. By doing so, the functional $\mathcal{J}[v]$ can be treated as a function of λ for any given w.

Inserting Eq. (3.29) into (3.26) gives

$$\begin{aligned}
\mathcal{J}[v] &= \iint_\Omega \left[\frac{1}{2}\left((u_x + \lambda w_x)^2 + \left(u_y + \lambda w_y\right)^2\right) - f(u + \lambda w)\right] \mathrm{d}x\mathrm{d}y \\
&= \iint_\Omega \left[\frac{1}{2}\left(u_x^2 + u_y^2\right) - fu\right] \mathrm{d}x\mathrm{d}y + \lambda \int_\Omega \left[u_x w_x + u_y w_y - fw\right] \mathrm{d}x\mathrm{d}y \\
&\quad + \frac{\lambda^2}{2} \int_\Omega \left(w_x^2 + w_y^2\right) \mathrm{d}x\mathrm{d}y.
\end{aligned} \tag{3.30}$$

Since u is the minimiser of Eq. (3.28), the functional $\mathcal{J}[u + \lambda w]$ should be minimised at $\lambda = 0$, for any $w \in V_0$. Hence

$$\left.\frac{\mathrm{d}\mathcal{J}[u+\lambda w]}{\mathrm{d}\lambda}\right|_{\lambda=0} = 0 \tag{3.31}$$

should hold for any $w \in V_0$. The derivative appearing in Eq. (3.31) is termed as the *Gâteaux derivative*.

Combining Eq. (3.31) with (3.30) suggests that

$$\iint_{\Omega} \left[u_x w_x + u_y w_y - fw\right] \mathrm{d}x\mathrm{d}y = 0 \tag{3.32}$$

holds for any $w \in V_0$.

With Green's formula, we have

$$\iint_{\Omega} \left(u_x w_x + u_y w_y\right) \mathrm{d}x\mathrm{d}y = \int_{\partial\Omega} w \frac{\partial u}{\partial n} \mathrm{d}s - \iint_{\Omega} w \left(u_{xx} + u_{yy}\right) \mathrm{d}x\mathrm{d}y.$$

As $w \in V_0$, the integral over $\partial\Omega$ should vanish, and we then reach

$$\iint_{\Omega} \left(u_x w_x + u_y w_y\right) \mathrm{d}x\mathrm{d}y = -\iint_{\Omega} w \left(u_{xx} + u_{yy}\right) \mathrm{d}x\mathrm{d}y.$$

Incorporating it with Eq. (3.32), we have

$$-\iint_{\Omega} w\left(\Delta u + f\right) \mathrm{d}x\mathrm{d}y = 0, \tag{3.33}$$

which should hold for any $w \in V_0$.

Given this arbitrariness in the choice of w, the integrand appearing in Eq. (3.33) must vanish, so as to make it hold. As a result, $-\Delta u = f$, which is just the governing equation of problem (3.25), and the statement (a) is therefore justified.

To justify the statement (b) of the variational principle, we start with Eq. (3.33), which is valid for u being the solution for problem (3.25). Then we reverse our derivation from Eq. (3.33) and thus reach Eq. (3.32). With Eq. (3.32), the term linear about λ in Eq. (3.30) vanishes. Thus, we have

$$\mathcal{J}[v] = \mathcal{J}[u+\lambda w] = \mathcal{J}[u] + \frac{\lambda^2}{2} \iint_{\Omega} \left(w_x^2 + w_y^2\right) \mathrm{d}x\mathrm{d}y \geq \mathcal{J}[u], \tag{3.34}$$

which hold for any $v \in V_0$. Therefore, the solution u for the PDE problem (3.25), if it exists, is the minimiser of problem (3.28), and the statement (b) is thus justified. □

In the proof for the variational principle here, the minimisation problem over functions $v \in V_0$ is transformed into a differentiation problem with respect to the

parameter λ. Thus, the term "variation", in the context of PDE solvers, can be envisaged as the "differentiation" of a functional (usually representing a rescaled energy quantity) with respect to its input function.

The variational principle addresses a key intuition from physics. When an equilibrium state can be described by a PDE problem [e.g. problem (3.25)], its solution should minimise the energy quantity dictating the evolution of the system. This energy quantity is often termed as the "free energy" of the system. From such a viewpoint, the conceptualisation of variation sees its vast applications in examining the behaviour of many physical, chemical and biological systems.

With the variational principle introduced here, PDE problem (3.25) is transformed into a minimisation problem. Another initiative for such transformation lies in the fact that, the requirement over the solution for the minimisation problem is weaker if compared with that for the original PDE problem. To be specific, when problem (3.25) is of our concern, the solution u must be differentiable at least twice. In contrast, the requirement on the minimiser u of Eq. (3.28) is much "weaker", as long as its first derivatives are square integrable within Ω. With such a perspective, the minimiser u of Eq. (3.28) is called the *weak solution* for problem (3.25). As the requirement on solution smoothness is weak for the minimisation problem, one may numerically approximate the actual solution for problem (3.25) by relatively simple functions, such as piecewisely linear functions (that are no longer differentiable twice). This is exactly the backbone idea underlying the powerful numerical scheme of the finite element method [17].

When the variational principle is justified, Eq. (3.32) plays a pivotal role in linking PDE problem (3.25) with minimisation problem (3.28). In fact, Eq. (3.32) serves to be the *weak formulation* of problem (3.28). Note that Eq. (3.32) qualifies for a weak formulation only when it holds for any $w \in V_0$, where w is called a *trial function* and V_0 the *trial space*.

Therefore, a PDE problem (describing an equilibrium state), along with its weak formulation and the corresponding energy minimisation problem, should form a firmed "triangle", as illustrated in Fig. 3.3. Knowing the information about one of its vertices should give rise to the derivations of the information about the other two (e.g. see Exercises 3.5 and 3.6).

3.3 Harmonic Functions in Polar System

In this section, we consider representing harmonic functions with polar coordinates. The first case concerns expressing the two-dimensional Laplace's equation in polar system. Then the situation is extended for three-dimensional cases with spherical coordinates. Finally, we look for the general expression for radically symmetric solutions to Laplace's equation.

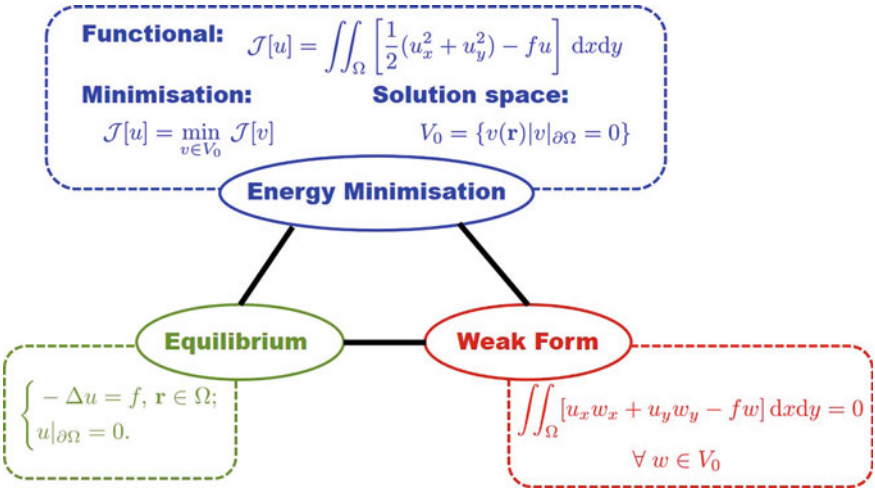

Fig. 3.3 A PDE problem (describing an equilibrium state), along with its weak formulation and the corresponding energy minimisation problem, should form a firmed "triangle". Knowing the information about one of its vertices should give rise to the derivation of the information about the other two

3.3.1 Laplace's Equation in Polar System

To this end, we consider rewriting Laplace's equation

$$\Delta u = 0$$

with polar coordinates, and the key is to transform Laplacian operator "Δ" from Cartesian to polar system.

We start with a two-dimensional case where $\Delta u = u_{xx} + u_{yy} = 0$. To this end, we introduce

$$\begin{cases} r = \sqrt{x^2 + y^2}; \\ \theta = \tan^{-1} \dfrac{y}{x}. \end{cases} \tag{3.35}$$

With Eq. (3.35), the Cartesian coordinates x and y are transformed into the polar coordinates of radius r and angle θ, and the associated Jacobean matrix is then given by

$$\begin{pmatrix} r_x & \theta_x \\ r_y & \theta_y \end{pmatrix} = \begin{pmatrix} \frac{x}{r} & -\frac{y}{r^2} \\ \frac{y}{r} & \frac{x}{r^2} \end{pmatrix}.$$

Now we need to re-express the derivatives of u with respect to the new variables r and θ. This is achieved by employing the multivariable chain rule. For instance,

$$\frac{\partial u}{\partial x} = \frac{\partial u}{\partial r} \cdot \frac{\partial r}{\partial x} + \frac{\partial u}{\partial \theta} \cdot \frac{\partial \theta}{\partial x} = \frac{\partial u}{\partial r} \cdot \frac{x}{r} - \frac{\partial u}{\partial \theta} \cdot \frac{y}{r^2}.$$

Differentiating it with respect to x again, we obtain

$$\begin{aligned}
\frac{\partial^2 u}{\partial x^2} &= \frac{\partial}{\partial x}\left(\frac{x}{r}\frac{\partial u}{\partial r} - \frac{y}{r^2}\frac{\partial u}{\partial \theta}\right) = x\frac{\partial}{\partial x}\left(\frac{1}{r}\frac{\partial u}{\partial r}\right) + \frac{1}{r}\frac{\partial u}{\partial r} - y\frac{\partial}{\partial x}\left(\frac{1}{r^2}\frac{\partial u}{\partial \theta}\right) \\
&= x\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial u}{\partial r}\right)\frac{\partial r}{\partial x} + \frac{x}{r}\frac{\partial^2 u}{\partial r \partial \theta}\frac{\partial \theta}{\partial x} + \frac{1}{r}\frac{\partial u}{\partial r} - y\frac{\partial}{\partial r}\left(\frac{1}{r^2}\frac{\partial u}{\partial \theta}\right)\frac{\partial r}{\partial x} - \frac{y}{r^2}\frac{\partial^2 u}{\partial \theta^2}\frac{\partial \theta}{\partial x} \\
&= \frac{x^2}{r^2}\left(\frac{\partial^2 u}{\partial r^2} - \frac{1}{r}\frac{\partial u}{\partial r}\right) - \frac{xy}{r^3}\frac{\partial^2 u}{\partial r \partial \theta} + \frac{1}{r}\frac{\partial u}{\partial r} - \frac{xy}{r^3}\left(\frac{\partial^2 u}{\partial r \partial \theta} - \frac{2}{r}\frac{\partial u}{\partial \theta}\right) + \frac{y^2}{r^4}\frac{\partial^2 u}{\partial \theta^2} \\
&= \frac{x^2}{r^2}\frac{\partial^2 u}{\partial r^2} - \frac{2xy}{r^3}\frac{\partial^2 u}{\partial r \partial \theta} + \frac{y^2}{r^4}\frac{\partial^2 u}{\partial \theta^2} + \left(\frac{1}{r} - \frac{x^2}{r^3}\right)\frac{\partial u}{\partial r} + \frac{2xy}{r^4}\frac{\partial u}{\partial \theta}.
\end{aligned}$$

Analogically, one may express u_{yy} by

$$\frac{\partial^2 u}{\partial y^2} = \frac{y^2}{r^2}\frac{\partial^2 u}{\partial r^2} + \frac{2xy}{r^3}\frac{\partial^2 u}{\partial r \partial \theta} + \frac{x^2}{r^4}\frac{\partial^2 u}{\partial \theta^2} + \left(\frac{1}{r} - \frac{y^2}{r^3}\right)\frac{\partial u}{\partial r} - \frac{2xy}{r^4}\frac{\partial u}{\partial \theta}.$$

Adding the above two identities returns the Laplacian operator in the two-dimensional polar system as

$$\Delta u = \frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2}. \tag{3.36}$$

The situation is now generalised to express Laplace's equation with spherical coordinates, which are related to the Cartesian coordinates by

$$\begin{cases} x = r\sin\theta\cos\varphi; \\ y = r\sin\theta\sin\varphi; \\ z = r\cos\theta, \end{cases} \tag{3.37}$$

where the radius $r > 0$; the latitude angle $\theta \in [0, \pi)$; the longitude angle $\varphi \in [0, 2\pi)$, as shown in Fig. 3.4.

Similar as the two-dimensional case, one may repeatedly employ the multivariable chain rule and obtain

$$\Delta u = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial u}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial u}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta} \cdot \frac{\partial^2 u}{\partial \varphi^2}, \tag{3.38}$$

and the derivation of Eq. (3.38) is omitted here.

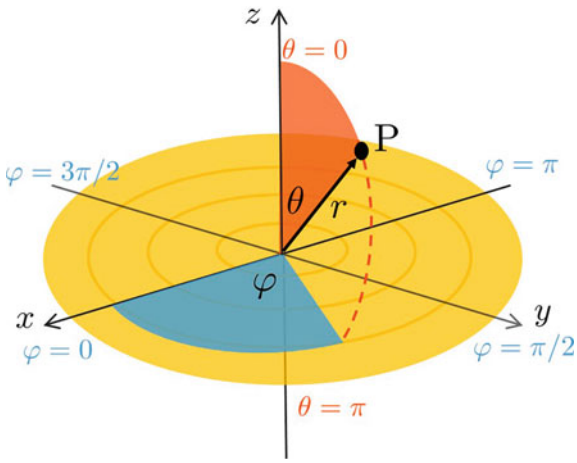

Fig. 3.4 An illustration about the spherical coordinates defined by Eq. (3.37)

3.3.2 Radial Solutions to Laplace's Equation

Now we are focused on a particular type of harmonic functions, which take a radially symmetric form. To this end, the concept of radial function should be introduced beforehand. Given a spatial point $\mathbf{r}^*$, if the value of a function at $\mathbf{r}$ is only dependent on the distance from $\mathbf{r}$ to $\mathbf{r}^*$, then we call the function a *radially symmetric function*, or simply a *radial function*. Mathematically, a radial function u is a unary function of the radius from the reference point $\mathbf{r}^*$ i.e. $u = u(|\mathbf{r} - \mathbf{r}^*|)$. For instance, the gravitational potential function ϕ defined by Eq. (3.5) is a radial function with regard to the point $\mathbf{r}^*$.

Note that when a radial function is introduced, the reference point $\mathbf{r}^*$ should be declared in advance. In other words, $\mathbf{r}^*$ serve as the parameters for the resulting radial functions. In this book, we use $u(\mathbf{r}; \mathbf{r}^*)$ to denote a function with $\mathbf{r}$ being its independent variables, and $\mathbf{r}^*$ being its parameters. Apparently, a radial function is a special case of $u(\mathbf{r}; \mathbf{r}^*)$.

A radial function that is a solution to a PDE is called a *radially symmetric solution*, or simply a *radial solution* to the PDE. If the PDE is Laplace's equation, the corresponding radial solution is also called a *radially symmetric harmonic function*. As discussed in Sect. 3.1, $1/|\mathbf{r} - \mathbf{r}^*|$ is a radial solution to three-dimensional Laplace's equation. Hence it is a radially symmetric harmonic function.

Now we look for the general form for radially symmetric harmonic functions irrespective of the dimensionality. Without loss of generalities, we set the reference point $\mathbf{r}^*$ to be the origin. Then the corresponding radial function u has only a single input of the radius r, i.e. $u = u(r)$, where $r^2 = |\mathbf{r}| = r_1^2 + \cdots + r_n^2$ with r_i the i-th independent variable (in Cartesian systems).

As from the multivariable chain rule,

$$\frac{\partial u}{\partial r_i} = \frac{\mathrm{d}u}{\mathrm{d}r} \cdot \frac{\partial r}{\partial r_i} = \frac{r_i}{r}\frac{\mathrm{d}u}{\mathrm{d}r}, \qquad \text{for } i = 1, 2, \ldots, n.$$

Note that since u is now a unary function of the radius r, the derivative of u with respect to r becomes a total derivative $\frac{\mathrm{d}u}{\mathrm{d}r}$. Differentiating the identity above with respect to r_i again gives

$$\frac{\partial^2 u}{\partial r_i^2} = \frac{\mathrm{d}^2 u}{\mathrm{d}r^2} \cdot \frac{r_i^2}{r^2} + \frac{\mathrm{d}u}{\mathrm{d}r} \cdot \left(\frac{1}{r} - \frac{r_i^2}{r^3}\right), \qquad \text{for } i = 1, 2, \ldots, n.$$

Adding the identities above together over i gives

$$\Delta u = \frac{\mathrm{d}^2 u}{\mathrm{d}r^2} + \frac{n-1}{r} \cdot \frac{\mathrm{d}u}{\mathrm{d}r} = 0.$$

Therefore, Laplace's equation gets transformed into an ordinary differential equation of the radius r. For its general solution, we re-write the ODE above by

$$\frac{1}{r^{n-1}} \frac{\mathrm{d}}{\mathrm{d}r}\left(r^{n-1} \frac{\mathrm{d}u}{\mathrm{d}r}\right) = 0. \tag{3.39}$$

When $n = 2$ or 3, the left side of Eq. (3.39) simply reproduces the derivative with respect to r in Eq. (3.36) or (3.38).

The general solution to Eq. (3.39) is thus found to be

$$u = \begin{cases} A \ln r + B, & n = 2; \\ \dfrac{A}{r^{n-2}} + B, & n \geq 3, \end{cases}$$

where A and B are coefficients to be determined.

When the reference point $\mathbf{r}^*$ is not at the origin, the general expression for radial solutions to Laplace's equation should be expressed by

$$u = \begin{cases} A \ln |\mathbf{r} - \mathbf{r}^*| + B, & n = 2; \\ A|\mathbf{r} - \mathbf{r}^*|^{n-2} + B, & n \geq 3, \end{cases}$$

for any constants A and B.

As its special cases, $u = \ln |\mathbf{r} - \mathbf{r}^*|$ is a useful two-dimensional radially symmetric harmonic function, and $u = 1/|\mathbf{r} - \mathbf{r}^*|$ is a useful three-dimensional radial solution to Laplace's equation. Both of them play a pivotal role in the derivation of the Green's function corresponding to Poisson's equation, which is to be discussed in the upcoming section.

3.4 The Method of Green's Function

In this section, we introduce the method of Green's function, another effective tool for solving linear PDE problems.

For illustration, we start with an interior boundary value problem for Laplace's equation, as given by

$$\begin{cases} \Delta u = 0, \ \mathbf{r} \in \Omega; \\ u|_{\partial\Omega} = h. \end{cases} \tag{3.40}$$

With the domain Ω fixed, the solution for problem (3.40) should be fully dependent on the boundary condition h. Thus, solving problem (3.40) is equivalent to determining the interrelationship between u and h on $\partial\Omega$.

At this stage, we have to state that the concept of Green's function offers a typical example where the motivation behind its introduction becomes quite clear only after its full derivation is given. Hence, we suggest reader follow the derivation (in patience) first, and its motivation is elucidated in the end.

3.4.1 Green's Formulae Related to Laplacian Operator

As a posterior observation, the solution u for problem (3.40) is expected to be formulated by means of an integral defined on the boundary $\partial\Omega$. For deriving that, we write

$$\int_{\Omega} u\Delta v \mathrm{d}\mathbf{r} = \int_{\partial\Omega} u\frac{\partial v}{\partial n}\mathrm{d}\Gamma - \int_{\Omega} \nabla u \cdot \nabla v \mathrm{d}\mathbf{r}, \tag{3.41}$$

where "$\frac{\partial v}{\partial n}$" denotes the derivative of v along the outer normal direction on the domain boundary $\partial\Omega$. For the derivation of Eq. (3.41), we refer to Green's formula (1.99) from the prerequisite part of Sect. 1.4. Hence, Eq. (3.41) is sometimes termed as the *first Green's formula*.

Swapping u with v in Eq. (3.41) gives

$$\int_{\Omega} v\Delta u \mathrm{d}\mathbf{r} = \int_{\partial\Omega} v\frac{\partial u}{\partial n}\mathrm{d}\Gamma - \int_{\Omega} \nabla u \cdot \nabla v \mathrm{d}\mathbf{r}.$$

Subtracting the identity above by Eq. (3.41) gives rise to the *second Green's formula*, which reads

$$\int_{\Omega} (u\Delta v - v\Delta u)\,\mathrm{d}\mathbf{r} = \int_{\partial\Omega} \left(u\frac{\partial v}{\partial n} - v\frac{\partial u}{\partial n}\right)\mathrm{d}\Gamma. \tag{3.42}$$

Note that the above derivations are conducted irrespective of the dimensionality of definition.

Now we are focused on three-dimensional cases. Our target is, for any given point $\mathbf{r}^* \in \Omega$, we seek to express the function value of the solution for problem (3.40) at $\mathbf{r}^*$, i.e. $u(\mathbf{r}^*)$, through an integral defined on $\partial\Omega$. This can be achieved with the use of the second Green's formula of Eq. (3.42), because the right side of Eq. (3.42) is already a boundary integral. Hence, the task now is to appropriately choose the function v, along with the corresponding domain of integration, so as to simplify the left side of Eq. (3.42).

3.4.2 Fundamental Solution

Here the function v in Eq. (3.42) is chosen to be the radial solution to three-dimensional Laplace's equation (with respect to the reference point $\mathbf{r}^*$), i.e.

$$v = \frac{1}{|\mathbf{r} - \mathbf{r}^*|} \triangleq \frac{1}{r},$$

where the radius $r = |\mathbf{r} - \mathbf{r}^*|$.

Since the radial function v is not well defined in the neighbourhoods of $\mathbf{r}^*$, a small sphere centred at $\mathbf{r}^*$ and of radius δ, denoted by $\mathcal{O}_\delta(\mathbf{r}^*)$, needs to be removed, when v is integrated. Thus, as shown by the shaded region in Fig. 3.5a, the domain of integration for Eq. (3.42) is set to be $\Omega \backslash \mathcal{O}_\delta(\mathbf{r}^*)$, and the second Green's formula (3.42) then reads

$$\begin{aligned} &\iiint\limits_{\Omega\backslash\mathcal{O}_\delta(\mathbf{r}^*)} \left(u\Delta\left(\frac{1}{r}\right) - \frac{1}{r}\Delta u\right) \mathrm{d}\mathbf{r} \\ &= \iint\limits_{\partial\Omega} \left[u\frac{\partial}{\partial n}\left(\frac{1}{r}\right) - \frac{1}{r}\frac{\partial u}{\partial n}\right] \mathrm{d}S_{\mathbf{r}} + \iint\limits_{\partial\mathcal{O}_\delta(\mathbf{r}^*)} \left[u\frac{\partial}{\partial n}\left(\frac{1}{r}\right) - \frac{1}{r}\frac{\partial u}{\partial n}\right] \mathrm{d}S_{\mathbf{r}}. \end{aligned} \tag{3.43}$$

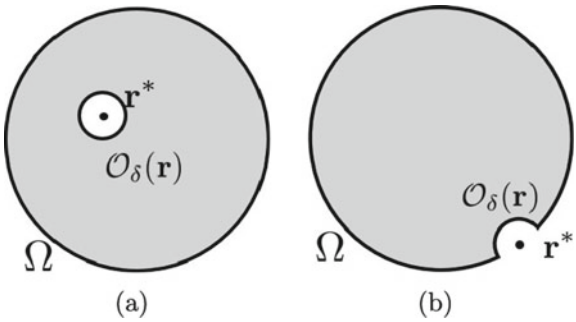

Fig. 3.5 An illustration on the domains of integration for implementing the second Green's formula (3.42): **a** that for an interior point $\mathbf{r}^*$; **b** that for a boundary point $\mathbf{r}^*$

It is worth stating again that $\mathbf{r}$ are the independent variables, and $\mathrm{d}S_{\mathbf{r}}$ calculates an infinitesimal area on the domain boundary measured in $\mathbf{r}$. Note that the domain of integration here consists of two parts: the original domain boundary $\partial\Omega$ and the spherical surface $\partial\mathcal{O}_\delta(\mathbf{r}^*)$. This is why there are two boundary integral terms appearing on the right side of Eq. (3.43).

Inside the region of $\Omega\backslash\mathcal{O}_\delta(\mathbf{r}^*)$, both u [which is harmonic as suggested by the governing equation of problem (3.40)] and v (which is a radial solution to Laplace's equation) are harmonic functions. Thus, the left side of Eq. (3.43) vanishes, and we obtain

$$\iint\limits_{\partial\Omega}\left[u\frac{\partial}{\partial n}\left(\frac{1}{r}\right)-\frac{1}{r}\frac{\partial u}{\partial n}\right]\mathrm{d}S_{\mathbf{r}}=\iint\limits_{\partial\mathcal{O}_\delta(\mathbf{r}^*)}\left[\frac{1}{r}\frac{\partial u}{\partial n}-u\frac{\partial}{\partial n}\left(\frac{1}{r}\right)\right]\mathrm{d}S_{\mathbf{r}}. \tag{3.44}$$

Now we examine the limiting behaviour of the right side of Eq. (3.44) as $\delta\to 0$. It is known that on the spherical surface $\partial\mathcal{O}_\delta(\mathbf{r}^*)$, the radius $r=|\mathbf{r}-\mathbf{r}^*|=\delta$. Thus, the first term on the right side of Eq. (3.44) is calculated by

$$\iint\limits_{\partial\mathcal{O}_\delta(\mathbf{r}^*)}\frac{1}{r}\frac{\partial u}{\partial n}\mathrm{d}S_{\mathbf{r}}=\frac{1}{\delta}\iint\limits_{\partial\mathcal{O}_\delta(\mathbf{r}^*)}\frac{\partial u}{\partial n}\mathrm{d}S_{\mathbf{r}}=\frac{1}{\delta}\left.\frac{\partial u}{\partial n}\right|_{\tilde{\mathbf{r}}\in\partial\mathcal{O}_\delta(\mathbf{r}^*)}4\pi\delta^2.$$

Here the second identity stems from the integral mean-value theorem, i.e. a continuous function integrated over a bounded domain should be equal to the area/volume of the domain multiplied by the function evaluated at a certain point in the domain (which is $\tilde{\mathbf{r}}$ here). Letting $\delta\to 0$, we have

$$\iint\limits_{\partial\mathcal{O}_\delta(\mathbf{r}^*)}\frac{1}{r}\frac{\partial u}{\partial n}\mathrm{d}S_{\mathbf{r}}=4\pi\delta\cdot\left.\frac{\partial u}{\partial n}\right|_{\tilde{\mathbf{r}}\in\partial\mathcal{O}_\delta(\mathbf{r}^*)}\to 0. \tag{3.45}$$

Now we evaluate the limiting behaviour, as $\delta\to 0$, of the second term on the right side of Eq. (3.44). Note that a normal vector on a spherical surface should always be in alignment with one of its radial directions. As suggested in Fig. 3.5a, the interior of the sphere $\mathcal{O}_\delta(\mathbf{r}^*)$ is outside the domain of integration $\Omega\backslash\mathcal{O}_\delta(\mathbf{r}^*)$. Therefore, the outer normal direction quoted by $\frac{\partial}{\partial n}$ in Eq. (3.44) should point towards the centre $\mathbf{r}^*$, that is, in opposition against the corresponding radial direction. Mathematically, $\frac{\partial}{\partial n}=-\frac{\partial}{\partial r}$. Thus, the second term in Eq. (3.44) reads

$$\begin{aligned}\iint\limits_{\partial\mathcal{O}_\delta(\mathbf{r}^*)}u\frac{\partial}{\partial n}\left(\frac{1}{r}\right)\mathrm{d}S_{\mathbf{r}}&=-\iint\limits_{\partial\mathcal{O}_\delta(\mathbf{r}^*)}u\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{1}{r}\right)\mathrm{d}S_{\mathbf{r}}=\iint\limits_{\partial\mathcal{O}_\delta(\mathbf{r}^*)}u\cdot\frac{1}{r^2}\,\mathrm{d}S_{\mathbf{r}}\\&=\frac{1}{\delta^2}\iint\limits_{\partial\mathcal{O}_\delta(\mathbf{r}^*)}u\,\mathrm{d}S_{\mathbf{r}}=\frac{1}{\delta^2}\cdot 4\pi\delta^2\cdot u|_{\tilde{\mathbf{r}}\in\partial\mathcal{O}_\delta(\mathbf{r}^*)},\end{aligned} \tag{3.46}$$

where the fact that $r = \delta$ on $\partial\mathcal{O}_\delta(\mathbf{r}^*)$ and the integral mean-value theorem is employed again.

Note that $\tilde{\mathbf{r}} \to \mathbf{r}^*$, as $\delta \to 0$. Therefore,

$$\iint\limits_{\partial\mathcal{O}_\delta(\mathbf{r}^*)} u\frac{\partial}{\partial n}\left(\frac{1}{r}\right)\mathrm{d}S_{\mathbf{r}} \to 4\pi u(\mathbf{r}^*), \text{ as } \delta \to 0. \tag{3.47}$$

Inserting Eqs. (3.45) and (3.47) into (3.44) and letting $r = |\mathbf{r} - \mathbf{r}^*|$, we derive its limiting case as $\delta \to 0$ by

$$u\left(\mathbf{r}^*\right) = \frac{1}{4\pi}\iint\limits_{\partial\Omega}\left[\frac{1}{|\mathbf{r}-\mathbf{r}^*|}\cdot\frac{\partial u}{\partial n} - u\frac{\partial}{\partial n}\left(\frac{1}{|\mathbf{r}-\mathbf{r}^*|}\right)\right]\mathrm{d}S_{\mathbf{r}}. \tag{3.48}$$

Up to this stage, our original goal, to express the solution by means of a boundary integral, is fulfilled. Note that the radial function $\frac{1}{4\pi|\mathbf{r}-\mathbf{r}^*|}$ plays an essential role in the derivation of Eq. (3.48). It is not only a harmonic equation in $\Omega\backslash\mathcal{O}_\delta(\mathbf{r}^*)$ [so as to make the left side of Eq. (3.43) vanish], but also help express $u(\mathbf{r}^*)$ through a limiting procedure [given by Eq. (3.47)].

By playing both roles mentioned above, the function $v = \frac{1}{4\pi|\mathbf{r}-\mathbf{r}^*|}$ is termed as a *fundamental solution* to three-dimensional Poisson's/Laplace's equation. Note that there can be infinitely many fundamental solutions to a PDE. For example, $\frac{1}{4\pi|\mathbf{r}-\mathbf{r}^*|}$ added by a three-dimensional harmonic function can still play the two roles mentioned above. Hence, it is also a fundamental solution to the corresponding harmonic equation.

If the reference point $\mathbf{r}^*$ falls on the domain boundary $\partial\Omega$, as suggested by Fig. 3.5b, a similar strategy as above should still be adopted. But this time, only a half sphere centred at $\mathbf{r}^*$ is removed when the second Green's formula is implemented. Consequently, when the integral mean-value theorem is used, the domain area is that of a half sphere, i.e. $2\pi\delta^2$. Thus, we derive

$$u|_{\mathbf{r}^*\in\partial\Omega} = \frac{1}{2\pi}\iint\limits_{\partial\Omega}\left[\frac{1}{|\mathbf{r}-\mathbf{r}^*|}\cdot\frac{\partial u}{\partial n} - u\frac{\partial}{\partial n}\left(\frac{1}{|\mathbf{r}-\mathbf{r}^*|}\right)\right]\mathrm{d}S_{\mathbf{r}}. \tag{3.49}$$

3.4.3 Derivation of Green's Function

If Eq. (3.48) is employed to express the solution u for problem (3.40), one is expected to know both the function values of u and its normal derivatives on the domain boundary $\partial\Omega$. As a result, the information needed goes beyond what an interior boundary value problem governed by Poisson's/Laplace's equation can provide. Exemplified by problem (3.40), only the function values are given on $\partial\Omega$, with $\frac{\partial u}{\partial n}$ on the boundary

still being left unknown. This severely limits the direct use of Eq. (3.48) for solving problem (3.40).

There are several ways proposed to overcome this issue. One is to use Eq. (3.49) to first compute the unknown piece of information on the boundary. Then Eq. (3.40) is adopted to compute the value of u in the domain interior. This forms the theoretical basis of the boundary element method, which is not mentioned further.

Another way to address the issue, is to analytically annihilate the boundary integral which contains the unknown information. For this purpose, another (unspecified yet) three-dimensional harmonic function $g(\mathbf{r}; \mathbf{r}^*)$ with $\mathbf{r}^*$ being its parameters is introduced. The second Green's formula (3.42) is employed again with $v = g$ this time. Since the harmonic function g is now well defined throughout the whole domain for $\mathbf{r} \in \Omega$, we write

$$0 = \iiint_{\Omega} (u\Delta g - g\Delta u)\,\mathrm{d}\mathbf{r} = \iint_{\partial\Omega} \left(u\frac{\partial g}{\partial n} - g\frac{\partial u}{\partial n}\right)\mathrm{d}S_{\mathbf{r}}. \tag{3.50}$$

To specify g, we further require that the function values of g on $\partial\Omega$ coincide with that of the fundamental solution $\frac{1}{4\pi|\mathbf{r}-\mathbf{r}^*|}$. In other words, $g(\mathbf{r}; \mathbf{r}^*)$ satisfies another PDE problem (parameterised by $\mathbf{r}^*$) formulated through

$$\begin{cases} \Delta g(\mathbf{r}; \mathbf{r}^*) = 0, \ \ \mathbf{r} \in \Omega; \\ g|_{\mathbf{r}\in\partial\Omega} = \left.\dfrac{1}{4\pi|\mathbf{r}-\mathbf{r}^*|}\right|_{\mathbf{r}\in\partial\Omega}. \end{cases} \tag{3.51}$$

Adding Eqs. (3.48) with (3.50), as g and $\frac{1}{4\pi|\mathbf{r}-\mathbf{r}^*|}$ coincide with each other on $\partial\Omega$, the terms containing $\frac{\partial u}{\partial n}$ are mutually cancelled, leading to

$$u\left(\mathbf{r}^*\right) = -\iint_{\partial\Omega} u \cdot \frac{\partial}{\partial n}\left(\frac{1}{4\pi|\mathbf{r}-\mathbf{r}^*|} - g(\mathbf{r}; \mathbf{r}^*)\right)\mathrm{d}S_{\mathbf{r}}. \tag{3.52}$$

To this stage, we define

$$G(\mathbf{r}; \mathbf{r}^*) = \frac{1}{4\pi|\mathbf{r}-\mathbf{r}^*|} - g(\mathbf{r}; \mathbf{r}^*). \tag{3.53}$$

Inserting it into Eq. (3.52) finally expresses the solution for problem (3.40) by

$$u\left(\mathbf{r}^*\right) = -\iint_{\partial\Omega} h \cdot \frac{\partial G}{\partial n}\,\mathrm{d}S_{\mathbf{r}}, \tag{3.54}$$

where the boundary condition $u|_{\partial\Omega} = h$ is adopted.

The function $G(\mathbf{r}; \mathbf{r}^*)$ is called the *Green's function* for problem (3.40). Equation (3.54) actually illustrates how the method of Green's function works for solving a linear PDE problem for Laplace's equation and imposed with Dirichlet boundary condition. The Green function G defined by Eq. (3.53) is independent of the boundary condition h, but only depends on the Laplacian operator, as well as the domain Ω. Therefore, if G is known in advance, the solution u for problem (3.40) can be literally expressed by means of Eq. (3.54) for any Dirichlet boundary condition given through h. More features shown by the method of Green's function are discussed in the upcoming subsection.

The derivation for the three-dimensional Green's function (3.54) can be generalised to devise the Green's function in various other problems for Laplace's equation. For the two-dimensional situation, for instance, one may follow the derivation procedure here to derive the corresponding *fundamental solution* of two-dimensional Poisson's equation to be

$$v(\mathbf{r}; \mathbf{r}^*) = -\frac{1}{2\pi} \ln |\mathbf{r} - \mathbf{r}^*|,$$

and the corresponding Green's function can be constructed accordingly (see Exercise 3.9).

When the boundary condition is no longer Dirichlet type, the boundary condition for the introduced function g [as defined by problem (3.51)] should be modified accordingly (also see Exercise 3.9). Moreover, when the domain of definition Ω becomes unbounded, the resulting PDE problem becomes an exterior boundary value problem. And Green's function for the case of three-dimensional half space, as illustrated in Sect. 3.5.1, may offer some hints on constructing the Green's function for general exterior boundary value problems.

3.4.4 Properties of Green's Function

Some properties exhibited by Green's function (3.53) are outlined as follows.
Property 3.1 As $\mathbf{r} \to \mathbf{r}^*$, G tends to infinity at a same rate as $\frac{1}{4\pi r}$, i.e.

$$G \sim \mathcal{O}\left(\frac{1}{4\pi|\mathbf{r} - \mathbf{r}^*|}\right), \text{ as } \mathbf{r} \to \mathbf{r}^*.$$

Property 3.2 $G|_{\partial\Omega} = 0$, as suggested from the boundary condition for $g(\mathbf{r}; \mathbf{r}^*)$ from problem (3.51).
Property 3.3 The inputs of G are communicative, i.e.

$$G(\mathbf{r}; \mathbf{s}) = G(\mathbf{s}; \mathbf{r})$$

hold for any spatial positions $\mathbf{r}$ and $\mathbf{s}$.

Property 3.4 For any domain Ω_0 enclosing the reference point $\mathbf{r}^*$, we have

$$\iint\limits_{\partial\Omega_0} \frac{\partial G}{\partial n} \mathrm{d}S_{\mathbf{r}} = -1. \tag{3.55}$$

These properties are not difficult to verify, and knowing their proof is helpful in the sense of developing more solid understanding over the concept of Green's function.

The above-listed properties in a physical viewpoint are worth being mentioned. We know that for a unit point charge located at $\mathbf{r}^*$, it induces an electric potential of $\frac{1}{4\pi|\mathbf{r}-\mathbf{r}^*|}$, while the electric permittivity is set to be unity. In this sense, G defined by Eq. (3.53) should correspond to the electric potential due to a certain charge distribution. Inside Ω, it can be verified that $\Delta G = 0$ for $\mathbf{r} \neq \mathbf{r}^*$, indicating that the charge density [as from Gauss's law (3.11)] is zero away from $\mathbf{r}^*$. Near the point $\mathbf{r}^*$, as from property 3.1, the electric charge distribution that induces G should be the same as a unit charge. Therefore, no other charges (apart from the unit charge at $\mathbf{r}^*$) are at present inside Ω.

Property 3.2 indicates that the boundary $\partial\Omega$ is an iso-potential surface of zero value. It corresponds to the situation where a metallic body is connected to the ground. By doing that, an extra charge distribution gets induced (outside the domain Ω), so as to keep the boundary surface being an iso-potential surface, which is known as the *electrostatic screening* effect. With reference to Eq. (3.51), the electric potential due to the corresponding induced charges (outside Ω) is just measured by $-g(\mathbf{r}; \mathbf{r}^*)$. Therefore, Green's function (3.53) simply formulates the superposed electric potential due to both a unit charge at $\mathbf{r}^*$ and the induced charges outside Ω, such that $\partial\Omega$ becomes an iso-potential surface.

From this viewpoint, the electric potential at $\mathbf{s}$ due to the corresponding induced charge at $\mathbf{r}$ should be identical to the electric potential at $\mathbf{r}$ due to a same charge at $\mathbf{s}$, and property 3.3 is thus justified. The communicativeness in the inputs of Green function defined by (3.53) offers one example about the *principles of reciprocity* in physics.

3.4.5 Problems for Poisson's Equation

When the governing equation in problem (3.40) is switched to Poisson's equation, i.e.

$$\begin{cases} -\Delta u = f, \ \mathbf{r} \in \Omega; \\ u|_{\partial\Omega} = h. \end{cases} \tag{3.56}$$

One may follow the derivation for Eq. (3.48) to obtain

$$u\left(\mathbf{r}^*\right) = \frac{1}{4\pi}\iint\limits_{\partial\Omega}\left[\frac{1}{|\mathbf{r}-\mathbf{r}^*|}\cdot\frac{\partial u}{\partial n} - u\cdot\frac{\partial}{\partial n}\left(\frac{1}{|\mathbf{r}-\mathbf{r}^*|}\right)\right]\mathrm{d}S_{\mathbf{r}} - \frac{1}{4\pi}\iiint\limits_{\Omega}\frac{f(\mathbf{r})\,\mathrm{d}\mathbf{r}}{|\mathbf{r}-\mathbf{r}^*|}, \tag{3.57}$$

where the last integral stems from the fact that Δu does not vanish this time. As a result, an extra term occurs from the left side of Eq. (3.43).

In particular, when $\Omega = \mathbb{R}^3$ and $u \sim \frac{1}{4\pi|\mathbf{r}-\mathbf{r}^*|}$ as $|\mathbf{r}| \to \infty$, Eq. (3.57) is thus simplified by

$$u\left(\mathbf{r}^*\right) = -\frac{1}{4\pi}\iiint\limits_{\mathbb{R}^3}\frac{f(\mathbf{r})\mathrm{d}\mathbf{r}}{|\mathbf{r}-\mathbf{r}^*|}. \tag{3.58}$$

which agrees with the discussion from the electrostatic case in Sect. 3.1.2. As from Eq. (3.58), the solution u is expressed by the convolution of $-f(\mathbf{r})$, the right side of the governing equation, with a fundamental solution of the homogeneous PDE, which is Laplace's equation here.

When Ω is bounded, if Eq. (3.57) is employed to express $u(\mathbf{r}^*)$, both function values of u and its partial derivatives on $\partial\Omega$ are needed. Hence similar as the case for Laplace's equation, the parameterised harmonic function $g(\mathbf{r}, \mathbf{r}^*)$ satisfying problem (3.51) should be introduced. In this scenario, the left side of Eq. (3.50) no longer vanishes, leading to

$$\iiint\limits_{\Omega} f(r)g(\mathbf{r};\mathbf{r}^*)\,\mathrm{d}\mathbf{r} = \iiint\limits_{\Omega}\left(u\Delta g - g\Delta u\right)\,\mathrm{d}\mathbf{r} = \iint\limits_{\partial\Omega}\left(u\frac{\partial g}{\partial n} - g\frac{\partial u}{\partial n}\right)\mathrm{d}S_{\mathbf{r}}. \tag{3.59}$$

Subtracting Eq. (3.57) by (3.59), and introducing the function $G(\mathbf{r};\mathbf{r}^*)$ defined by Eq. (3.53), we finally express the solution to problem (3.56) by

$$u\left(\mathbf{r}^*\right) = -\iint\limits_{\partial\Omega} h(\mathbf{r})\cdot\frac{\partial G}{\partial n}\,\mathrm{d}S_{\mathbf{r}} - \iiint\limits_{\Omega} f(\mathbf{r})G(\mathbf{r};\mathbf{r}^*)\,\mathrm{d}\mathbf{r}. \tag{3.60}$$

It is observed that, when the domain Ω and the type of boundary conditions are fixed, Laplace's equation shares a same Green's formula with Poisson's equation. The concept is generalisable for general linear PDE problems. The Green's function of a linear PDE depends on the involved differential operator, but not whether the PDE is homogeneous.

3.4.6 Final Remarks

Green's function provides an effective means for solving linear PDE problems. For the present case, once G defined by Eq. (3.53) is available, one can then solve problem (3.56) with Eq. (3.53), for any $f(\mathbf{r})$ and boundary condition $h(\mathbf{r})$.

Based on the derivations above, the formulation of Green' function $G(\mathbf{r}; \mathbf{r}^*)$ is found to depend on three key factors. The first factor is the type of the (linear) differential operator defining the PDE of interest. In the present case, it is the Laplacian operator. The second factor is the type of imposed boundary conditions. For the present case, Dirichlet boundary condition is concerned, while formulation for other types should be worked out analogically (see Exercise 3.9). The third key factor co-determining the Green's function for a PDE problem is the domain of definition Ω. This means, even though the previous two factors stay unchanged, a change in the shape of Ω should result in a different Green's function. This turns out to be a disadvantageous feature regarding applying the method of Green's function. When the domain of definition keeps changing, the corresponding Green's function should be calculated repeatedly, resulting in rather high computational costs.

Another issue limiting the implementation of the method of Green's function is that, one needs to solve an extra PDE problem (3.51) for $g(\mathbf{r}, \mathbf{r}^*)$, so as to express $G(\mathbf{r}, \mathbf{r}^*)$. In most cases especially when Ω is geometrically irregular, solving for the parametric function $g(\mathbf{r}, \mathbf{r}^*)$ seems to be far more difficult than solving the original problem (3.56), which contains no parameters. Therefore, being an analytical approach, the method of Green's function may be quite effective when the domain Ω is geometrically regular. This motivates the discussion in the upcoming section, where two regular-shape domains, the half space and the spherical domains, are of our attentions.

3.5 Image Method for Electric Potentials

In this section, we consider deriving the Green's functions for problems governed by Poisson's equation, which are defined in domains of regular shape, such as the three-dimensional half space and spheres.

When the governing equation is Poisson's equation with Dirichlet boundary condition imposed on the boundary, as suggested in Sect. 3.4, the associated Green's function is generally expressed by

$$G(\mathbf{r}; \mathbf{r}^*) = \frac{1}{4\pi|\mathbf{r} - \mathbf{r}^*|} - g(\mathbf{r}; \mathbf{r}^*), \tag{3.61}$$

where g is recalled to be a harmonic function that solves problem (3.51).

The physical implication of Green's function (3.61) has been discussed in Sect. 3.4.4. Suppose that a unit point charge is located at $\mathbf{r}^*$. When the domain

is connected to the ground, a redistribution of charges outside Ω is induced, leading to an extra electric potential of $-g(\mathbf{r};\mathbf{r}^*)$. As a result, the domain boundary $\partial\Omega$ becomes an iso-potential surface of zero value. This just summarises the key idea underlying the *image method for electric potentials* to be introduced in this section. We seek to determine, from a physical viewpoint, the expression for Green's function (3.61), by identifying the corresponding induced charge distribution outside Ω, such that $\partial\Omega$ becomes an iso-potential surface.

3.5.1 The Case in Three-Dimensional Half Space

Let us consider

$$\begin{cases} \Delta u = 0, \ (x, y, z) \in \mathbb{R} \times \mathbb{R} \times \mathbb{R}^+; \\ u|_{z=0} = h(x, y); \\ \lim\limits_{\sqrt{x^2+y^2+z^2}\to\infty} u(x, y, z) = 0. \end{cases} \tag{3.62}$$

Here the domain of definition Ω is the three-dimensional half space $\{(x, y, z)|z > 0\}$. Note that Ω becomes unbounded now. Hence being a part of an exterior boundary value problem, the behaviour at infinity should be declared in addition to the boundary condition imposed on the plane of $z = 0$.

Then we seek to express the Green's function for problem (3.62). Our aim is to determine the distribution of the induced charges in the other half plane ($z < 0$), such that the plane of $z = 0$ is an iso-potential surface.

It is known that for a pair of electric dipole, the equi-distant plane of the two consisting particles is an iso-potential surface of zero value. Suppose that a unit charge is located at $\mathbf{r}^*$, as shown in Fig. 3.6. Then the $z = 0$ plane should become an iso-potential plane, when a negative unit charge is put at the mirrored position of $\mathbf{r}^*$ about $z = 0$.

Mathematically, this mirrored position is given by $\tilde{\mathbf{r}}^* = (x^*, y^*, -z^*)$, and the induced (negative unit) charge there exerts an electric potential of

$$-g(\mathbf{r};\mathbf{r}^*) = -\frac{1}{4\pi\sqrt{(x-x^*)^2+(y-y^*)^2+(z+z^*)^2}}. \tag{3.63}$$

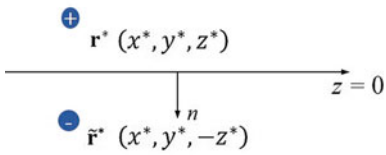

Fig. 3.6 The electrostatic image of a half space

Inserting Eq. (3.63) into (3.61) gives

$$G = \frac{1}{4\pi}\left(\frac{1}{\sqrt{(x-x^*)^2+(y-y^*)^2+(z-z^*)^2}} - \frac{1}{\sqrt{(x-x^*)^2+(y-y^*)^2+(z+z^*)^2}}\right). \tag{3.64}$$

Equation (3.64) is introduced in a physical aspect. We still need to verify [with reference to problem (3.51)] that it is actually the Green's function desired. Thus, one needs to show that g given by Eq. (3.63) should meet the following conditions: (a) g is a harmonic function for $\mathbf{r} \in \mathbb{R} \times \mathbb{R} \times \mathbb{R}^+$; (b) g equals $\frac{1}{4\pi|\mathbf{r}-\mathbf{r}^*|}$ on $z = 0$ [in comparison with Problem (3.51)]; (c) g tends to 0 at infinity.

As for condition (a), Eq. (3.63) is actually a radial solution to Laplace's equation, with its reference point outside the half space of interest. Thus, condition (a) is met. Condition (b) can be checked straight forward by letting $z = 0$ in g, i.e.

$$g|_{z=0} = \frac{1}{4\pi\sqrt{(x-x^*)^2+(y-y^*)^2+(z^*)^2}} = \left.\frac{1}{4\pi|\mathbf{r}-\mathbf{r}^*|}\right|_{z=0}.$$

Meanwhile, it can be calculated that $\lim_{|\mathbf{r}|\to\infty} g = 0$, and thus condition (c) is also met.

Therefore, we conclude that Eq. (3.64) serves to be the Green's function for problem (3.62). With reference to Eq. (3.54), the solution for problem (3.62) is then expressed by

$$u(x^*, y^*, z^*) = -\iint\limits_{z=0} h\frac{\partial G}{\partial n}\mathrm{d}S_{\mathbf{r}}. \tag{3.65}$$

On the $z = 0$ plane, $\mathrm{d}S_{\mathbf{r}} = \mathrm{d}x\mathrm{d}y$, and the outer normal vector lies in the same direction of $-z$. Thus, we have

$$\left.\frac{\partial G}{\partial n}\right|_{z=0} = -\left.\frac{\partial G}{\partial z}\right|_{z=0} = -\frac{z^*}{2\pi((x-x^*)^2+(y-y^*)^2+(z^*)^2)^{\frac{3}{2}}}.$$

Inserting it into Eq. (3.65) finally expresses the solution for problem (3.62) by

$$u(x^*, y^*, z^*) = \frac{z^*}{2\pi}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\frac{h(x,y)\mathrm{d}x\mathrm{d}y}{[(x-x^*)^2+(y-y^*)^2+(z^*)^2]^{\frac{3}{2}}}. \tag{3.66}$$

3.5.2 The Case in a Spherical Domain

When the domain of definition becomes a spherical region, say, $\Omega = \{\mathbf{r}||\mathbf{r}| < R\}$, the corresponding interior boundary value problem can be formulated by

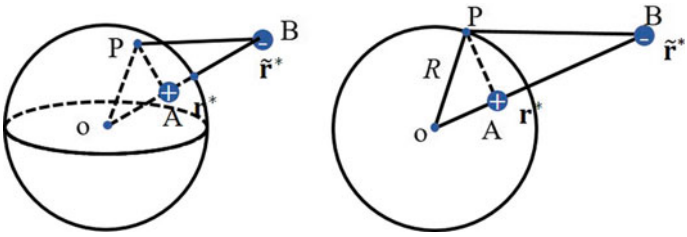

Fig. 3.7 Electrostatic image about a spherical surface. The point B which makes Eq. (3.68) hold is the inversion point of A about the spherical surface

$$\begin{cases} \Delta u = 0, \ \mathbf{r} \in \Omega; \\ u|_{\partial\Omega} = h(\mathbf{r}). \end{cases} \tag{3.67}$$

Here the domain Ω, as shown in Fig. 3.7a, is a sphere centred at the origin, which is denoted by O.

Now we derive the corresponding Green's formula with reference to an arbitrary reference point inside the sphere, say $\mathbf{r}^*$ at point A in Fig. 3.7a.

We then extend the vector $\overrightarrow{\mathrm{OA}}$ outside the sphere to point B, such that

$$|\overrightarrow{\mathrm{OA}}| \cdot |\overrightarrow{\mathrm{OB}}| = R^2, \tag{3.68}$$

where $|\overrightarrow{\mathrm{OA}}|$ denotes the length of the vector $\overrightarrow{\mathrm{OA}}$, and so on. Here the point B is called the *inversion point* of A about the spherical surface. Suppose that the coordinates of B are given by $\tilde{\mathbf{r}}^*$. Then according to Eq. (3.68), we have

$$\tilde{\mathbf{r}}^* = \frac{R^2}{|\mathbf{r}^*|^2}\mathbf{r}^*. \tag{3.69}$$

Now let us suppose that the Green's formula in this scenario has the form of

$$G(\mathbf{r}; \mathbf{r}^*) = \frac{1}{4\pi}\left(\frac{1}{|\mathbf{r} - \mathbf{r}^*|} - \frac{q}{|\mathbf{r} - \tilde{\mathbf{r}}^*|}\right). \tag{3.70}$$

Eq. (3.70) corresponds to the situation where a unit charge is located at A, while another point charge of electric quantity $-q$ is put at its inversion point B.

But we still need to determine q, such that the spherical surface becomes isopotential. To this end, a point P on $\partial\Omega$ is arbitrarily chosen, as shown in Fig. 3.7b. Based on Eq. (3.68) and the fact that $\angle\mathrm{POA} = \angle\mathrm{BOP}$, one should conclude that the triangle formed by POA is similar to the triangle formed by BOP. Hence

$$\frac{|\overrightarrow{\mathrm{PB}}|}{|\overrightarrow{\mathrm{PA}}|} = \frac{|\overrightarrow{\mathrm{OP}}|}{|\overrightarrow{\mathrm{OA}}|}.$$

Given that $|\overrightarrow{\mathrm{OP}}| = R$; $|\overrightarrow{\mathrm{OA}}| = |\mathbf{r}^*|$; $|\overrightarrow{\mathrm{PA}}| = |\mathbf{r}_\mathrm{P} - \mathbf{r}^*|$; $|\overrightarrow{\mathrm{PB}}| = |\mathbf{r}_\mathrm{P} - \tilde{\mathbf{r}}^*|$ with $\mathbf{r}_\mathrm{P}$ being the coordinates of P, the identity above is then reformulated by

$$\frac{1}{|\mathbf{r}_\mathrm{P} - \mathbf{r}^*|} - \frac{1}{|\mathbf{r}_\mathrm{P} - \tilde{\mathbf{r}}^*|} \cdot \frac{R}{|\mathbf{r}^*|} = 0. \tag{3.71}$$

Comparing Eq. (3.71) with (3.70), we see that as long as $q = \frac{R}{|\mathbf{r}^*|}$, $G|_{\mathbf{r}=\mathbf{r}_\mathrm{P}} = 0$ holds for any $\mathbf{r}_\mathrm{P} \in \partial\Omega$, and $\partial\Omega$ thus becomes an iso-potential surface.

Therefore, the Green's function corresponding to problem (3.67) is expressed by

$$G(\mathbf{r}; \mathbf{r}^*) = \frac{1}{4\pi}\left(\frac{1}{|\mathbf{r} - \mathbf{r}^*|} - \frac{R}{|\mathbf{r}^*|} \cdot \frac{1}{|\mathbf{r} - \tilde{\mathbf{r}}^*|}\right). \tag{3.72}$$

To fully solve problem (3.67) with Eq. (3.54), one also needs to express the normal derivative of G on $\partial\Omega$. But the normal direction $\mathbf{n}$ coincides with the radial direction here. For simplicity, we introduce a spherical coordinate system (ρ, θ, φ) defined by

$$\begin{cases} x = \rho \sin\theta \cos\varphi; \\ y = \rho \sin\theta \sin\varphi; \\ z = \rho \cos\theta, \end{cases}$$

where $\rho \in [0, R]$, $\theta \in [0, \pi)$, and $\varphi \in [0, 2\pi)$. Further we let

$$\rho = |\mathbf{r}|, \qquad \rho^* = |\overrightarrow{\mathrm{OA}}| = |\mathbf{r}^*|, \qquad \tilde{\rho}^* = |\overrightarrow{\mathrm{OB}}| = |\tilde{\mathbf{r}}^*| = \frac{R^2}{\rho^*}.$$

Then the Green's function (3.72) is re-expressed in this spherical system by

$$G = \frac{1}{4\pi}\left(\frac{1}{\sqrt{\rho^2 + (\rho^*)^2 - 2\rho^*\rho\cos\gamma}} - \frac{R}{\sqrt{(\rho\rho^*)^2 + 2R^2\rho\rho^*\cos\gamma + R^4}}\right), \tag{3.73}$$

where γ measures the angle between $\mathbf{r}$ and $\mathbf{r}^*$.[1] Then we have

$$\left.\frac{\partial G}{\partial n}\right|_{\partial\Omega} = \left.\frac{\partial G}{\partial \rho}\right|_{\rho=R} = \frac{1}{4\pi R} \cdot \frac{R^2 - (\rho^*)^2}{(R^2 + (\rho^*)^2 - 2R\rho^*\cos\gamma)^{\frac{3}{2}}}.$$

[1] Since $\mathbf{r} = \rho(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)^\mathrm{T}$, $\mathbf{r}^* = \rho^*(\sin\theta^*\cos\varphi^*, \sin\theta^*\sin\varphi^*, \cos\theta^*)^\mathrm{T}$ the angle between them given by γ satisfies

$$\cos\gamma = \cos\theta\cos\theta^* + \sin\theta\sin\theta^*\cos(\varphi - \varphi^*).$$

.

Incorporating it with Eq. (3.60) solves problem (3.67) by

$$u(\mathbf{r}^*) = \frac{1}{4\pi R} \iint\limits_{|\mathbf{r}|=R} \frac{(R^2 - (\rho^*)^2)h(\mathbf{r})\mathrm{d}S_{\mathbf{r}}}{(R^2 + (\rho^*)^2 - 2R\rho^* \cos\gamma)^{\frac{3}{2}}}. \tag{3.74}$$

Eq. (3.74) is sometimes called *Poisson's formula*.

The key to the derivation of the Green's function (3.72) is to find the inversion point B of an interior point A in Fig. 3.7. The idea also works for deriving Green's function for the problem governed by Poisson's equation defined in a two-dimensional circle, and one may refer to Exercise 3.12 for practice.

3.6 Solution Uniqueness

The uniqueness of solutions for problems governed by Poisson's equation is discussed in this section. Several intrinsic properties of harmonic functions, as indicated by the mean-value formula and the (strong) maximum principle, are also mentioned. Similar as other linear cases, when demonstrating solution uniqueness, one simply looks into problems with everything being homogeneous.

3.6.1 Mean-Value Formula

Lemma 1 *If a function u is harmonic in* Ω*, and it is continuous towards the boundary* $\partial\Omega$*, then*

$$\int\limits_{\partial\Omega} \frac{\partial u}{\partial n}\,\mathrm{d}\Gamma = 0$$

holds, where $\mathrm{d}\Gamma$ *is an infinitesimal boundary element.*

Proof On using Green's formula:

$$0 = \int\limits_{\Omega} \Delta u \mathrm{d}\mathbf{r} = \int\limits_{\partial\Omega} \frac{\partial u}{\partial n}\,\mathrm{d}\Gamma. \qquad \square$$

The lemma above may be perceived from a physical viewpoint. When no electric charges are inside Ω, according to Eq. (3.13), the electric potential should satisfy Laplace's equation in Ω, and the electric flux over the boundary $\partial\Omega$, which is calculated by the boundary integral appearing in the lemma, should be conserved to be zero. The lemma can also be understood in the context of heat conduction. If u denotes the temperature distribution within Ω, $\int_{\partial\Omega} \frac{\partial u}{\partial n}\,\mathrm{d}\Gamma$ is proportional to the rate of the heat units flowing across the surface $\partial\Omega$. When u is harmonic, it describes a

thermally equilibrated state in the absence of heat sources/sinks inside Ω. Hence the net heat flow across $\partial\Omega$ should vanish all the time. Otherwise the equilibrated state cannot be maintained.

The lemma sees one of its applications in ensuring the (non-)existence of a harmonic equation with its normal derivative prescribed on the boundary of a closed region. Suppose that Neumann boundary condition (3.19b) is considered, i.e. $\frac{\partial u}{\partial n}\Big|_{\partial\Omega} = h$. If u is harmonic in Ω, from the lemma, we obtain $\int_{\partial\Omega} h \mathrm{d}\Gamma = \int_{\partial\Omega} \frac{\partial u}{\partial n}\,\mathrm{d}\Gamma = 0$. Therefore, when $\int_{\partial\Omega} h \mathrm{d}\Gamma \neq 0$, the corresponding PDE problem should yield no solutions.

On using the lemma, a *mean-value formula* for three-dimensional harmonic function is introduced.

Mean-value formula for three-dimensional cases. Suppose that u is harmonic in a three-dimensional domain, say, Ω. Then for any balls falling inside Ω, i.e. $\mathcal{O}_a(\mathbf{r}^*) \subset \Omega$, the following mean-value formula should hold:

$$u(\mathbf{r}^*) = \frac{1}{4\pi a^2} \iint\limits_{\partial\mathcal{O}_a(\mathbf{r}^*)} u(\mathbf{r}) \mathrm{d}S_{\mathbf{r}}. \tag{3.75}$$

Proof On specifying the domain Ω in Eq. (3.48) to be $\mathcal{O}_a(\mathbf{r}^*)$, we have

$$u(\mathbf{r}^*) = \frac{1}{4\pi} \iint\limits_{\partial\mathcal{O}_a(\mathbf{r}^*)} \left[\frac{1}{r}\frac{\partial u}{\partial n} - u\frac{\partial}{\partial n}\left(\frac{1}{r}\right)\right] \mathrm{d}S_{\mathbf{r}}, \tag{3.76}$$

where $r = |\mathbf{r} - \mathbf{r}^*|$. Note that on $\partial\mathcal{O}_a(\mathbf{r}^*)$, $r = a$. Thus, combining the lemma above, the first term on the right side of Eq. (3.76) is calculated by

$$\frac{1}{4\pi} \iint\limits_{\partial\mathcal{O}_a(\mathbf{r}^*)} \frac{1}{r}\frac{\partial u}{\partial n} \mathrm{d}S_{\mathbf{r}} = \frac{1}{4\pi a} \iint\limits_{\partial\mathcal{O}_a(\mathbf{r}^*)} \frac{\partial u}{\partial n} \mathrm{d}S = 0.$$

Meanwhile, the second term on the right side of Eq. (3.76) is calculated by

$$\frac{1}{4\pi} \int\limits_{\partial\mathcal{O}_a(\mathbf{r}^*)} u\frac{\partial}{\partial n}\left(\frac{1}{r}\right) \mathrm{d}S_{\mathbf{r}} = \frac{1}{4\pi} \int\limits_{\partial\mathcal{O}_a(\mathbf{r}^*)} u\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{1}{r}\right) \mathrm{d}S_{\mathbf{r}} = -\frac{1}{4\pi a^2} \int\limits_{\partial\mathcal{O}_a(\mathbf{r}^*)} u\,\mathrm{d}S_{\mathbf{r}},$$

where we have made use of the fact that the outer normal vector on $\partial\mathcal{O}_a(\mathbf{r}^*)$ should coincide with the corresponding radial direction. Incorporating the results above into Eq. (3.76) verifies the mean-value formula (3.75). □

The mean-value formula also sees its two-dimensional counterpart, as more details can be found in Exercise 3.15.

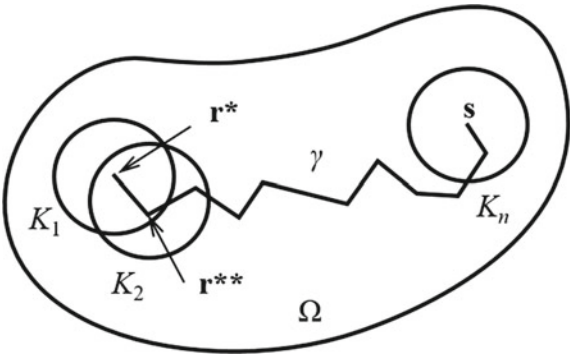

Fig. 3.8 A diagram showing the idea for justifying the maximum principle in Sect. 3.6.2

3.6.2 Maximum Principle

The **maximum principle** for harmonic functions. If u is a non-constant harmonic function in Ω, and u is continuous towards its boundary, then u cannot be maximised in the interior part of Ω.

Proof Assume that u can be maximised at an interior point, say $\mathbf{r}^* \in \Omega$, and we seek for contradiction. There should exist $a > 0$, such that $\mathcal{O}_a(\mathbf{r}^*) \subset \Omega$. Suppose $u(\mathbf{r}^*) = M = \max_{\Omega} u$. As from the mean-value formula,

$$u(\mathbf{r}^*) = \frac{1}{4\pi a^2} \iint_{\partial \mathcal{O}_a(\mathbf{r}^*)} u(\mathbf{r}) \mathrm{d}S_{\mathbf{r}} = M .$$

This implies that the average value of u over $\partial \mathcal{O}_a(\mathbf{r}^*)$ equals the maximum value M of the whole domain. Then the only possible situation is $u|_{\partial \mathcal{O}_a(\mathbf{r}^*)} = M$. As the radius a varies, one should show that there exists a sphere, say K_1, centred at $\mathbf{r}^*$, such that the function u uniformly equals M in K_1.

Now we show that for any $\mathbf{s} \in \Omega$, $u(\mathbf{s}) = M$ holds. If $\mathbf{s} \in K_1$, it is already the case. We are then focused on the situation where $\mathbf{s} \notin K_1$. As shown in Fig. 3.8, one may choose another point, say $\mathbf{r}^{**}$, in K_1. As the function values stay constant in Ω, $u(\mathbf{r}^{**}) = M$. Repeating the discussion above, one should conclude that there exists another sphere centred at $\mathbf{r}^{**}$, say K_2, such that u is uniformly equal to M in K_2. But K_2 is now "closer" to the target point $\mathbf{s}$ than K_1, as schematically shown in Fig. 3.8. One may carry on to generate a series of spheres K_i, $i = 1, \ldots, n$, such that $u|_{K_i} = M$.

This procedure is continued until $\mathbf{s}$ falls inside one ball from the series.

Therefore, we have shown that for any $\mathbf{s} \in \Omega$, $u(\mathbf{s}) \equiv M$. This is contradictory to the fact that u is not a constant in Ω. Thus, the maximum principle is proved. □

Several issues concerning the proof are mentioned here. First, the proof is given in a three-dimensional context, but it can be generalised to show that the maximum principle also works for two-dimensional harmonic functions. Second, as Ω is treated as an open set by default, its boundary Ω is not contained in Ω. Hence, more rigorous terms to state the maximum principle here are the supremum/infimum values of u over Ω, denoted by $\sup_\Omega u$ and $\inf_\Omega u$, respectively. For a bounded domain of Ω, an intuitive way to distinguish $\sup_\Omega u$ from $\max_\Omega u$ is as follows. For $\max_\Omega u$, the maximiser $\mathbf{r}^*$ must belong to Ω, while this is not necessary for $\sup_\Omega u$, as "maximisation" may take place on $\partial\Omega$ which is not necessarily in Ω. For the present case, as u is continuous towards its boundary,

$$\sup_\Omega u = \max_{\Omega\cup\partial\Omega} u, \qquad \inf_\Omega u = \min_{\Omega\cup\partial\Omega} u,$$

and the use of two sets of terms should not cause confusion.

The proof of the maximum principle here helps us to develop further understanding over the profile of a harmonic function. For instance, there are no local extrema for a non-constant harmonic function inside its domain of definition. Otherwise, the maximum principle is violated in the neighbourhood of any of the local maximiser/minimiser.

As for solution uniqueness imposed with Dirichlet boundary conditions, we simply need to show that if a harmonic function is constantly equal to zero on the boundary $\partial\Omega$, it must be uniformly zero inside Ω. This can be justified straight forward with the use of the maximum principle here. Besides, one may extend the present discussion to examine the stability of problems governed by Poisson's equation with Dirichlet boundary condition. The underlying idea is similar as that discussed in Sect. 2.4.

3.6.3 Strong Maximum Principle

Now we examine the case with Neumann boundary conditions. To this end, we consider

$$\begin{cases} \Delta u = 0, \ \mathbf{r} \in \Omega; \\ \left.\dfrac{\partial u}{\partial n}\right|_{\partial\Omega} = 0. \end{cases} \tag{3.77}$$

Note that any constant-valued functions in Ω serve to be a solution for problem (3.77). So our target here is to show that problem (3.77) only yields constant-valued solutions. In other words, the solution for problem (3.77) will be shown *unique up to a constant*. In this case, as the values of u on $\partial\Omega$ are not specified, the maximum principle introduced in Sect. 3.6.2 does not apply, and we need to introduce the *Hopf maximum principle*, which is also termed as the *strong maximum principle*.

The strong maximum principle for harmonic functions. Suppose that the boundary of a bounded domain Ω is sufficiently smooth, that is, for any $\mathbf{s} \in \partial\Omega$, there exists a ball belonging to the closure of Ω (which contains both Ω and its boundary $\partial\Omega$). If $\sup\limits_{\Omega} u$ is attained at $\mathbf{r}^* \in \partial\Omega$, then $\frac{\partial u}{\partial m}\Big|_{\mathbf{r}^*} > 0$; if $\inf\limits_{\Omega} u$ is attained at $\mathbf{r}^* \in \partial\Omega$, then $\frac{\partial u}{\partial m}\Big|_{\mathbf{r}^*} < 0$, where $\frac{\partial u}{\partial m}$ denotes the derivative of u along the direction $\mathbf{m}$, where $\mathbf{m} \cdot \mathbf{n} > 0$ with $\mathbf{n}$ being the normal vector at $\mathbf{r}^*$ pointing outward the domain Ω.

The reason that this maximum principle is "strong" can be summarised as follows. For a general function defined in a closed region Ω, if it is maximised at the domain boundary, say at $\mathbf{r}^* \in \partial\Omega$, then $\frac{\partial u}{\partial n}\Big|_{\mathbf{r}^*} \geqslant 0$ should hold. But for a harmonic function, the Hopf maximum principle excludes the situation of $\frac{\partial u}{\partial n}\Big|_{\mathbf{r}^*} = 0$, implying that the values of a harmonic function cannot transit "horizontally" towards the maximiser on the boundary.

It generally takes two steps to prove this strong maximum principle. First, one demonstrates its validity in a sphere. Then the proof is generalised to arbitrary domains enclosed by sufficiently smooth boundaries. But the details of the proof are not mentioned here. With this strong maximum principle, one is able to demonstrate the corresponding solution uniqueness (up to a constant) as follows.

Solution uniqueness (up to a constant) for problems governed by Poisson's equation with Neumann boundary conditions. If the boundary of Ω is sufficiently smooth as required by the strong maximum principle, problem (3.77) only yields constant-valued solutions.

Proof If u is not a constant-valued solution for problem (3.77), its outer normal derivative at the maximiser at the boundary, as from the strong maximum principle, should not vanish. This contradicts with the imposed homogeneous Neumann boundary condition. Therefore, problem (3.77) yields only constant-valued solutions. □

3.6.4 Energy Method

The maximum principles introduced here exhibit certain extents of similarities with that introduced for the heat equation in Sect. 2.4. This should not be surprising, as Poisson's equation can be used to describe a steady state of heat conduction. On the other hand, Poisson's equation can also be employed to represent a mechanistically-static state governed by the wave equation. Thus, the corresponding energy method, as introduced in Sect. 1.5, should also work for examining the solution uniqueness for problems governed by Poisson's equation.

For illustration, we here consider the spatially two-dimensional case. As discussed in Sect. 3.2, the (rescaled) system energy of a membrane in equilibrium (in the absence of external loads) is formulated by

$$\begin{aligned}\mathcal{E} &= \frac{a^2}{2}\iint\limits_{\Omega}\left[\left(\frac{\partial u}{\partial x}\right)^2+\left(\frac{\partial u}{\partial y}\right)^2\right]\mathrm{d}x\mathrm{d}y\\ &= \frac{a^2}{2}\iint\limits_{\Omega}\left[\frac{\partial}{\partial x}\left(u\frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(u\frac{\partial u}{\partial y}\right)-u\Delta u\right]\mathrm{d}x\mathrm{d}y\\ &= \frac{a^2}{2}\int\limits_{\partial\Omega}u\frac{\partial u}{\partial n}\,\mathrm{d}s-\frac{a^2}{2}\iint\limits_{\Omega}u\Delta u\,\mathrm{d}x\mathrm{d}y,\end{aligned}\tag{3.78}$$

where $\mathrm{d}s$ measures an infinitesimally short arc-length on the boundary $\partial\Omega$. Since u is harmonic, the double integral on the right side of Eq. (3.78) vanishes. Thus,

$$\mathcal{E}=\frac{a^2}{2}\int\limits_{\partial\Omega}u\frac{\partial u}{\partial n}\,\mathrm{d}s.\tag{3.79}$$

With either homogeneous Dirichlet boundary condition ($u|_{\partial\Omega}=0$) or Neumann boundary condition ($\frac{\partial u}{\partial n}\big|_{\partial\Omega}=0$), the right side of Eq. (3.79) vanishes. Hence $\mathcal{E}=0$, and $u_x=u_y\equiv 0$ holds for any points in Ω. Thus, u can only be constant-valued functions, and this demonstrates the solution uniqueness for the case with Neumann boundary condition. As for the case with Dirichlet boundary condition, this constant should coincide with the boundary condition, i.e. $u=0$, and the corresponding solution uniqueness is thus demonstrated.

Exercise

1. Write down the general form of the binary polynomials of degree 3, which satisfies the harmonic equation.
2. Verify that the following binary functions are harmonic functions in $\mathbb{R}^2$:

   (a) $(x^2+y^2)^{\frac{n}{2}}\cos nx$.
   (b) $(e^{bx}+e^{-bx})\sin by$, where b is a constant.

3. Verify that the following binary functions satisfy harmonic equations in $\mathbb{R}^2\backslash\{(0,0)\}$:

   (a) $\log(x^2+y^2)$.
   (b) $\tan^{-1}\frac{y}{x}$.

4. Use the method of separation of variables to solve the following PDE problem defined in a unit square:

$$\begin{cases} u_{xx} + u_{yy} = 0, \ (x, y) \in [0, 1] \times [0, 1]; \\ u|_{x=0} = u|_{x=1} = 0; \\ u|_{y=0} = \sin \pi x, \quad u|_{y=1} = 0. \end{cases}$$

5. Consider the steady-state solution of the membrane vibration problem:

$$\begin{cases} u_{xx} + u_{yy} = -f(x, y), \ (x, y) \in \Omega; \\ \left.\dfrac{\partial u}{\partial n}\right|_{\partial\Omega} = g(x, y), \end{cases}$$

where "$\frac{\partial}{\partial n}$" means taking the outer normal derivative on the domain boundary. Consider the corresponding energy functional given by

$$\mathcal{J}[u] = \frac{1}{2} \iint_{\Omega} \left[\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial y}\right)^2 \right] \mathrm{d}x\mathrm{d}y - \iint_{\Omega} fu \, \mathrm{d}x\mathrm{d}y - \int_{\partial\Omega} gu \, \mathrm{d}s.$$

(a) Interpret the physical meaning of the energy functional in the context of membrane vibration.
(b) Show that if u minimises the energy functional among all displacement states meeting the Neumann boundary condition imposed to the PDE problem above, that is,

$$\mathcal{J}[u] = \min_{v \in V_g} \mathcal{J}[v],$$

where $V_g = \{v | \left.\frac{\partial v}{\partial n}\right|_{\partial\Omega} = g\}$, then u is the solution to this PDE problem. (Tips: Set $v = u + \lambda w$, where $\left.\frac{\partial w}{\partial n}\right|_{\partial\Omega} = 0$.)

6. Consider the case for Laplace's equation imposed with Robin boundary condition as follows,

$$\begin{cases} u_{xx} + u_{yy} + u_{zz} = 0, \ (x, y, z) \in \Omega; \\ \left.\left(\dfrac{\partial u}{\partial n} + \sigma u\right)\right|_{\partial\Omega} = g(x, y, z). \end{cases}$$

(a) Derive the weak formulation of this PDE problem taking a similar form as Eq. (3.32). For that purpose, one may multiply both sides of the governing equation by an arbitrary trial function w, and integrate the result over Ω. (Note that there may be non-vanishing boundary integrals arising in the weak formulation, which is different from the case examined in the main text.)
(b) Express the energy functional corresponding to this PDE problem, and state the corresponding variational principle.

7. Show that in the spherical coordinate system of (r, θ, φ) [as defined by Eq. (3.37)], the Laplacian operator with Cartesian coordinates can be written in the form of Eq. (3.38) with spherical coordinates, that is,

$$\Delta u = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial u}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial u}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 u}{\partial \varphi^2}.$$

8. Show that in the cylindrical coordinate system (r, θ, z), the Laplacian operator is expressed by

$$\Delta u = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2} + \frac{\partial^2 u}{\partial z^2}.$$

9. Assume that $u(x, y)$ is a harmonic function defined in a two-dimensional region Ω. Substitute $v = \log r^2 = \log((x - x^*)^2 + (y - y^*)^2)$ into the second Green's formula (3.42).

   (a) With reference to Eq. (3.48), express the function value of u at any point $\mathbf{r}^* = (x^*, y^*)^{\mathrm{T}}$ inside Ω in the form of a boundary integral.
   (b) If u satisfies Robin boundary condition on the regional boundary, that is

$$\left(\frac{\partial u}{\partial n} + \sigma u\right)\bigg|_{\partial\Omega} = g(x, y),$$

   give the resulting expression for the Green's function for the resulting definite PDE problem.

10. For a harmonic function u defined in a three-dimensional region Ω, show that if $\mathbf{r}^* \in \partial\Omega$, Eq. (3.49) holds.
11. Solve the following PDE problem defined in the half plane with the image method for electric potentials:

$$\begin{cases} u_{xx} + u_{yy} = 0, \ \ y > 0; \\ \dfrac{\partial u}{\partial n}\bigg|_{y=0} = \phi(x); \\ \lim\limits_{x^2+y^2\to\infty} u(x, y) = 0. \end{cases}$$

12. Use the image method for electric potentials to construct the Green's function corresponding to problems governed by Poisson's equation in a two-dimensional circle, with Dirichlet boundary condition imposed on the circular boundary.
13. Consider a hemispherical region of $\Omega = \{(x, y, z)|x^2 + y^2 + z^2 < R, \ z > 0\}$ with R being the radius. Use the image method of electric potentials to construct the Green's function corresponding to problems for Poisson's equation imposed with Dirichlet boundary conditions imposed both on the hemispherical surface and the base.

14. Consider a second-order linear differential operator $\mathcal{L}$. Assume that V_0 is a set containing all functions that are twice differentiable and vanish on the boundary of a given region Ω, that is

$$V_0 = \left\{ v | v \in C^2,\ v|_{\partial\Omega} = 0 \right\}.$$

If there exists a differential operator $\mathcal{L}^*$, such that,

$$\int_\Omega v\mathcal{L}[u]\,\mathrm{d}\mathbf{r} = \int_\Omega u\mathcal{L}^*[v]\,\mathrm{d}\mathbf{r}$$

holds for any $u, v \in V_0$, then $\mathcal{L}^*$ is called the *adjoint operator* of $\mathcal{L}$. Specially, if $\mathcal{L}^* = \mathcal{L}$, then $\mathcal{L}$ is called a *self-adjoint operator*.

(a) If $\mathcal{L} = \frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\mathrm{d}}{\mathrm{d}x}$, where $x \in \Omega = (0, 1)$, determine its adjoint operator $\mathcal{L}^*$.
(b) Show that the differential operator inducing the Sturm–Liouville equation [with reference to Sect. 2.3.2], i.e.

$$\mathcal{L} = \frac{\mathrm{d}}{\mathrm{d}x}\left(k(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) - q(x) + \lambda\rho(x),$$

where $x \in \Omega = (a, b)$ is always self-adjoint.
(c) Show that the Laplacian operator is a self-adjoint operator.
(d) Show that the solution to

$$\begin{cases} \mathcal{L}[u] = f(\mathbf{r}),\ \ \mathbf{r} \in \Omega; \\ u|_{\partial\Omega} = 0 \end{cases}$$

can be expressed as

$$u(\mathbf{r}^*) = \int_\Omega G(\mathbf{r}; \mathbf{r}^*) f(\mathbf{r})\,\mathrm{d}\mathbf{r},$$

where $G(\mathbf{r}; \mathbf{r}^*)$ is the Green function corresponding to the fixed solution problem, satisfies

$$\begin{cases} \mathcal{L}^*[G(\mathbf{r}; \mathbf{r}^*)] = \delta(\mathbf{r} - \mathbf{r}^*),\ \ \mathbf{r} \in \Omega; \\ G|_{\mathbf{r}\in\partial\Omega} = 0. \end{cases}$$

Here $\delta(\mathbf{r} - \mathbf{r}^*)$ is the Dirac-δ function. A not fully rigorous definition of the Dirac-δ function is given by

$$\int_{\Omega} \delta(\mathbf{r} - \mathbf{r}^*) f(\mathbf{r})\, \mathrm{d}\mathbf{r} = f(\mathbf{r}^*),$$

for any continuous function f and $\mathbf{r}^* \in \Omega$.

15. Refer to the three-dimensional mean-value formula given by Eq. (3.75).

    (a) Derive the corresponding *mean-value formula for two-dimensional harmonic function*, i.e.

    $$u(\mathbf{r}^*) = \frac{1}{2\pi a} \int_{\mathcal{O}_a(\mathbf{r}^*)} u(\mathbf{r})\, \mathrm{d}s,$$

    where $\mathcal{O}_a(\mathbf{r}^*)$ is a two-dimensional circle; $\mathrm{d}s$ measures an infinitesimally short arc-length taken from the circular boundary.

    (b) If a harmonic function $u(x, y)$ satisfies

    $$u|_{x^2+y^2=1} = \frac{y^2}{x^2 + y^2},$$

    evaluate $u(0, 0)$.

16. If a continuous function u satisfies the mean-value formula at any point $\mathbf{r}^*$ in the region Ω, that is

    $$u(\mathbf{r}^*) = \frac{1}{4\pi a^2} \iint_{\partial\mathcal{O}_a(\mathbf{r}^*)} u \mathrm{d}S$$

    for all $\mathbf{r}^* \in \Omega$ and for any a such that $\mathcal{O}_a(\mathbf{r}^*) \subset \Omega$, show that u must be a harmonic function Ω.

17. If a function u satisfies

    $$4u_{xx} + u_{yy} + u_{zz} = 0, \text{ in } \Omega,$$

    derive a mean-value formula satisfied by u in comparison with Eq. (3.75), and explain the meaning behind it.

Chapter 4
Summary over Second-Order Linear Partial Differential Equation

In the previous three chapters, the wave equation, the heat equation and Poisson's equation are investigated in turn. The topics cover their motivations, initial/boundary conditions, methods for solutions and solution properties. Actually, these three types of equations are typical representatives of second-order linear partial differential equations. In this chapter, we will discuss the classification of general second-order linear partial differential equations. Then the features exhibited by various groups of PDEs are comparatively summarised, with reference to the knowledge introduced in the previous three chapters. The contents in this chapter are summarised in the knowledge map charted by Fig. 4.1.

4.1 Classification of Second-Order Linear Partial Differential Equations

4.1.1 Cases with Two Variables

Recalling from the definition over linear differential operators in Sect. 1.1.3, the wave equation, the heat equation and Poisson's equation are all second-order linear partial differential equations. Here the term "second-order" means the involved highest derivatives are second-order; "linear" means the differential operators inducing the resulting PDEs are linear about the unknown function u.

We start with the cases involving two independent variables. Note that a second-order linear PDE containing two independent variables has a *general form* of

$$a_{11}u_{xx} + 2a_{12}u_{xy} + a_{22}u_{yy} + b_1u_x + b_2u_y + cu = f, \tag{4.1}$$

where $a_{11}, a_{12}, a_{22}, b_1, b_2, c, f$ can all be known functions of x and y.

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Y. Zhu, *Equations and Analytical Tools in Mathematical Physics*,
https://doi.org/10.1007/978-981-16-5441-1_4

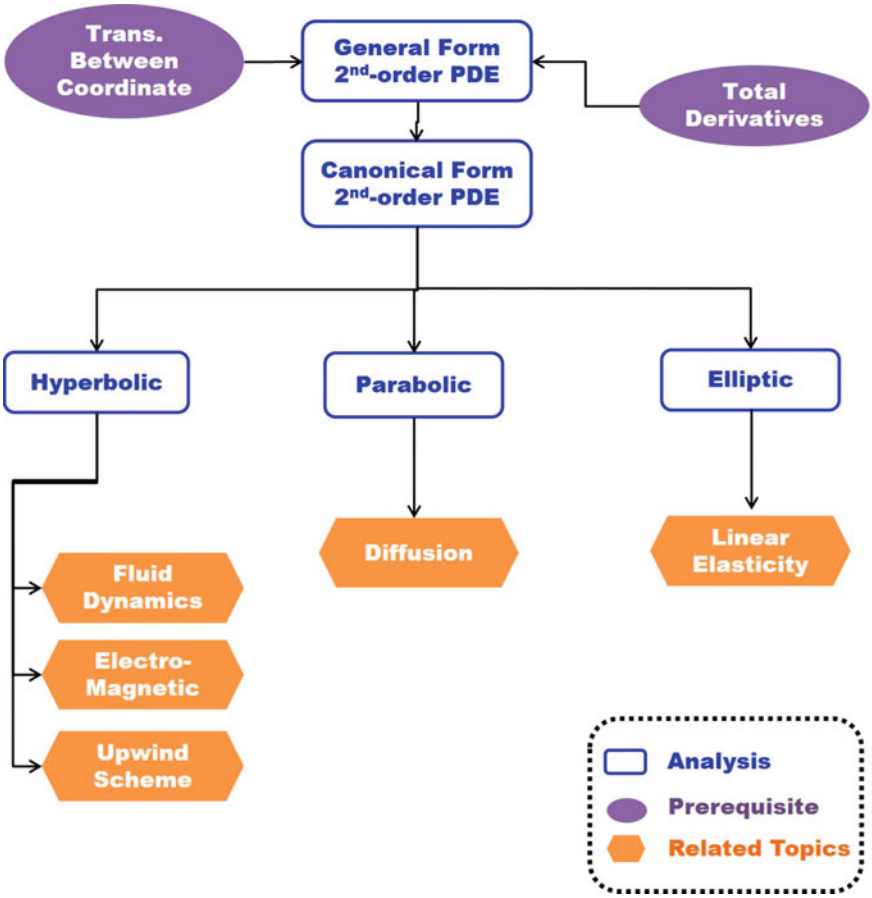

Fig. 4.1 Knowledge map—a summary over second-order linear PDEs

Our aim here is to rewrite the general form of Eq. (4.1) in a new coordinate system in a simplified form, which is later specified as the canonical form. To this end, we introduce

$$\begin{cases} \xi = \xi(x, y); \\ \eta = \eta(x, y). \end{cases} \tag{4.2}$$

To make transformation (4.2) meaningful, the associated Jacobean determinant should not vanish, i.e.

$$\xi_x \eta_y - \xi_y \eta_x \neq 0. \tag{4.3}$$

As an example, if $\xi(x, y) = \sqrt{x^2 + y^2}$, $\eta(x, y) = \tan^{-1} \frac{y}{x}$, Eq. (4.2) effectively transforms a PDE from Cartesian system to the polar system.

On using the multivariable chain rule, the derivatives of u with respect to x and y can be expressed by means of that to ξ and η by

$$\begin{cases} u_x = u_\xi \xi_x + u_\eta \eta_x; \\ u_y = u_\xi \xi_y + u_\eta \eta_y, \end{cases} \tag{4.4}$$

and also its second derivatives by

$$\begin{cases} u_{xx} = u_{\xi\xi}\xi_x^2 + 2u_{\xi\eta}\xi_x\eta_x + u_{\eta\eta}\eta_x^2 + u_\xi \xi_{xx} + u_\eta \eta_{xx}; \\ u_{xy} = u_{\xi\xi}\xi_x\xi_y + u_{\xi\eta}(\xi_x\eta_y + \xi_y\eta_x) + u_{\eta\eta}\eta_x\eta_y + u_\xi \xi_{xy} + u_\eta \eta_{xy}; \\ u_{yy} = u_{\xi\xi}\xi_y^2 + 2u_{\xi\eta}\xi_y\eta_y + u_{\eta\eta}\eta_y^2 + u_\xi \xi_{yy} + u_\eta \eta_{yy}. \end{cases} \tag{4.5}$$

Incorporating Eqs. (4.4) and (4.5) with (4.1) gives

$$\tilde{a}_{11}u_{\xi\xi} + 2\tilde{a}_{12}u_{\xi\eta} + \tilde{a}_{22}u_{\eta\eta} + \tilde{b}_1 u_\xi + \tilde{b}_2 u_\eta + \tilde{c}u = \tilde{f}, \tag{4.6}$$

where we are mainly focused on the coefficients before the second derivatives with the other coefficients, such as $\tilde{b}_1$, etc. unspecified for the moment, i.e.

$$\begin{cases} \tilde{a}_{11} = a_{11}\xi_x^2 + 2a_{12}\xi_x\xi_y + a_{22}\xi_y^2; \\ \tilde{a}_{12} = a_{11}\xi_x\eta_x + a_{12}\xi_x\eta_y + a_{12}\xi_y\eta_x + a_{22}\xi_y\eta_y; \\ \tilde{a}_{22} = a_{11}\eta_x^2 + 2a_{12}\eta_x\eta_y + a_{22}\eta_y^2. \end{cases} \tag{4.7}$$

Equation (4.6) simply re-expresses the general form (4.1) in the new system of ξ and η. Our goal now is to determine the mapping rule (4.2), so as to diminish some of the coefficients $\tilde{a}_{11}$, $\tilde{a}_{12}$ and $\tilde{a}_{22}$.

A key observation here is that the expressions for $\tilde{a}_{11}$ and $\tilde{a}_{22}$ are identical, if one swaps ξ with η. Therefore, a natural way to simplify Eq. (4.6) is to let $\tilde{a}_{11} = \tilde{a}_{22} = 0$. In other words, we consider another PDE for the binary function $\phi(x, y)$ governed by

$$a_{11}\phi_x^2 + 2a_{12}\phi_x\phi_y + a_{22}\phi_y^2 = 0. \tag{4.8}$$

Suppose that one is able to find two mutually independent solutions to Eq. (4.8), say, $\phi = \phi_1(x, y)$ and $\phi = \phi_2(x, y)$. Then we can set up the mapping rule (4.2) by

$$\begin{cases} \xi = \phi_1(x, y); \\ \eta = \phi_2(x, y). \end{cases} \tag{4.9}$$

The resulting equation (4.6) should thus be greatly simplified. Here we say that the two solutions are "mutually independent", meaning that Eq. (4.3) holds, i.e.

$$\phi_{1x}\phi_{2y} - \phi_{1y}\phi_{2x} \neq 0, \tag{4.10}$$

where ϕ_{1x} denotes the derivative of ϕ_1 with respect to x, and so on.

Equation (4.8) is effectively a nonlinear PDE, which is generally even harder to solve. But one can readily identify certain features shown by its solutions. Note that ϕ_x and ϕ_y cannot vanish simultaneously. Otherwise condition (4.10) is not met. Here without loss of generalities, we let $\phi_y \neq 0$. Dividing ϕ_y^2 on both sides of Eq. (4.8) leads to

$$a_{11}\left(\frac{\phi_x}{\phi_y}\right)^2 + 2a_{12}\left(\frac{\phi_x}{\phi_y}\right) + a_{22} = 0, \tag{4.11}$$

which can be treated as an algebraic equation for $\frac{\phi_x}{\phi_y}$ (for each pair of x and y).

Being an algebraic equation of degree 2, the behaviour of Eq. (4.11) should fall into one of the following three categories.

Case 1 $a_{12}^2 - a_{11}a_{22} > 0$.
In this case, the algebraic equation (4.11) yields two real roots represented by

$$\frac{\phi_{1x}}{\phi_{1y}} = \frac{-a_{12} + \sqrt{a_{12}^2 - a_{11}a_{22}}}{a_{11}}; \tag{4.12a}$$

$$\frac{\phi_{2x}}{\phi_{2y}} = \frac{-a_{12} - \sqrt{a_{12}^2 - a_{11}a_{22}}}{a_{11}}. \tag{4.12b}$$

Eqs. (4.12a) and (4.12b) become two first-order PDEs for ϕ_1 and ϕ_2, respectively. Here we take Eq. (4.12a) as an example to briefly illustrate the key idea for solving them. There are two alternative ways to solve Eq. (4.12a).

The first way is based on the concept of total differential, whose details are referred to in the prerequisite part concluding this section. Equation (4.12a) suggests that

$$\phi_{1x} = \mu(x, y) \cdot \frac{-a_{12} + \sqrt{a_{12}^2 - a_{11}a_{22}}}{a_{11}}, \quad \phi_{1y} = \mu(x, y) \cdot \frac{-a_{12} + \sqrt{a_{12}^2 - a_{11}a_{22}}}{a_{11}},$$

where $\mu(x, y)$ is still an arbitrary function, and one needs to choose the integrating factor $\mu(x, y)$, such that

$$\mathrm{d}\phi_1 = \mu(x, y) \cdot \left(\frac{-a_{12} + \sqrt{a_{12}^2 - a_{11}a_{22}}}{a_{11}} \cdot \mathrm{d}x + \frac{-a_{12} + \sqrt{a_{12}^2 - a_{11}a_{22}}}{a_{11}} \cdot \mathrm{d}y\right)$$

becomes a total differential. For solving $\mu(x, y)$, another PDE has to be introduced. But one may finally integrate for $\phi_1(x, y)$ then, regardless the path of integration in the x-y plane.

The second way to solve Eq. (4.12a) is based on the concept of integral curves, whose features are also summarised in the prerequisite part. From that viewpoint, Eq. (4.12a) is equivalent to an ordinary differential equation given by

$$\frac{\mathrm{d}y}{\mathrm{d}x} = -\frac{\phi_x}{\phi_y} = \frac{a_{12} - \sqrt{a_{12}^2 - a_{11}a_{22}}}{a_{11}}, \tag{4.13}$$

which defines a family of parametric curves $\phi_1(x, y) = C_1$ with C_1 being the parameter. Being an ordinary differential equation, the chance in finding the solutions to Eq. (4.13) should be enhanced.

Suppose that we manage to solve Eqs. (4.12a) and (4.12b). We simply let $\xi = \phi_1(x, y)$ and $\eta = \phi_2(x, y)$ to establish the mapping rule given by Eq. (4.2). In this case, both $\tilde{a}_{11}$ and $\tilde{a}_{22}$ in Eq. (4.6) should vanish.

Note that one also needs to check with condition (4.10). Inserting Eqs. (4.12a) and (4.12b) into (4.10) gives

$$\phi_{1x}\phi_{2y} - \phi_{1y}\phi_{2x} = \frac{\sqrt{a_{12}^2 - a_{11}a_{22}}}{a_{11}}\phi_{1y}\phi_{2y}.$$

Since ϕ_y in Eq. (4.11) is set nonzero, $\phi_{1y}\phi_{2y} \neq 0$. Thus, condition (4.10) is automatically met.

Now we insert Eqs. (4.12a) and (4.12b) into (4.7), and $\tilde{a}_{12}$ is re-expressed by

$$\tilde{a}_{12} = \frac{2(a_{11}a_{22} - a_{12}^2)}{a_{11}} \cdot \phi_{1y}\phi_{2y} \neq 0.$$

Therefore, with $\xi = \phi_1(x, y)$ and $\eta = \phi_2(x, y)$, Eq. (4.6) is simplified to be

$$2\tilde{a}_{12}u_{\xi\eta} + \tilde{b}_1 u_\xi + \tilde{b}_2 u_\eta + \tilde{c}u = \tilde{f}.$$

Dividing it on both sides by $2\tilde{a}_{12}$, we finally reach

$$u_{\xi\eta} = Au_\xi + Bu_\eta + Cu + D, \tag{4.14}$$

where A, B, C and D are all functions of ξ and η.

If we further introduce

$$t = \xi + \eta, \qquad s = \xi - \eta,$$

Eq. (4.14) can be rewritten in $s - t$ coordinates by

$$u_{tt} - u_{ss} = A_1 u_t + B_1 u_s + C_1 u + D_1, \tag{4.15}$$

where A_1, B_1, C_1 and D_1 are functions of s and t.

If a second linear PDE, upon coordinate transformation, can be transformed to the form given either by Eq. (4.14) or (4.15), it is called a second-order linear *hyperbolic* PDE. Equation (4.14) is called the *canonical form* of second-order linear hyperbolic PDEs.

To see the origin of the term "hyperbolic" used here, we replace the partial derivatives in Eq. (4.15) by power functions of the corresponding variables. For instance, u_{tt} is replaced by t^2; u_s is replaced by s; u is replaced by 1, D_1 which is the term independent of the unknown u is replaced by 0, and so on. By doing so, Eq. (4.15) corresponds an algebraic equation of degree 2:

$$t^2 - s^2 = A_1 t + B_1 s + C_1.$$

which describes a hyperbola in the $s - t$ plane.

Here the similarities in sorting algebraic curves with the classification of PDEs are addressed. In fact, other comparable issues exist between polynomials and linear operators, and keeping their linkages in mind is quite helpful for analysing linear PDEs. For example, it can be verified that

$$\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} = \left(\frac{\partial}{\partial t} + \frac{\partial}{\partial x}\right)\left(\frac{\partial}{\partial t} - \frac{\partial}{\partial x}\right).$$

which echoes with factorisation of the difference of two squared numbers.

As a special case, when $A_1 = B_1 = C_1 = 0$, $s = x$, and $D_1 = f$ in Eq. (4.15), we end up with the wave equation (with $a^2 = 1$), which is one of the most typical representatives of second-order linear hyperbolic PDEs.

Case 2 $a_{12}^2 - a_{11}a_{22} = 0$.
In this scenario, a_{11} and a_{22} are of same sign. Thus without loss of generalities, we let a_{11}, a_{12}, and a_{22} all be positive. Letting $a_{12} = \sqrt{a_{11}a_{22}}$ in Eq. (4.8), we write

$$(\sqrt{a_{11}}\phi_x + \sqrt{a_{22}}\phi_y)^2 = 0. \tag{4.16}$$

In this case, only one family of parametric curves, say, $\phi = \phi_1(x, y) = C$, satisfy Eq. (4.16). One coordinate can thus be determined by letting $\xi = \phi_1(x, y)$. Then $\tilde{a}_{11} = 0$ in Eq. (4.6).

For the other coordinate η, we choose an arbitrary binary function, say $\phi_2(x, y)$, provided that it is independent of $\phi_1(x, y)$, and let $\eta = \phi_2(x, y)$. In this case, the coefficient $\tilde{a}_{12}$ given by Eq. (4.7) becomes

$$\tilde{a}_{12} = (\sqrt{a_{11}}\phi_{1x} + \sqrt{a_{22}}\phi_{1y})(\sqrt{a_{11}}\phi_{2x} + \sqrt{a_{22}}\phi_{2y}) = 0,$$

where Eq. (4.16) is employed.

Therefore, in $\xi - \eta$ system, Eq. (4.6) is simplified to be

$$\tilde{a}_{22}u_{\eta\eta} = A_1 u_\xi + B_1 u_\eta + C_1 u + D_1.$$

As $\tilde{a}_{22} \neq 0$, it can be divided on both sides and we reach

$$u_{\eta\eta} = Au_{\xi} + Bu_{\eta} + Cu + D. \tag{4.17}$$

Based on the mapping rule between polynomials and differential operators as introduced in Case 1, Eq. (4.17) corresponds to $\eta^2 = A\xi + B\eta + C$, which defines a parabola. Therefore, upon coordinate transformation, a PDE that can be transformed into the canonical form given by Eq. (4.17) is called a second-order linear *parabolic* PDE.

In particular, when $A = 1$, $B = C = 0$, Eq. (4.17) becomes the spatially one-dimensional heat equation, with ξ measuring the time and η measuring the space. Actually, the heat equation is one of the most typical representatives of second-order linear parabolic PDEs.

Case 3 $a_{12}^2 - a_{11}a_{22} < 0$.
In this scenario, Eq. (4.11) yields no real roots for $\frac{\phi_x}{\phi_y}$, but a pair of complex roots. Assume that Eq. (4.8) can be solved by

$$\phi(x, y) = \phi_1(x, y) + \mathrm{i}\phi_2(x, y), \tag{4.18}$$

where ϕ_1 and ϕ_2 are both real functions.

Inserting Eq. (4.18) into (4.8) and separating the real parts from the imaginary parts, we have

$$\begin{cases} a_{11}\phi_{1x}^2 + 2a_{12}\phi_{1x}\phi_{1y} + a_{22}\phi_{1y}^2 = a_{11}\phi_{2x}^2 + 2a_{12}\phi_{2x}\phi_{2y} + a_{22}\phi_{2y}^2 \\ a_{11}\phi_{1x}\phi_{2x} + a_{12}(\phi_{1x}\phi_{2y} + \phi_{1y}\phi_{2x}) + a_{22}\phi_{1y}\phi_{2y} = 0. \end{cases} \tag{4.19}$$

which form a PDE system for ϕ_1 and ϕ_2. Given solution existence for Eq. (4.19), we introduce the coordinate transformation as follows, $\xi = \phi_1(x, y)$ and $\eta = \phi_2(x, y)$.

Before carrying on with further calculations, one should first ensure that condition (4.3) is met. As ϕ in Eq. (4.8) is now written by $\phi = \xi + \mathrm{i}\eta$, we have

$$\frac{\phi_x}{\phi_y} = \frac{\xi_x + \mathrm{i}\eta_x}{\xi_y + \mathrm{i}\eta_y} = -\frac{a_{12} + \sqrt{a_{11}a_{22} - a_{12}^2}}{a_{11}}.$$

Then, we separate the real part from the imaginary part, and obtain

$$\begin{vmatrix} \xi_x & \xi_y \\ \eta_x & \eta_y \end{vmatrix} = \frac{\sqrt{a_{11}a_{22} - a_{12}^2}}{a_{11}} \cdot (\xi_y^2 + \eta_y^2).$$

Since at least one of ξ and η is dependent on y, the determinant above does not vanish. Therefore, the choices for ξ and η here are mutually independent.

Upon such coordinate transformation, Eq. (4.19) can be further written by

$$a_{11}\xi_x^2 + 2a_{12}\xi_x\xi_y + a_{22}\xi_y^2 = a_{11}\eta_x^2 + 2a_{12}\eta_x\eta_y + a_{22}\eta_y^2; \tag{4.20a}$$

$$a_{11}\xi_x\eta_x + a_{12}(\xi_x\eta_y + \xi_y\eta_x) + a_{22}\xi_y\eta_y = 0. \tag{4.20b}$$

A comparison of Eqs. (4.20) with Eq. (4.7) suggests that $\tilde{a}_{11} = \tilde{a}_{22} \neq 0$ and $\tilde{a}_{12} = 0$. Hence, Eq. (4.6) is simplified to be

$$u_{\xi\xi} + u_{\eta\eta} = Au_\xi + Bu_\eta + Cu + D. \tag{4.21}$$

which corresponds to an elliptic curve given by $\xi^2 + \eta^2 = A\xi + B\eta + C$. Therefore, a PDE that can be transformed into the canonical form given by Eq. (4.21) is called a second-order linear *elliptic* PDE.

In particular, if $A = B = C = 0$ and $D = f$, Eq. (4.21) becomes Poisson's equation, which is the most typical representative of second-order linear elliptic PDEs.

4.1.2 Summary and Examples

To summarise, a second-order linear partial differential equation with two independent variables is generally represented by

$$a_{11}u_{xx} + 2a_{12}u_{xy} + a_{22}u_{yy} + b_1u_x + b_2u_y + cu = f.$$

At any point falling inside its domain of definition, say, (x_0, y_0), it can be classified into one of the following three groups.

- If the coefficients satisfy
$$a_{12}^2 - a_{11}a_{22} > 0,$$
then the equation is hyperbolic at (x_0, y_0). Upon appropriate coordinate transformation, it can be transformed into the canonical form (4.14).
- If the coefficients satisfy
$$a_{12}^2 - a_{11}a_{22} = 0,$$
then the equation is parabolic at (x_0, y_0). Upon appropriate coordinate transformation, it can be transformed into the canonical form (4.17).
- If the coefficients satisfy
$$a_{12}^2 - a_{11}a_{22} < 0,$$
then the equation is elliptic at (x_0, y_0). Upon appropriate coordinate transformation, it can be transformed into the canonical form (4.21).

Several examples are provided to enhance our understanding over this classification rule.

Example 1 Euler–Tricomi equation plays an important role in the development of vehicles travelling at a speed close to that of sound [4], and it is given by

$$u_{xx} + xu_{yy} = 0. \tag{4.22}$$

Compared to Eq. (4.1), we have $a_{11} = 1$, $a_{12} = 0$, and $a_{22} = x$. Thus $a_{12}^2 - a_{11}a_{22} = -x$. Therefore, Euler–Tricomi equation is elliptic in the region of $x > 0$, and it is hyperbolic in the region of $x < 0$. □

Suggested by this example, a same PDE may be of different types in different regions. When a PDE is hyperbolic at every point in a region Ω, the PDE is also called a hyperbolic PDE in Ω. Similar definitions also apply for the other two types.

Example 2 Transform the wave equation $u_{tt} - a^2 u_{xx} = 0$ into its canonical form.

Replacing the variable y in Eq. (4.1) by the temporal variable t, we have $a_{11} = -a^2$, $a_{12} = 0$ and $a_{22} = 1$. Thus, $a_{12}^2 - a_{11}a_{22} = a^2 > 0$. Hence, the wave equation, as discussed above, is hyperbolic for $(x, t) \in \mathbb{R} \times \mathbb{R}^+$.

It is expected to be transformed into the canonical form (4.14). For that purpose, Eqs. (4.12a) and (4.12b) are considered:

$$\frac{\phi_{1x}}{\phi_{1t}} = \frac{1}{a}, \qquad \frac{\phi_{2x}}{\phi_{2t}} = -\frac{1}{a}, \tag{4.23}$$

respectively.

It can be verified that

$$\begin{cases} \xi = \phi_1(x, t) = x + at; \\ \eta = \phi_2(x, t) = x - at, \end{cases} \tag{4.24}$$

naturally satisfy Eq. (4.23). Incorporating Eq. (4.24) with (4.7), we obtain $\tilde{a}_{11} = \tilde{a}_{22} = 0$, $\tilde{a}_{12} = -2a^2$. And the corresponding canonical form is $u_{\xi\eta} = 0$, which is just Eq. (1.22), where the wave equation gets simplified during the derivation for D'Alembert's formula in Sect. 1.2.

Moreover, Eq. (4.24) actually identifies two families of parametric curves: $\phi_1(x, y) = x + at = C_1$ and $\phi_2(x, y) = x - at = C_2$, with C_1 and C_2 being parameters. In fact, they just correspond to the two families of characteristics for the wave equation, as detailed in Sect. 1.2.2. □

Therefore, the concept of characteristics is generalisable to other second-order linear hyperbolic PDEs. When being transformed to their canonical form, Eqs. (4.12a) and (4.12b) are introduced. Each of them should identify a family of parametric curves, which just define a set of characteristics for the corresponding hyperbolic PDE. As shown in Sect. 1.2.2, characteristics provide an effective means for captur-

ing the feature of wave propagation at finite speeds exhibited by the wave equation. In a similar sense, the method of characteristics is also expected to work for studying general second-order linear hyperbolic PDEs.

4.1.3 Multivariable Situations

Now the discussion is extended to cover second-order linear PDEs containing n independent variables, whose general form is given by

$$\sum_{i,j}^{n} a_{ij} \frac{\partial^2 u}{\partial r_i \partial r_j} + \sum_{i}^{n} b_i \frac{\partial u}{\partial r_i} + cu = f, \tag{4.25}$$

where a_{ij}, b_i, c and f are functions of $\mathbf{r} = (r_1, r_2, \ldots, r_n)^{\mathrm{T}}$. Here without loss of generalities, we let $a_{ij} = a_{ij}$. This is because $\frac{\partial^2 u}{\partial r_i \partial r_j} = \frac{\partial^2 u}{\partial r_j \partial r_i}$. Hence even though $a_{ij} \neq a_{ji}$ originally, one can always introduce $(a_{ij} + a_{ji})/2$ as the new coefficients for a_{ij} and a_{ji}.

The coefficients a_{ij} can be summarised in an $n \times n$ (symmetric) matrix given by

$$A(\mathbf{r}) = \begin{pmatrix} a_{11}(\mathbf{r}) & a_{12}(\mathbf{r}) & \cdots & a_{1n}(\mathbf{r}) \\ a_{12}(\mathbf{r}) & a_{22}(\mathbf{r}) & \cdots & a_{2n}(\mathbf{r}) \\ \vdots & \vdots & \ddots & \vdots \\ a_{1n} & a_{2n} & \cdots & a_{nn} \end{pmatrix} \tag{4.26}$$

Given its symmetry at any point $\mathbf{r}$, the matrix A always yields n real eigenvalues, say, $\lambda_1(\mathbf{r})$, …, $\lambda_n(\mathbf{r})$. The classification of second-order linear PDEs for multidimensional cases is just based on the sign of these eigenvalues, detailed as follows.

- If all n eigenvalues are of same sign, i.e. they are all positive or all negative at $\mathbf{r}$, the PDE (4.25) is elliptic at $\mathbf{r}$.
- If one of the eigenvalue is zero, while the other eigenvalues are of same sign at $\mathbf{r}$, the PDE (4.25) is parabolic at $\mathbf{r}$.
- If $n - 1$ eigenvalues are of same sign, while the other is of opposite sign, the PDE (4.25) is hyperbolic at $\mathbf{r}$.

This classification rule also complies with the two-dimensional cases discussed in Sect. 4.1.1.

Some simple examples are mentioned. For three-dimensional Poisson's equation, $u_{xx} + u_{yy} + u_{zz} = f$, the coefficient matrix (4.26) is the 3-by-3 identify matrix. Since the eigenvalues are identically equal to 1, it is of elliptic type. In contrast, for the three-dimensional heat equation $u_t - a^2(u_{xx} + u_{yy} + u_{zz}) = f$, its coefficient matrix is a 4-by-4 diagonal matrix. Three of its eigenvalues are equal to $-a^2$, while the other equals 0. Hence, it is of parabolic type.

Example 3 Determine the type of the PDE given by

$$u_{xx} + u_{yy} + u_{xz} + u_{zz} = 0$$

A comparison with Eq. (4.25), the matrix A is expressed by

$$A = \begin{pmatrix} 1 & 0 & 1/2 \\ 0 & 1 & 0 \\ 1/2 & 0 & 1 \end{pmatrix}$$

Its eigenvalues equal $1/2$, 1 and $3/2$, respectively. Hence, the equation is of elliptic type.

Example 4 Maxwell's equations

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}; \tag{4.27a}$$

$$\nabla \cdot \mathbf{B} = 0; \tag{4.27b}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}; \tag{4.27c}$$

$$\nabla \times \mathbf{B} = \mu_0 \left(\mathbf{J} + \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right) \tag{4.27d}$$

form the fundamental equation system underpinning the electromagnetism science. The physical quantities appearing in Maxwell's equations are summarised in Table 4.1. Here "$\nabla\cdot$" denotes finding the divergence of a vector; "$\nabla\times$" denotes finding the curl of a vector field. More details about linear differential operators can be found in the prerequisite knowledge part of Sect. 3.1.

Maxwell's equations effectively formulate key observations in classical electromagnetism. Equation (4.27a) comes from Gauss's law; Eq. (4.27b) comes from *Gauss's law for magnetism*; Eq. (4.27c) comes from *Faraday's law of induction*; Eq. (4.27d) comes from *Ampère's circuital law*.

When the medium is homogeneous, Maxwell's equations form a system of first-order, constant-coefficient, vector-valued PDEs for the involved vector fields. Note that both Eqs. (4.27c) and (4.27d) contain the electric field $\mathbf{E}$ and the magnetic field $\mathbf{B}$. One may incorporate them so as to eliminate one of them, and thus derive an equation solely for the other. To be specific, taking the curl on both sides of Eq. (4.27c) gives

$$\nabla \times (\nabla \times \mathbf{E}) = \nabla(\nabla \cdot \mathbf{E}) - \Delta \mathbf{E} = \frac{1}{\epsilon_0} \nabla \rho - \Delta \mathbf{E} = -\frac{\partial}{\partial t} (\nabla \times \mathbf{B}), \tag{4.28}$$

Table 4.1 Physical quantities appearing in Maxwell's equations

Symbol	Type	Physical meaning	Quantity unit
$\mathbf{E}$	Vector field	Electric field	N/C
$\mathbf{B}$	Vector field	Magnetic field	T
$\mathbf{J}$	Vector field	Electric current	A/m^2
ρ	Scalar field	Charge distribution	C/m^3
ϵ_0	Material constant	Electric permittivity	$C^2\,m^2/N$
μ_0	Material constant	Magnetic conductivity	N/A^2

where Eq. (4.27a) is also employed and $\Delta\mathbf{E}$ denotes the Laplacian operator applied on each entry of $\mathbf{E}$. On the other hand, differentiating Eq. (4.27d) with respect to t gives

$$\frac{\partial}{\partial t}(\nabla \times \mathbf{B}) = \mu_0\left(\frac{\partial \mathbf{J}}{\partial t} + \epsilon_0\frac{\partial^2 \mathbf{E}}{\partial t^2}\right). \tag{4.29}$$

Adding Eq. (4.29) by (4.28) eliminates $\mathbf{B}$, and we obtain

$$\mu_0\epsilon_0\frac{\partial^2 \mathbf{E}}{\partial t^2} - \Delta\mathbf{E} = -\mu_0\frac{\partial \mathbf{J}}{\partial t} - \frac{1}{\epsilon_0}\nabla\rho.$$

Analogically, a second-order PDE for $\mathbf{B}$ can also be derived as

$$\mu_0\epsilon_0\frac{\partial^2 \mathbf{B}}{\partial t^2} - \Delta\mathbf{B} = -\mu_0\nabla \times \mathbf{J}.$$

In particular, when $\mathbf{J} = \mathbf{0}$ and $\rho = 0$, we have

$$\frac{\partial^2 \mathbf{E}}{\partial t^2} - \frac{1}{\mu_0\epsilon_0}\Delta\mathbf{E} = \mathbf{0}; \tag{4.30}$$

$$\frac{\partial^2 \mathbf{B}}{\partial t^2} - \frac{1}{\mu_0\epsilon_0}\Delta\mathbf{B} = \mathbf{0}, \tag{4.31}$$

indicating that each component of the electric field $\mathbf{E}$ and the magnetic field $\mathbf{B}$ satisfies the wave equation. This provides evidence that the electromagnetic field evolves like a wave in space. Besides, as from the discussion in Sect. 1.4.3, the wave speed should be calculated by $1/\sqrt{\mu_0\epsilon_0}$. In vacuum, it equals the light speed, confirming the fact that electromagnetic wave propagates at the light speed in vacuum.

Implied by this example, first-order vector-valued PDE systems may sometimes be analysed based on the tools introduced for investigating second-order linear PDEs.

Prerequisite knowledge

Total differential

Given a point mass in two-dimensional space, it moves from point (x_0, y_0) to (x_1, y_1) driven by a force field of $\mathbf{f} = (f_1, f_2)^{\mathrm{T}}$. The work done by this background force is calculated by

$$\int_C f_1(x, y)\mathrm{d}x + f_2(x, y)\mathrm{d}y,$$

where C is a curve describing the trajectory of the point mass. In general, the integral not only depends on the starting/end points, but also the path identified by C.

But there are exceptions where the integral is fully independent on the choice of the path, that is, there exists a differentiable binary function $\phi = \phi(x, y)$, such that, $f_1 = \phi_x$ and $f_2 = \phi_y$. And the resulting differential

$$\mathrm{d}\phi = f_1\mathrm{d}x + f_2\mathrm{d}y = \mathbf{f} \cdot \mathrm{d}\mathbf{r} \tag{4.32}$$

is known as the total differential of the binary function ϕ. Here the function ϕ becomes a potential function of the system, and $\mathbf{f}$ is called a *conservative force* then.

Given $\mathbf{f}$, one condition to ensure that Eq. (4.32) is a total differential (for two-dimensional cases) is

$$\frac{\partial f_1}{\partial y} = \frac{\partial f_2}{\partial x}. \tag{4.33}$$

The concept is generalisable to n-dimensional cases. For an n-dimensional field $\mathbf{f}$ defined in $\mathbb{R}^n$, if there exists a function of n variables, say $\phi = \phi(\mathbf{r})$, such that $\mathbf{f} = \nabla\phi$. Then

$$\mathrm{d}\phi = \mathbf{f} \cdot \mathrm{d}\mathbf{r} \tag{4.34}$$

defines the total differential of ϕ.

To ensure that Eq. (4.34) defines a total differential in $\mathbb{R}^3$, we require

$$\mathbf{curl}\,[\mathbf{f}] = \nabla \times \mathbf{f} = \mathbf{0},$$

where the definition of the **curl** operation can be found in the prerequisite knowledge of Sect. 3.1.

Parametric curves

Given a binary function $\phi(x, y)$ and a constant C, $\phi(x, y) = C$ provides an implicit representation of a curve in $\mathbb{R}^2$. As C varies, $\{\phi(x, y) = C\}$ represent a family of *parametric curves* in $\mathbb{R}^2$.

For instance, two families of parametric curves formulated by

$$\phi_1(x, y) = \sqrt{x^2 + y^2} = C_1, \quad \phi_2(x, y) = \arctan\frac{y}{x} = C_2$$

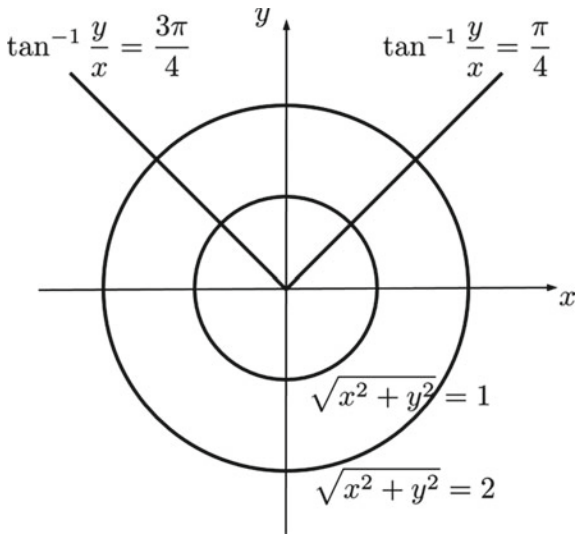

Fig. 4.2 Examples on parametric curves

are schematically shown in Fig. 4.2. The first family $\{\phi_1(x, y) = C_1\}$ represents a family of concentric circles. The second family $\{\phi_2(x, y) = C_2\}$ is formed by half-lines ending at the origin. If one sets the parameters C_1 and C_2 as the new spatial variables, the two families of curves effectively identify the transformation from Cartesian system to the two-dimensional polar system.

When the parameter C is fixed, the tangent at each point on the curve $\phi(x, y) = C$ can be calculated based on the chain rule for implicit functions by

$$\frac{\mathrm{d}y}{\mathrm{d}x} = -\frac{\phi_x}{\phi_y}. \tag{4.35}$$

The right side of Eq. (4.35) should be formulated as explicit functions of x and y, as the expression for ϕ is presumably known. Thus, Eq. (4.35) becomes an ordinary differential equation for y with x being its independent variable. This is just the case shown by Eq. (4.13).

Moreover, if $y = f(x)$ solves Eq. (4.35), $y = f(x) + C$ also solves it for any constant C. The corresponding parametric curves, in this case, are formulated by $\phi(x, y) = y - f(x) = C$, which explicitly expresses the family of *integral curves* corresponding to Eq. (4.35).

Parametric curves see their wide applications in physical science. In fluid dynamics, for instance, the trajectories of the constituting fluidic particles form a family of parametric curves originated from the corresponding governing equations, and these parametric curves are known as the *streamlines* of the fluid.

4.2 Topical Discussion

In the previous three chapters, contents on the wave equation, the heat equation and Poisson's equation are given, respectively. Through the discussion in Sect. 4.1, we know that they are effectively the representatives of second-order linear partial differential equations of hyperbolic, parabolic and elliptic types, respectively. In this section, key features shown by these three types of second-order linear PDEs are comparatively summarised topic by topic. For each topic, the focus is always first laid on these representative PDEs, i.e. the wave equation, the heat equation and Poisson's equation. Then, the features shared by other PDEs belonging to their own categories are discussed. The aim of this section is to draw inferences about other cases from one instance, so as to help reader develop a sense in picking appropriate methods to analyse (possibly new) PDE problems arising in their own fields.

Physical background

Hyperbolic PDE

The wave equation is employed mainly to describe the behaviour of certain vibrating systems undertaking small vibrations. It is derived based on the conservation of momentum, and the causation of vibration is the inertial effect. To be specific, when any part of the system is away from its equilibrium position, it feels a restoring force from its neighbouring parts, which is proportional to the second temporal derivative of the local displacement field. As a result, when this moving object arrives at its equilibrium position, it does not stop, but keeps on moving, and vibration thus persists.

The phenomena that can be formulated by the wave equation exhibit a key feature of propagation, that is, the information at one point propagates at a finite speed along certain (characteristics) directions. For a general second-order linear hyperbolic PDE, it has the wave equation as its canonical form. Hence, it should inherit this feature of propagation. As discussed in Sect. 4.1, when a second-order hyperbolic PDE (of two variables) gets transformed to its canonical form, two families of parametric curves are introduced, which just define the corresponding two families of characteristics. Actually, a first-order PDE may also be hyperbolic, which normally corresponds to one family of characteristics. The physical processes it describes should also yield propagating behaviour. For instance, many PDEs widely used in fluid mechanics are first-order hyperbolic PDEs (e.g. [5]).

Parabolic PDE

The heat equation mainly describes how the temperature distribution of a system evolves. The driving mechanism is Fourier's law of heat transfer. Heat flows down side temperature gradient. In other words, the evolution is caused by spatial heterogeneities in certain physical quantities. Such a mechanism of gradient-driven diffusion also underlies several other physical phenomena, such as the spread of chemical elements [6], the diffusion of nutrient irons in human bodies [6], the evolution of crystalline point defects [3, 14], etc. These phenomena also see second-order

parabolic PDEs in their modellings. Besides, parabolic PDEs also see their applications in modelling stochastic processes, such as in the Black–Scholes option pricing model [9].

Elliptic PDE

Poisson's equation describes the behaviour of a potential function, most notably in electrostatic and gravitational cases. As summarised in the end of 3.1.2, it is derived by integrating two parts: a gradient-based constitutive relation usually determined through experimentation, and a divergence-based equilibrium law resulting from the conservation of certain physical quantities. Such modelling strategies are clearly demonstrated from the case of flow in porous media as detailed in Sect. 3.1.2. The experimentally validated Darcy's law (3.17) suggests that the local average fluid velocity is proportional to the spatial gradient of the hydrostatic pressure, and the proportionality is purely determined by the medium of interest. Meanwhile, mass conservation of the fluid yields Eq. (3.18), which brings a closure to the model. This also provides a rationale to the fact that a thermally equilibrated state can also be formulated by Poisson's equation. Fourier's law of heat transfer plays the role of the constitutive relation, because the heat flux is proportional to the negative temperature gradient, as suggested by Eq. (2.2). At the thermally equilibrated state, the net change in thermal energy within any closed region is zero, which sets up a conservation relation. Therefore, Poisson's equation formulates a gradient-based equilibrium state.

Such a feature is inherited by other second-order linear elliptic PDEs. For instance, the basic governing equations of linear elastostatic problems can be viewed as an elliptic PDE system for the displacement field. The constitutive relation is the Hooke's law, saying that the stress (tensor) is linearly dependent on the displacement gradient, and the proportionality is measured by the so-called elastic constants. The local force balance introduces an equilibrium relation. Therefore, many methods that are shown effective in solving problems for Poisson's equation, such as the variational principle, also work for solving linear elastostatic problems.

Initial/boundary conditions

To establish a PDE problem, certain initial and/or boundary conditions are also needed. Since both the wave equation and the heat equation evolve in time, initial conditions should be imposed accordingly. But for Poisson's equation which is normally used for describing a steady state, no initial conditions are needed. For the wave equation, one needs two initial conditions: the initial displacement and the initial speed. As for the heat equation, one initial condition suffices, that is, the initial temperature distribution.

As for boundary conditions imposed for defining PDE problems, there are normally three choices: Dirichlet (the first kind) boundary condition which specifies the values of the unknown function on the boundary; Neumann (the second kind) boundary condition which evaluates the outward normal derivatives of the unknown function on the boundary; Robin (the third type) boundary condition which can be

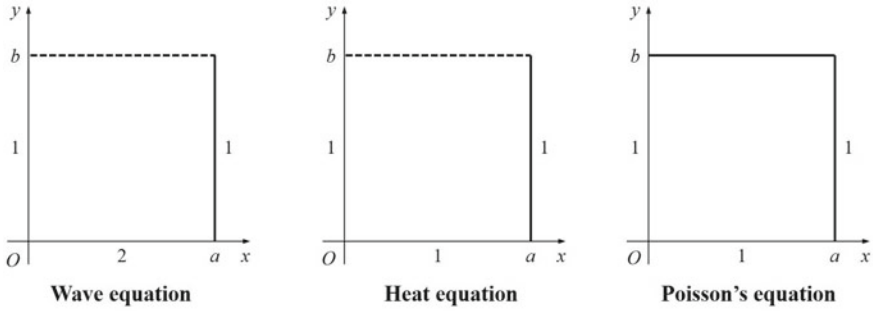

Fig. 4.3 Appropriate declaration of initial and/or boundary conditions for the three typical PDEs. The numbers of initial/boundary conditions that should be imposed are declared accordingly

considered as a linear combination of the above two types. Note that boundary conditions should be imposed everywhere on the boundary. For the case of Poisson's equation, in particular, when the domain of definition is bounded, a boundary condition should be declared at every single point on the boundary, and the resulting PDE problem is called an interior boundary value problem.

When the domain of definition is unbounded, the corresponding problem for Poisson's equation is called an exterior boundary value problem. In this case, the behaviour of the unknown function at infinity should also be specified to ensure solution uniqueness. As for the wave equation or the heat equation that are defined in unbounded domains, we only consider the cases defined throughout the full Euclidean space $\mathbb{R}^n$, i.e. the Cauchy problems. In these cases, the behaviour of the unknown function at infinity is already inferred by the initial conditions. Thus there is no need to specify the behaviour at infinity as time evolves.

Figure 4.3 comparatively summarises the condition profiles imposed with different types of second-order linear PDEs in a same prescribed domain of $(x, y) \in [0, a] \times [0, b]$. Note that the variable x represents space in all the three cases. As for the other independent variable y, it serves to be a temporal variable for the cases with the wave equation and the heat equation, while it becomes a spatial variable for the case with Poisson's equation. As discussed above, boundary conditions should definitely be imposed at the boundary points at $x = 0$ and $x = a$, corresponding to the vertical solid lines in the three figures. At $y = 0$, two initial conditions are needed for the wave equation, and one initial condition for the heat equation. But in both cases, no conditions need to be specified at $y = b$ when the evolution terminates. Its physical indication is clear. To make predictions over time, one should specify the initial state of a system, while the terminal state is a natural outcome from the evolution. But for Poisson's equation, boundary conditions are needed at both ends at $y = 0$ and $y = b$.

For generalisation, as discussed in Sect. 4.1, second-order hyperbolic PDEs bear two families of characteristics, inferring that the information translates downstream at a finite speed. As for second-order parabolic PDEs of two variables, it corresponds to

one family of integral curves, or characteristics. Hence, the concept of "up-to-down stream" still prevails. Therefore, one criterion for imposing initial conditions for hyperbolic/parabolic equations is to provide sufficient information on the boundary of the temporal domain that sits in the upstream direction. But for elliptic equations, they do not yield any characteristics, indicating that the information transition is accomplished "instantaneously". There is no upstream direction, and all boundaries have the same weight in terms of imposing conditions on them. These criteria for appropriately imposing boundary conditions are also generalisable to problems for PDEs defined in higher dimensions.

Solution for Cauchy problem

The solution for the Cauchy problem for the wave equation, i.e. D'Alembert's formula, is derived in Sect. 1.2. The derivation can be considered as a realisation of the procedure of finding the canonical form of a second-order linear hyperbolic PDE discussed in Sect. 4.1. Two families of characteristics are introduced through coordinate transformation. Therefore, when the domain of interest is the full space of $\mathbb{R}^n$, finding the corresponding characteristics offers an effective means for analysing hyperbolic PDEs. When the domain is not the full Euclidean space, the presence of boundaries may deflect or absorb a travelling wave, which complicates the situation when the method of characteristics is employed. Nevertheless, there are certain scenarios, e.g. the case with the half space, where the method of characteristics, upon modification, is still effective (see the discussion in Sect. 1.2.3).

In Sect. 2.2, the Cauchy problem for the heat equation is solved on using the method of integral transform, which is actually irrespective of the dimensionality in consideration. The key idea is to apply Fourier transform so as to transform the heat equation into an ordinary differential equation in time, whose solution is found to be in a convolution form. Note that Fourier transform is an operation that is linear with its input function. Hence, the treatments of integral transform should be generalised to solving problems governed by other linear PDEs defined in $\mathbb{R}^n$. For instance, D'Alembert's formula (1.27) can also be derived through integral transform. Note that when Fourier transform is used, the domain of definition should be the full space of $\mathbb{R}^n$. When the domain becomes the half space, Laplace transform should be employed, which is not discussed in detail here.

Method of separation of variables

The method of separation of variables is discussed in both Sect. 1.3 and 2.3, where the initial–boundary value problems governed by the wave equation and the spatially one-dimensional heat equation are solved, respectively. The key idea is to express the solution by means of a series given by

$$u(x;t) \sim \sum_{n\in\mathbb{Z}^+} A_n X_n(x) T_n(t),$$

where each term takes a variable-separated form defined as a product of unary functions. A further discussion in Sect. 2.3.2 shows that the spatial function $X_n(x)$,

$n = 1, 2, \ldots,$ are just the eigenfunctions of a Sturm–Liouville system. Guaranteed by the general properties of Sturm–Liouville systems, these eigenfunctions naturally form a complete set of orthogonal functions. The coefficients A_n are then determined by projecting the initial conditions onto X_n (see Sect. 2.3.2 for details). This establishes part of the theoretical foundation underpinning the method of separation of variables. The method is also applicable for problems governed by Laplace's equation (see Exercise 3.4).

The method of separation of variables sees its limitation on the fact that the domain (in both time and space) must take a rectangle or cuboid shape. Otherwise, the variables cannot be fully separated on the domain boundaries. It is noted that some regions that do not take a rectangle or cuboid shape in Cartesian systems may become regular in other coordinate systems. For instance, a circle corresponds to a rectangle region represented by the two-dimensional polar coordinates given by the radius r and the angle θ. This motivates the discussion in Chap. 5. Besides, the number of eigenvalue problems to be solved for increases when the method of separation of variables is applied for solving problems in higher dimensions. Still, the method of separation of variables offers an effective tool for analysing initial–boundary value problems for linear PDEs.

Variational method

The variational principle for Poisson's equation is introduced in Sect. 3.2. For a self-equilibrated system, its physical implication is clear. At the self-equilibrated state, the energy quantity driving the system must be minimised among all possible states satisfying the imposed boundary conditions. Normally, a variational method leads to a weak formulation, e.g. Eq. (3.32), which is often expressed by means of an integral that is valid for all trial functions belonging to a certain function space. The term "weak" stems from the fact that the requirement over the solution satisfying the derived integral formulation is weak in the sense of function differentiability. For instance, a classical solution to Poisson's equation should be differentiable at least twice, but its weak formulation yields solutions whose first derivatives are simply required to be integrable in the domain of interest. Technically, this is because the differentiation over the original unknown function is moved to the trial function with the use of integration by parts.

Note that finding analytical solutions from weak formulations is normally even harder than for their original PDE problems. But the variational method offers a solid theoretical foundation beneath certain numerical PDE solvers, most notably, the finite element method [17], which exhibits a number of distinguished features as a PDE solver. For instance, it works even though the domain of definition is quite irregular and has thus been implemented in many commercial softwares for engineering use. In fact, variational principles work especially well for self-equilibrated problems, normally governed by elliptic PDEs [15]. But the idea can also be implemented, upon modification, for solving problems of linear hyperbolic and parabolic PDEs, and even nonlinear problems [16].

Green's function

In Sect. 3.4, we derived the Green's function for a problem governed by Poisson's equation and imposed with Dirichlet boundary condition. The derivation starts with the implementation of the second Green's formula (3.42). When its two input functions are chosen as the solution for the problem of interest and a fundamental solution to Laplace's equation, the solution for the original PDE problem can thus be expressed as an integral defined simply on the domain boundary $\partial\Omega$, i.e. Eq. (3.48). But both the values of the solution u and its normal derivatives on $\partial\Omega$ are required if Eq. (3.48) is used. This exceeds the number of boundary conditions a problem for Poisson's equation can offer. Hence, another problem for Laplace's equation, i.e. Eq. (3.51), has to be introduced, so as to annihilate the unknown terms appearing in the boundary integral. Combining the fundamental solution with the obtained harmonic function finally defines the Green's function in need. For any Dirichlet boundary conditions and the function f on the right side of the governing equation, the solution can always be expressed through Green's function, i.e. Eq. (3.60). The derivations can be naturally generalised to cover cases with other types of boundary conditions. However, solving for the Green's function (parameterised by $\mathbf{r}^*$) is generally more difficult than solving the original PDE problem. But for domains of regular shape, such as the half space, a sphere, etc., analytical expressions for Green's function become feasible, with the use of the image method for electric potentials.

Actually, apart from problems governed by linear elliptic PDEs, the concept of Green's function can also be implemented for analysing other linear PDEs. The key procedure stays the same as discussed in Sect. 3.4. But one needs to find a more general alternative to the second Green's formula (3.42). This encompasses the concept of adjoint differential operator, which is not discussed in this book. Finally, it is noted that the boundary element method is a numerical realisation of the concept of fundamental solutions to linear PDEs.

Maximum principles

The maximum principle for the heat equation is introduced in Sect. 2.4. It suggests that in the absence of interior heat sources/sinks, the maximum/minimum temperature throughout a process of heat conduction arises either initially or on the domain boundaries. The maximum principle for the heat equation is rather physically intuitive. As suggested by Fourier's law of heat transfer, heat flows downside the temperature gradient. Therefore, in the absence of heat sources, the net heat units transferred to the position where the temperature is maximised must be non-positive, and the temperature there cannot rise as a result. This property is inherited by solutions to the steady-state (homogeneous) heat equation, i.e. harmonic functions. Literally, the maximum principle for harmonic functions is even stronger. Given a bounded domain, a non-constant harmonic function must be maximised on the boundary. Moreover, as suggested by the strong maximum principle in Sect. 3.6, the normal derivative of the harmonic function cannot even vanish at the maximiser. The uniqueness and stability of solutions for problems governed by the heat equation/Poisson's equation are demonstrated with the use of corresponding maximum principles.

Note that the solution to a hyperbolic PDE does not comply with any maximum principles. As a representative, the wave equation formulates the propagation of wave (along the characteristics). Thus, the peaks of two wave may occasionally superpose to form an even higher peak, which can take place at an interior point that is not in its initial state. From a mathematical perspective, the heat equation is affiliated with a maximum principle, because the rate of change in the unknown quantity (which is the temperature) is affected by its negative spatial gradient. In contrast, the wave equation is derived where the spatial gradient of the displacement is proportional to its acceleration, and no maximum principle can be declared then.

Energy method

The solution uniqueness of a problem governed by the wave equation is analysed with the use of energy expression given by Eq. (1.106). Actually, the energy estimation approach offers an effective means for predicting the behaviour of second-order hyperbolic PDEs. Note that the wave equation can degenerate to Poisson's equation, when the unknown function becomes independent of time. Therefore, the energy method is also applicable to demonstrate the solution uniqueness of problems for Poisson's equation as stated in Sect. 3.6.4.

Summary

A comparative discussion on the behaviours of the three canonical second-order linear PDEs has been conducted over various topics. In Table 4.2, a final summary over the key concepts discussed is outlined here.

Table 4.2 A comparative summary about the concepts related to the three canonical second-order linear PDEs

Type	Hyperbolic (Sect. 4.1)	Parabolic (Sect. 4.1)	Elliptic (Sect. 4.1)
Physical background	Propagation	Diffusion	Equilibrium
Representative	$u_{tt} - a^2\Delta u = f$ Wave (Sect. 1.1, Sect. 1.4)	$u_t - a^2\Delta u = f$ Heat (Sect. 2.1)	$-\Delta u = f$ Electrostatic (Sect. 3.1)
Initial/boundary conditions	2ICs, 2BCs (Sect. 1.1)	1ICs,2BCs (Sect. 2.1)	Interior and exterior problem (Sect. 3.1)
Cauchy problem	Characteristics (Sect. 1.2)	Integral transform (Sect. 2.2)	
Separation of variables	Sturm–Liouville system (Sect. 1.3, Sect. 2.3)		Also applicable
Variational principle	Applicable	Applicable	Energy minimisation (Sect. 3.2)
Green's function	Applicable	Applicable	Electrostatic (Sect. 3.5)
Solution uniqueness	Energy method (Sect. 1.5)	Maximum principle (Sect. 2.4)	Both and stronger (Sect. 3.6)
Other concepts	Infinitesimal (Sect. 1.1) Duhamel's principle (Sect. 1.2)	Fourier transform Convolution (Sect. 2.2)	Radial solution (Sect. 3.3)

One may refer to the labelled section for greater details about the corresponding concepts

Exercise

1. Determine the type of the following PDEs:

   (a) $y^2 u_{xx} - x^2 u_{yy} = 0$;
   (b) $\sin^2 x u_{xx} + u_{yy} = 0$;
   (c) $xy u_{xx} + u_{yy} = 0$;
   (d) $u_{xx} + u_{yy} + 4u_{zz} + 2u_{xy} - 4u_{xz} = 0$.

2. Transform the following PDEs into their canonical forms [Eqs. (4.14), (4.17) or (4.21)].

   a. $5u_{xx} + 4u_{xy} + u_{yy} + 2u_x + 3u_y = 0$;
   b. $y^2 u_{xx} + 2xy u_{xy} + x^2 u_{yy} = 0$;
   c. $x u_{xx} + u_{yy} = 0$;
   d. $(3 + \sin^2 y) u_{xx} + 2\cos y\, u_{xy} - u_{yy} = 0$.

Part II
Special Functions

Chapter 5
Bessel Functions

From this chapter on, several mathematical tools for solving linear PDE problems will be introduced. The next three chapters are focused on special functions, which are conceptualised in contrast with elementary functions. Being a general term, a special function is a function having a particular use in mathematical physics or some other branch of mathematics.[1] Special functions are sometimes discussed in contrast with the elementary functions, including algebraic, exponential, logarithm, trigonometric functions and their combination and composition for finite times.[2] In this chapter, an important family of special functions, Bessel functions, will be discussed in detail. The contents in this chapter are summarised in the knowledge map charted by Fig. 5.1.

5.1 Bessel Equation and Bessel Functions

5.1.1 Physical Motivation

We start with the motivation of the Bessel differential equation from the modelling of heat conduction within a circular domain. To this end, we consider a (two-dimensional) circular region of radius R defined by $\mathcal{O}_R = \{(x, y)|x^2 + y^2 \leq R^2\}$. The heat transfer process within $\mathcal{O}_R$ is thus modelled by

[1] This definition is taken from mathworld.wolfram.com/SpecialFunction.

[2] For a more rigorous definition for elementary function, one may refer to p. 145 of [10].

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Y. Zhu, *Equations and Analytical Tools in Mathematical Physics*,
https://doi.org/10.1007/978-981-16-5441-1_5

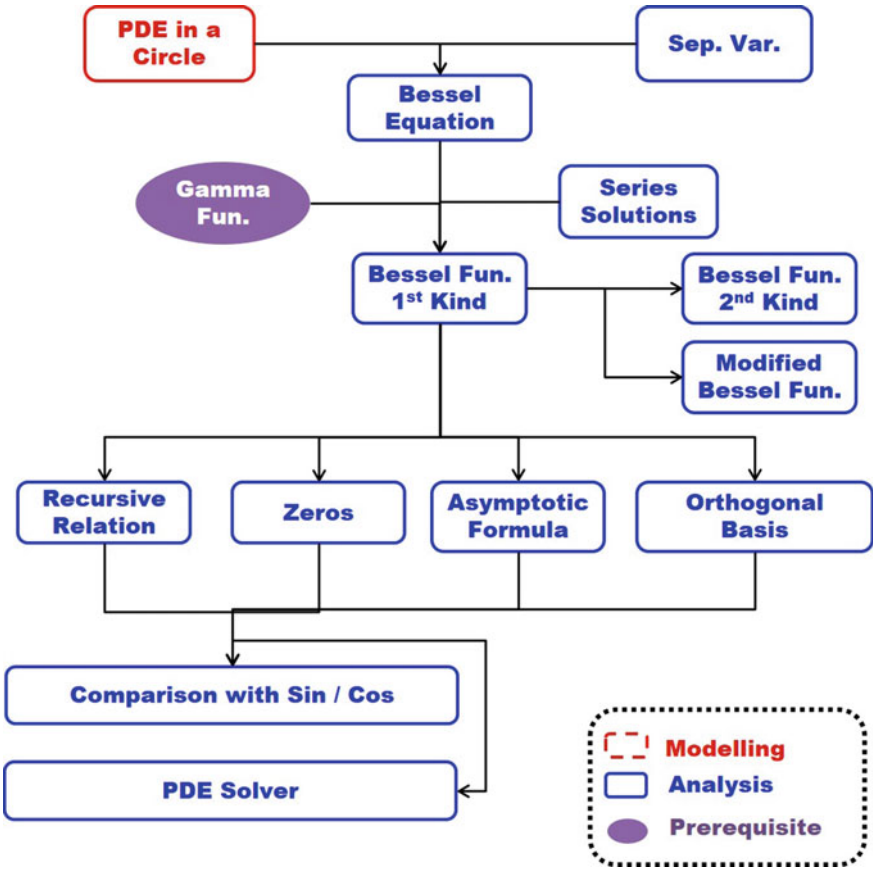


Fig. 5.1 Knowledge map—Bessel functions

$$\begin{cases} u_t - a^2(u_{xx} + u_{yy}) = 0, \ (x, y) \in \mathcal{O}_R, \ t > 0; \\ u|_{t=0} = \phi(x, y); \\ u|_{\partial \mathcal{O}_R} = 0. \end{cases} \tag{5.1}$$

Problem (5.1) is effectively an initial–boundary value PDE problem, and we are then inclined to use the method of separation of variables for its solution. The present example is distinguished from the previous cases discussed in Sects. 1.3 and 2.3.1. First, more than two independent variables are involved here, indicating that the variables may be separated more than once. Second, the domain of definition here does not take a rectangular shape in space, and the variables x and y cannot be fully dissociated on the circular boundary. The present subsection is aimed to overcome these two challenging issues.

As a trial, we assume that the unknown function u take a variable-separated form of

$$u(x, y; t) = T(t)V(x, y),$$

where the temporal variable is separated from the two spatial variables. Inserting it into the governing PDE of problem (5.1) gives

$$\frac{T'}{a^2 T} = \frac{1}{V}(V_{xx} + V_{yy}) = -\lambda,$$

where a constant λ is introduced.

To this stage, we end up with an ordinary differential equation in time:

$$T' + a^2 \lambda T = 0$$

and a partial differential equation in space:

$$\begin{cases} \Delta V + \lambda V = 0, (x, y) \in \mathcal{O}_R; \\ V|_{\sqrt{x^2+y^2}=R} = 0, \end{cases} \tag{5.2}$$

where $\Delta V = V_{xx} + V_{yy}$ is recalled to be the (two-dimensional) Laplacian operation as defined in Sect. 3.1.1. The governing equation of problem (5.2) is called the (two-dimensional) *Helmholtz equation*.

We consider solving problem (5.2). Since the domain of definition is a circle now, it is natural to consider the problem with the two-dimensional polar coordinates introduced by

$$\begin{cases} r = \sqrt{x^2 + y^2}; \\ \theta = \tan^{-1}\left(\frac{y}{x}\right). \end{cases}$$

As suggested by Eq. (3.35), problem (5.2) can be rewritten in the two-dimensional polar system by

$$\begin{cases} V_{rr} + \frac{1}{r}V_r + \frac{1}{r^2}V_{\theta\theta} + \lambda V = 0; \\ V|_{r=R} = 0. \end{cases} \tag{5.3}$$

Note that with polar coordinates r and θ, the domain of definition becomes $(r, \theta) \in [0, R] \times [0, 2\pi]$, which now takes a rectangle shape. Hence, one may separate the variables again by assuming

$$V(r, \theta) = \mathcal{P}(r)\Theta(\theta).$$

Inserting it into the Helmholtz equation of problem (5.3) and dividing $\mathcal{P}\Theta$ on both sides, we manage to separate the variable r from θ and then obtain

$$-\frac{r^2\mathcal{P}'' + rP'}{\mathcal{P}} - \lambda r^2 = \frac{\Theta''}{\Theta} = -\nu,$$

where ν is another constant introduced during this round of separation of variables. Note that the variables have been separated twice. As a result, two constants λ and ν are sequentially introduced, and they should be carefully distinguished from each other in the upcoming derivations.

Therefore, we establish an ODE problem for $\Theta(\theta)$ given by

$$\begin{cases} \Theta'' + \nu\Theta = 0, \quad \theta \in [0, 2\pi]; \\ \Theta(0) = \Theta(2\pi), \ \Theta'(0) = \Theta'(2\pi), \end{cases} \tag{5.4}$$

and an ODE problem for $\mathcal{P}(r)$ given by

$$\begin{cases} r^2\mathcal{P}'' + r\mathcal{P}' + (\lambda r^2 - \nu)\mathcal{P} = 0, \quad r \in (0, R); \\ \mathcal{P}|_{r=R} = 0. \end{cases} \tag{5.5}$$

Note that the boundary conditions in problem (5.4) stems from the fact that $\Theta(\theta)$ is periodic in θ with 2π being the period.

Now we need to decide which one of problems (5.4) and (5.5) should be solved first. Recalling from the previous attempts on using the method of separation of variables, the two introduced constants λ and ν are expected to be the eigenvalues of the corresponding problems. It is observed that problem (5.4) only contains ν, while both λ and ν appear in problem (5.5). Hence, a feasible strategy is to solve the eigenvalue problem (5.4) for ν first, then solve the other problem for λ (with ν given). This principle also applies in other situations where variables get progressively separated.

As discussed in the prerequisite knowledge part of Sect. 1.3, the solutions to the ODE of problem (5.4) can be generally expressed by $\Theta(\theta) = A\cos\sqrt{\nu}\theta + B\sin\sqrt{\nu}\theta$. But only when $\nu = n^2$, the periodic conditions are satisfied for arbitrary constants A and B. In other words, non-trivial solutions to problem (5.4) exist with $\nu = \nu_n = n^2$, and the resulting eigenfunctions (corresponding to the eigenvalue ν_n) are then calculated by

$$\Theta_n(\theta) = A_n\cos n\theta + B_n\sin n\theta, \ \text{for } n = 0, 1, \ldots.$$

Inserting $\nu = n^2$ into problem Eq. (5.5) gives

$$\begin{cases} r^2\mathcal{P}'' + r\mathcal{P}' + (\lambda r^2 - n^2)\mathcal{P} = 0, \ r \in (0, R); \\ \mathcal{P}|_{r=R} = 0. \end{cases} \tag{5.6}$$

Problem (5.6) is governed by a second-order linear ODE. Thus, it can be analytically solved, provided that its two mutually independent solutions can be derived.

To this end, we introduce

$$x^2\frac{\mathrm{d}^2y}{\mathrm{d}x^2} + x\frac{\mathrm{d}y}{\mathrm{d}x} + (x^2 - n^2)y = 0. \tag{5.7}$$

It can be verified that if $y = F(x)$ is a solution to ODE (5.7), then $\mathcal{P}(r) = F(\sqrt{\lambda}r)$ solves the governing equation of problem (5.6). Note that Eq. (5.7) is slightly simpler as it only contains one parameter n.

Therefore, instead of solving the original problem (5.6), we look for solutions to Eq. (5.7), which is called the nth order *Bessel differential equation*, or simply the *Bessel equation*.

5.1.2 Bessel Function of the First Kind

Now we consider a more general situation, with the integer n in Eq. (5.7) changed to be any number α. The resulting equation

$$x^2\frac{\mathrm{d}^2y}{\mathrm{d}x^2} + x\frac{\mathrm{d}y}{\mathrm{d}x} + (x^2 - \alpha^2)y = 0 \tag{5.8}$$

becomes an αth *order* Bessel equation. Note that here we set $\alpha > 0$, and it will be seen later this setting does not lose generalities. The Bessel equation (5.8) is effectively a second-order, linear, and homogeneous ODE. Hence, we seek for two of its mutually independent solutions, so as to derive its fundamental solution system.

The strategy here is to find a solution to Eq. (5.8) which has a series expansion of

$$y = \left(a_0 + a_1x + a_2x^2 + \cdots\right)x^c = \left(\sum_{m=0}^{\infty} a_m x^m\right)x^c. \tag{5.9}$$

Several issues are noted regarding the formulation given by Eq. (5.9). Firstly, compared to the Taylor series, a common factor x^c is introduced. The reason is as follows. It is possible that $y = 0$ at $x = 0$. If that is the case, we do not know beforehand the rate of y tending to 0 as $x \to 0$, i.e. $y \sim x^c$ with the exponent c also being an unknown number. In particular, when c is equal to a non-negative integer, Eq. (5.9) becomes a conventional Taylor series.

Secondly, without loss of generalities, we let the coefficient $a_0 \neq 0$. If a_0 happens to be zero, we can always let a_1 replace a_0, and let $c + 1$ replace c. Then the assumption of $a_0 \neq 0$ still holds, provided that the original $a_1 \neq 0$. If the original a_1 happens to be zero, too, we carry on this process until encountering a nonzero a_n.

Thirdly, we only consider the situation for all x, such that the series in Eq. (5.9) is uniformly convergent. Since the series in Eq. (5.9) differs from Taylor series only by a common factor of x^c, the concept of convergent radius still apply here; i.e. there should exist $R > 0$, such that series (5.9) is uniformly convergent as long as $|x| < R$.

With the series set by Eq. (5.9), the unknowns now become a family of coefficients $\{a_m\}_{m=0}^{\infty}$ and the exponent c. They should be determined through inserting Eq. (5.9) into (5.8) and equating coefficients order by order. For doing that, one needs to

interchange the operations of differentiation with combination about a uniformly convergent series. For instance, we have

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{\mathrm{d}}{\mathrm{d}x}\left(a_m \sum_{m=0}^{\infty} x^{m+c}\right) = \sum_{m=0}^{\infty} a_m \frac{\mathrm{d}x^{m+c}}{\mathrm{d}x} = \sum_{m=0}^{\infty} a_m (m+c) x^{m+c-1}.$$

Differentiating it with respect to x again gives

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} = \sum_{m=0}^{\infty} a_m (m+c)(m+c-1) x^{m+c-2}.$$

Thus, the following identity should hold:

$$\begin{aligned} & x^2 \frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + x \frac{\mathrm{d}y}{\mathrm{d}x} - \alpha^2 y \\ &= \sum_{m=0}^{\infty} \left(a_m (m+c)(m+c-1) + a_m (m+c) - a_m \alpha^2\right) x^{m+c} \\ &= \sum_{m=0}^{\infty} a_m \left[(m+c)^2 - \alpha^2\right] x^{m+c}. \end{aligned} \tag{5.10}$$

Besides,

$$x^2 y = \sum_{m=0}^{\infty} a_m x^{m+c+2} = \sum_{m=2}^{\infty} a_{m-2} x^{m+c}, \tag{5.11}$$

where the second identity is obtained by index shift; i.e. the series starting with $m = 0$ is first re-indexed by letting $k = m + 2$, and then the resulting series is re-indexed back by m instead of k. The reason is that a change in the symbol for indexation in a series does not vary its output. Such a way of index shift enables direct summation of the two series given by Eqs. (5.10) and (5.11). To be specific, the sum of these two (uniformly convergent) series is carried out by adding together the corresponding coefficients of x^{m+c} with $m = 2, 3, \ldots$.

Adding Eqs. (5.10) by (5.11) simply reproduces the left side of Bessel equation (5.8), which is finally expressed in a series form by

$$a_0 (c^2 - \alpha^2) x^c + a_1 \left[(c+1)^2 - \alpha^2\right] x^{c+1} + \sum_{m=2}^{\infty} \left(a_m \left((m+c)^2 - \alpha^2\right) + a_{m-2}\right) x^{m+c} = 0. \tag{5.12}$$

Note that the summation in Eq. (5.12) starts from $m = 2$, which inherits the behaviour of the series in Eq. (5.11), and the terms involving x^c and x^{c+1} in Eq. (5.10) should be singled out individually.

For Eq. (5.12) to hold, the coefficients for x^{m+c} should vanish for any $m \geq 0$. This results in a series of algebraic equations for c and a_m ($m \geq 0$), and we should start from the lowest order, i.e.

$$a_0(c^2 - \alpha^2) = 0. \tag{5.13}$$

Because a_0 is set non-vanishing, $c = \pm\alpha$, and the situation with $c = \alpha$ is considered first.

Inserting $c = \alpha$ into Eq. (5.12) gives

$$a_1\left[(\alpha+1)^2 - \alpha^2\right]x^{\alpha+1} + \sum_{m=2}^{\infty}\left(a_m\left((m+\alpha)^2 - \alpha^2\right) + a_{m-2}\right)x^{\alpha+m} = 0. \tag{5.14}$$

Letting the coefficient for $x^{\alpha+1}$ vanish gives $a_1(2\alpha+1) = 0$, which suggests

$$a_1 = 0.$$

Then we carry on with the coefficients for $x^{\alpha+m}$ ($m \geq 2$) and derive

$$a_m\left((m+\alpha)^2 - \alpha^2\right) + a_{m-2} = 0,$$

which indicates a recurrence relation formulated by

$$a_m = -\frac{a_{m-2}}{m(2\alpha+m)}. \tag{5.15}$$

Originating from the fact that $a_1 = 0$, one quickly concludes that $a_3 = a_5 = \cdots = 0$ from Eq. (5.15). In other words, when m is an odd number, $a_m = 0$.

When m is an even number, we set $m = 2k$, $k = 0, 1, \ldots$. The recurrence formula (5.15) is rewritten by

$$a_{2k} = -\frac{a_{2k-2}}{2^2(\alpha+k)k}. \tag{5.16}$$

This sequentially suggests

$$a_2 = -\frac{a_0}{2^2(\alpha+1)1},\ a_4 = \frac{a_0}{2^2\cdot 2^2(\alpha+1)(\alpha+2)1\cdot 2}, \ldots.$$

Or a general expression for a_{2k} is summarised by

$$a_{2k} = \frac{(-1)^k a_0}{2^{2k}(\alpha+1)(\alpha+2)\cdots(\alpha+k)k!}, \tag{5.17}$$

indicating that all a_{2k} see its roots in a_0.

Up to now, a_0 is still an arbitrary nonzero constant left unspecified. This is reasonable, as for a linear homogeneous differential equation, a solution multiplied by

any constant is still its solution. But here, we may assign a certain value to a_0, so as to simplify the expressions for a_{2k} given by Eq. (5.17). To this end, we set

$$a_0 = \frac{1}{2^\alpha \Gamma(\alpha+1)},$$

where $\Gamma(\cdot)$ is the Gamma function, whose properties are briefly summarised in the prerequisite part concluding this section. On repeatedly using the recurrence relation (5.26) exhibited by Γ-function, we have

$$\Gamma(\alpha+1)\cdot((\alpha+1)(\alpha+2)\cdots(\alpha+k)) = \Gamma(\alpha+k+1).$$

The coefficients a_{2k} in Eq. (5.17) can thus be expressed by

$$a_{2k} = \frac{(-1)^k a_0}{2^{\alpha+2k}\Gamma(\alpha+k+1)k!}. \tag{5.18}$$

Finally, through inserting the results of $c=\alpha$, $a_{2k+1}=0$ and Eq. (5.18) into (5.9), a solution to Bessel equation (5.8) is eventually derived to be

$$y = \sum_{k=0}^{\infty} \frac{(-1)^k x^{\alpha+2k}}{2^{\alpha+2k}k!\Gamma(\alpha+k+1)} = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!\Gamma(\alpha+k+1)}\cdot\left(\frac{x}{2}\right)^{\alpha+2k}.$$

It can be readily verified that the series above is uniformly convergent for all $x\in\mathbb{R}$. In fact, this series effectively defines a family of functions parameterised by their order α, which can be collectively denoted by a symbol $\mathrm{J}_\alpha(x)$, i.e.

$$\mathrm{J}_\alpha(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!\Gamma(\alpha+k+1)}\cdot\left(\frac{x}{2}\right)^{\alpha+2k}. \tag{5.19}$$

$\mathrm{J}_\alpha(x)$ defined by Eq. (5.19) is known as the αth order *Bessel function of the first kind*, which satisfies the corresponding Bessel equation of order α. In particular, when α becomes an integer, say n, $\mathrm{J}_n(x)$ becomes a *Bessel function of integer order*. When α is a half-integer, i.e. $\alpha = n+\frac{1}{2}$, the resulting function $\mathrm{J}_{n+\frac{1}{2}}(x)$ is a *Bessel function of half-integer order*.

Here the Bessel function of the first kind is defined by means of its series expression, as in Eq. (5.19). This seems to be different from the way of introducing elementary functions, where their series expansions are often introduced successive to their definitions. But for a special function, it is usually introduced by its series form. This is because a special function is often a solution to a practically useful ODE, whose solution is available mainly from its series form. In fact, the idea of representing an important number/function through infinite summation is not new. For

instance, being one of the most important irrational number, the circular constant π is normally introduced through an infinite decimal number $3.1415926\cdots$. In a similar sense, Bessel functions of the first kind are defined by means of an infinite summation, that is, a series.

5.1.3 Bessel Function of the Second Kind

Besides the Bessel function of the first kind $\mathrm{J}_\alpha(x)$, another solution to Bessel equation (5.8) is still needed, so as to determine its fundamental system of solutions. A natural choice for this solution [which should be independent of $\mathrm{J}_\alpha(x)$] is to let $c = -\alpha$ in Eq. (5.13). Repeating the above procedure, we should derive a Bessel function of negative order expressed by

$$\mathrm{J}_{-\alpha}(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!\Gamma(-\alpha+k+1)} \cdot \left(\frac{x}{2}\right)^{-\alpha+2k}. \tag{5.20}$$

As long as $\mathrm{J}_{-\alpha}(x)$ and $\mathrm{J}_\alpha(x)$ are mutually independent, their linear combination should express any solution to Eq. (5.8). However, this is not the case. For example, when $\alpha = 0$, $\mathrm{J}_{-\alpha}(x) = \mathrm{J}_\alpha(x) = \mathrm{J}_0(x)$. Actually, we have the following lemma.

Lemma Being of integer order, the Bessel function of the first kind $\mathrm{J}_n(x)$ is linearly dependent on $\mathrm{J}_{-n}(x)$ by

$$\mathrm{J}_{-n}(x) = (-1)^n \mathrm{J}_n(x). \tag{5.21}$$

Proof Replacing $-\alpha$ in Eq. (5.20) by $-n$ gives

$$\mathrm{J}_{-n}(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!\Gamma(-n+k+1)} \cdot \left(\frac{x}{2}\right)^{-n+2k}.$$

As discussed in the prerequisite part of this section about Γ-function, $1/\Gamma(m) = 0$ for any non-positive integer input. Therefore, the coefficients of the first n terms in the above series (from $k = 0$ to $k = n-1$) are effectively all zero. Hence, the series above can be rewritten by

$$\mathrm{J}_{-n}(x) = \sum_{k=n}^{\infty} \frac{(-1)^k}{k!\Gamma(-n+k+1)} \cdot \left(\frac{x}{2}\right)^{-n+2k} = \sum_{m=0}^{\infty} \frac{(-1)^{m+n}}{(m+n)!\Gamma(m+1)} \cdot \left(\frac{x}{2}\right)^{n+2m},$$

where the treatment of index shift is employed again to derive the second identity.

Given $(m+n)! = m! \cdot (m+1)\cdots(m+n)$ and

$$(m+1)(m+2)\cdots(m+n)\Gamma(m+1) = \Gamma(n+m+1),$$

$\mathrm{J}_{-n}(x)$ can be eventually expressed by

$$\mathrm{J}_{-n}(x) = (-1)^n \sum_{k=0}^{\infty} \frac{(-1)^m}{m!\Gamma(n+m+1)} \cdot \left(\frac{x}{2}\right)^{n+2m}.$$

Comparing this expression with that by Eq. (5.19) proves the lemma. □

Therefore, we still need to seek for another solution to Eq. (5.8), which is linearly independent of $\mathrm{J}_\alpha(x)$ for all α. For this purpose, we introduce

$$\mathrm{N}_\alpha(x) = \lim_{\nu \to \alpha} \frac{\mathrm{J}_\nu(x)\cos\nu\pi - \mathrm{J}_{-\nu}(x)}{\sin\nu\pi}. \tag{5.22}$$

When α is not an integer, the fraction in Eq. (5.22) is well-defined with ν being replaced by α. As both $\mathrm{J}_\alpha(x)$ and $\mathrm{J}_{-\alpha}(x)$ are both solutions to the Bessel equation of order α, $\mathrm{N}_\alpha(x)$ given as their linear combination naturally solves Eq. (5.8), and the resulting $\mathrm{N}_\alpha(x)$ is independent of $\mathrm{J}_\alpha(x)$ given the presence of $\mathrm{J}_{-n}(x)$.

When $\alpha = n$ is an integer in Eq. (5.22), as from the lemma above, the limit defined by Eq. (5.22) is of "0/0" type, and $\mathrm{N}_n(x)$ should be further expressed with the use of L'Hôpital's rule. Without detailed proof, it can be verified that $\mathrm{N}_\alpha(x)$ also solves the αth order Bessel equation, and it is now independent of $\mathrm{J}_n(x)$.

The function $\mathrm{N}_\alpha(x)$ defined through Eq. (5.22) is called the α-th order *Bessel equation of the second kind*, or the *Neumann function*. Therefore, α-th order Bessel equation (5.8) yields a fundamental system of solutions that is formed by Bessel functions of both kinds, $\mathrm{J}_\alpha(x)$ and $\mathrm{N}_\alpha(x)$, i.e.

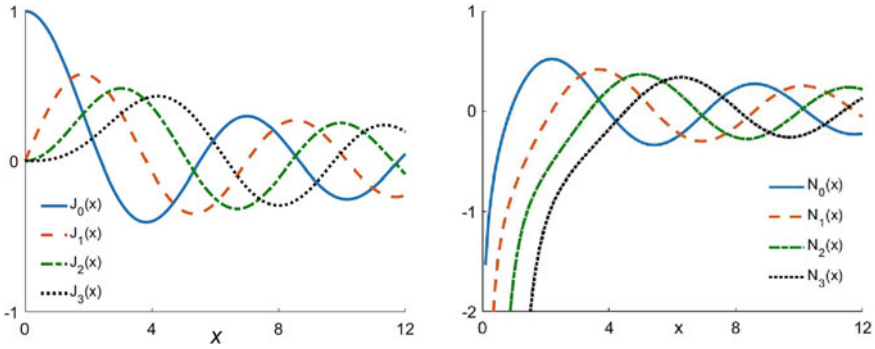
$$y = C_1\mathrm{J}_\alpha(x) + C_2\mathrm{N}_\alpha(x) \tag{5.23}$$

solves Eq. (5.8) with C_1 and C_2 being the coefficients to be determined.

Figure 5.2 shows the profiles of $\mathrm{J}_\alpha(x)$ and $\mathrm{N}_\alpha(x)$ with $\alpha = 0, 1, 2$ and 3. It can be observed that when $x \to 0^+$, $\mathrm{N}_\alpha(x)$ tends to negative infinity, i.e.

$$\lim_{x \to 0^+} \frac{1}{\mathrm{N}_\alpha(x)} = 0. \tag{5.24}$$

To this stage, the Bessel functions of both kinds are defined. They are actually induced by a differential equation, i.e. the Bessel equation. Moreover, they are expressed in a series form. This way of function introduction seems to be different from that for elementary functions. But actually, Bessel functions share strong analogies with sinusoidal functions, a typical class of elementary functions, in many aspects. For instance, sinusoidal functions can also be induced as solutions to an ODE of $\Theta''(x) + \alpha^2\Theta(x) = 0$. In the next section, similarities shared by Bessel functions and sinusoidal functions will be discussed in a more systematic manner.



(a) $\mathrm{J}_n(x)$ (b) $\mathrm{N}_n(x)$

Fig. 5.2 Profiles of $\mathrm{J}_n(x)$ and $\mathrm{N}_n(x)$ for $n = 0, 1, 2$ and 3

Prerequisite Knowledge

The concept of the *Gamma function* has been mentioned in a number of advanced calculus textbooks. It is defined by

$$\Gamma(z) = \int_0^\infty e^{-x} x^{z-1} \mathrm{d}x. \tag{5.25}$$

Two most prominent properties of the Gamma function are summarised as follows

- *recurrence formula*:

$$\Gamma(z+1) = z\Gamma(z); \tag{5.26}$$

- *reflection formula*:

$$\Gamma(z)\Gamma(1-z) = -z\Gamma(z)\Gamma(-z) = \frac{\pi}{\sin \pi z}. \tag{5.27}$$

Both of the properties above can be verified based on its definition (5.25). Moreover, the above-listed formulations can be generalised to the case where the input z takes complex values.

With these properties, $\Gamma(z)$ can be analytically expressed for certain input values of z. For instance, $\Gamma(1) = 1$ as checked directly with the definition (5.25). Then with the recurrence formula (5.26), we have $\Gamma(2) = \Gamma(1) \cdot 1 = 1$, and

$$\Gamma(z+n) = (z+n-1)\cdots(z+1)\Gamma(z+1) \tag{5.28}$$

for any positive integer n.

By letting $z = 1$ in Eq. (5.28), we obtain

$$\Gamma(n+1) = n!.$$

Then using reflection formula (5.27), we have

$$\frac{1}{\Gamma(-n)} = -\frac{n\Gamma(n)\sin \pi n}{\pi} = 0,$$

It can also be verified that $1/\Gamma(0) = 0$. This indicates that $\Gamma(z)$ is not well-defined for any negative integer inputs.

Moreover, letting $z = 1/2$ in Eq. (5.27) gives

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi},$$

and then letting $z = 1/2$ in Eq. (5.28) gives

$$\Gamma\left(n+\frac{1}{2}\right) = \left(n-\frac{1}{2}\right)\cdots\frac{1}{2}\cdot\Gamma\left(\frac{1}{2}\right) = \frac{1\cdot 3\cdot 5\cdots(2n-1)\sqrt{\pi}}{2^n} = \frac{(2n)!\sqrt{\pi}}{2^{2n}n!}. \tag{5.29}$$

On using the reflection formula (5.27), we have

$$\begin{aligned}\Gamma\left(-n+\frac{1}{2}\right) &= -\left(n+\frac{1}{2}\right)\Gamma\left(-n-\frac{1}{2}\right) = \frac{\pi}{\sin\left(n\pi+\frac{\pi}{2}\right)\Gamma\left(n+\frac{1}{2}\right)} \\ &= (-1)^n\frac{2^{2n}n!}{(2n)!}\cdot\sqrt{\pi}.\end{aligned} \tag{5.30}$$

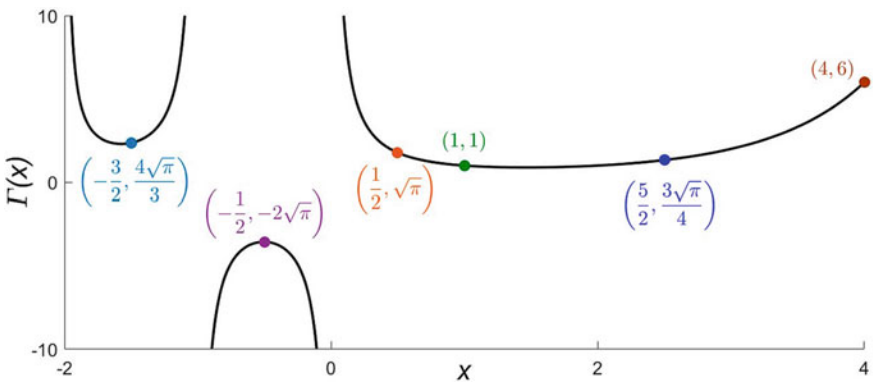


Fig. 5.3 Profile of the Gamma function $\Gamma(x)$, with several of its typical output values identified

To summarise, Gamma function can be analytically evaluated when its input becomes a positive integer or a half-integer. Figure 5.3 shows the profile of $\Gamma(x)$, with several of its key output values specified.

5.2 Properties of Bessel Functions

In this section, several interesting properties of Bessel functions of both kinds are discussed. For developing more solid understanding over the topic, these properties are comparatively summarised against similar properties shown by sinusoidal functions in the end of this section.

5.2.1 Recurrence Formulae

The recurrence formulae for Bessel functions describe how an αth-order Bessel function is related to Bessel functions of adjacent orders, i.e. $(\alpha \pm 1)$th order. We start with two recurrence relations for the Bessel functions of the first kind:

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(x^{\alpha}\mathrm{J}_{\alpha}(x)\right) = x^{\alpha}\mathrm{J}_{\alpha-1}(x), \qquad \frac{\mathrm{d}}{\mathrm{d}x}\left(x^{-\alpha}\mathrm{J}_{\alpha}(x)\right) = -x^{-\alpha}\mathrm{J}_{\alpha+1}(x). \tag{5.31}$$

The proof of the first identity above is presented here. The idea is to write the involved Bessel functions in series form and then establish the identity sequentially.

Inserting Eq. (5.19) into the left side of the first identity in Eq. (5.31) gives

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}x}\left(x^{\alpha}\mathrm{J}_{\alpha}(x)\right) &= \frac{\mathrm{d}}{\mathrm{d}x}\left(\sum_{k=0}^{\infty}\frac{(-1)^k 2^{\alpha}}{k!\Gamma(\alpha+k+1)}\cdot\left(\frac{x}{2}\right)^{2\alpha+2k}\right)\\ &= \sum_{k=0}^{\infty}\frac{(-1)^k\cdot 2^{\alpha+1}(\alpha+k)}{2^{2\alpha+2k}k!\Gamma(\alpha+k+1)}\cdot x^{2\alpha+2k-1}\\ &= \sum_{k=0}^{\infty}\frac{(-1)^k(\alpha+k)2^{\alpha}}{k!\Gamma(\alpha+k+1)}\cdot\left(\frac{x}{2}\right)^{2\alpha+2k-1}.\end{aligned} \tag{5.32}$$

On using $\Gamma(\alpha+k+1) = (\alpha+k)\Gamma(\alpha+k)$, the factor $(\alpha+k)$ on the right side of Eq. (5.32) gets eliminated, leading to

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(x^{\alpha}\mathrm{J}_{\alpha}(x)\right) = x^{\alpha}\sum_{k=0}^{\infty}\frac{(-1)^k}{k!\Gamma(\alpha+k)}\cdot\left(\frac{x}{2}\right)^{\alpha-1+2k}. \tag{5.33}$$

A comparison between Eqs. (5.19) and (5.33) suggests that the series on the right side of Eq. (5.33) is just $\mathrm{J}_{\alpha-1}(x)$. Thus, the first identity of Eq. (5.31) is proved, and the second one should be proved likewise.

Expanding the derivatives in Eq. (5.31) gives

$$x\mathrm{J}_{\alpha}^{'}(x) + \alpha\mathrm{J}_{\alpha}(x) = x\mathrm{J}_{\alpha-1}(x); \tag{5.34a}$$

$$x\mathrm{J}_{\alpha}^{'}(x) - \alpha\mathrm{J}_{\alpha}(x) = -x\mathrm{J}_{\alpha+1}(x). \tag{5.34b}$$

Adding and subtracting these two identities result in another pair of recurrence formulae given by

$$\mathrm{J}_{\alpha-1}(x) + \mathrm{J}_{\alpha+1}(x) = \frac{2\alpha}{x} \cdot \mathrm{J}_{\alpha}(x); \tag{5.35a}$$

$$\mathrm{J}_{\alpha-1}(x) - \mathrm{J}_{\alpha+1}(x) = 2\mathrm{J}_{\alpha}'(x), \tag{5.35b}$$

where $\mathrm{J}_{\alpha}'(x)$ denotes the derivative of $\mathrm{J}_{\alpha}(x)$.

Bessel functions of the second kind satisfy same recurrence relations, i.e.

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(x^{\pm\alpha}\mathrm{N}_{\alpha}(x)\right) = \pm x^{\pm\alpha}\mathrm{N}_{\alpha\mp1}(x). \tag{5.36}$$

As one application of the recurrence formulae listed above, the expressions for Bessel functions of the first kind of half-integer orders can be analytically derived. We start with letting $\alpha = \frac{1}{2}$ in series form (5.19) and obtain

$$\mathrm{J}_{\frac{1}{2}}(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!\Gamma(k+\frac{3}{2})}\left(\frac{x}{2}\right)^{\frac{1}{2}+2k}.$$

As from recurrence formula (5.29) for the Gamma function, i.e. $\Gamma\left(k+\frac{3}{2}\right) = \frac{(2(k+1))!\sqrt{\pi}}{2^{2(k+1)}(k+1)!}$, the above identity is rewritten by

$$\mathrm{J}_{\frac{1}{2}}(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \cdot \frac{2^{2(k+1)}(k+1)!}{(2(k+1))!\sqrt{\pi}}\left(\frac{x}{2}\right)^{\frac{1}{2}+2k} = \sqrt{\frac{2}{\pi x}} \cdot \sum_{k=0}^{\infty} \frac{(-1)^k x^{2k+1}}{(2k+1)!}.$$

Note that the series above is just equal to $\sin x$. Hence, we have

$$\mathrm{J}_{\frac{1}{2}}(x) = \sqrt{\frac{2}{\pi x}} \cdot \sin x. \tag{5.37}$$

Analogically, we obtain

$$\mathrm{J}_{-\frac{1}{2}}(x) = \sqrt{\frac{2}{\pi x}} \cdot \cos x. \tag{5.38}$$

On using recurrence formula (5.35a) with $\alpha = 1/2$, we have

$$\mathrm{J}_{\frac{3}{2}}(x) = \frac{1}{x} \cdot \mathrm{J}_{\frac{1}{2}}(x) - \mathrm{J}_{-\frac{1}{2}}(x) = \sqrt{\frac{2}{\pi x}} \cdot \left(\frac{\sin x}{x} - \cos x\right), \tag{5.39}$$

where Eqs. (5.37) and (5.38) are employed.

Similarly, one derives

$$\mathrm{J}_{-\frac{3}{2}}(x) = -\frac{1}{x} \cdot \mathrm{J}_{-\frac{1}{2}}(x) - \mathrm{J}_{\frac{1}{2}}(x) = -\sqrt{\frac{2}{\pi x}} \cdot \left(\frac{\cos x}{x} - \sin x\right). \tag{5.40}$$

This treatment can be extended for arbitrary half-integer orders. Without providing their proofs, the results are outlined as follows

$$\mathrm{J}_{n+\frac{1}{2}}(x) = (-1)^n \sqrt{\frac{2x}{\pi}} x^n \left(\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \left(\frac{\sin x}{x}\right); \tag{5.41a}$$

$$\mathrm{J}_{-n-\frac{1}{2}}(x) = \sqrt{\frac{2x}{\pi}} x^n \left(\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \left(\frac{\cos x}{x}\right), \tag{5.41b}$$

where an nth differential operator of $\left(\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\right)^n$ is introduced. For instance,

$$\left(\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\right)^2 f(x) = \frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{x}\frac{\mathrm{d}f}{\mathrm{d}x}\right) = \frac{1}{x}\left(\frac{f'(x)}{x}\right)'.$$

As suggested by Eq. (5.41), Bessel functions of the first kind with half-integer orders are actually elementary functions, and so are Bessel functions of the second kind. It will be seen in Chap. 6 that $\mathrm{J}_{\frac{1}{2}}(x)$ and $\mathrm{N}_{\frac{1}{2}}(x)$ are frequently used for analysing PDE problems defined in spherical regions.

5.2.2 Zeros

Here the focus is laid on the zeros of Bessel functions of the first kind of positive integer orders. A first glance at the series defined by Eq. (5.19) suggests, $\mathrm{J}_n(x)$ is an odd function when n is odd, while $\mathrm{J}_n(x)$ is an even function as n is even. Therefore, the zeros of $\mathrm{J}_n(x)$ are symmetric about the origin. Moreover, $x = 0$ is always a zero of $\mathrm{J}_n(x)$ provided that $n > 0$. Given such symmetry, only positive zeros of $\mathrm{J}_n(x)$ are considered in the following discussion.

Here the symbol $\zeta_s^{(n)}$ is introduced to denote the s-th zero of $\mathrm{J}_n(x)$. Here the super-/subindices should be distinguished from each other. The superindex n indicates which order for the Bessel function of the first kind is of our concern, while the subindex s labels the zeros sequentially.

Several key properties of the zeros of $J_n(x)$ are outlined as follows.

1. **Infiniteness**: $J_n(x)$ has infinitely many positive zeros, i.e. $\left\{\zeta_s^{(n)}\right\}_{s=1}^{\infty}$.
2. **Alternativeness**: Between any two neighbouring zeros of $J_n(x)$, there must exist only one zero of $J_{n+1}(x)$, and so does a single zero for $J_{n-1}(x)$.
3. **Asymptopic behaviour**: The larger two neighbouring zeros are, the closer their difference is towards π, i.e.

$$\lim_{s\to\infty}\left(\zeta_{s+1}^{(n)}-\zeta_s^{(n)}\right)=\pi.$$

Certain issues should be mentioned regarding the aforementioned properties. Firstly, they can be intuitively observed from the profiles of $J_n(x)$ as shown in Fig. 5.1a. Secondly, these properties also work for $N_n(x)$, the Neumann function of integer orders, and they should be observed from Fig. 5.2b.

The zeros of Bessel functions of integer orders are of great importance for engineering applications, and they can be evaluated in advance for further use. In Tables 5.1 and 5.2 list the first five positive zeros of $J_n(x)$ and $N_n(x)$, respectively, for $n = 0, 1, 2, 3$ and 4.

Table 5.1 First five positive zeros of $J_n(x)$, $n = 0, 1, 2, 3$ and 4 [1]

n	s				
	1	2	3	4	5
0	2.4048	5.5201	8.6537	11.7915	14.9309
1	3.8317	7.0156	10.1735	13.3237	16.4706
2	5.1356	8.41723	11.6198	14.7960	17.9598
3	6.3802	9.7610	13.0152	16.2235	19.4094
4	7.5883	11.0647	14.3725	17.6160	20.8269

Table 5.2 First five positive zeros of $N_n(x)$, $n = 0, 1, 2, 3$ and 4 [1]

n	s				
	1	2	3	4	5
0	0.8936	3.9577	7.0861	10.2223	13.3611
1	2.1971	5.4297	8.5960	11.7492	14.8974
2	3.3847	6.7938	10.0235	13.2100	16.3790
3	4.5270	8.0976	11.3965	14.6231	17.8185
4	5.6452	9.3616	12.7301	15.9996	19.2244

5.2.3 Approximating Formula

If the series form (5.19) is used for approximately evaluating $\mathrm{J}_n(x)$, many terms in the series are needed when the input x is large. Thus to substantially reduce the computational cost for evaluating $\mathrm{J}_n(x)$ with large input entries, certain approximating formula to Bessel functions is desired. Analysis suggests that, when x is large, the following approximating formula should hold:

$$\mathrm{J}_\alpha(x) \approx \sqrt{\frac{2}{\pi x}} \cos\left(x - \frac{\pi}{4} - \frac{\alpha\pi}{2}\right); \tag{5.42a}$$

$$\mathrm{N}_\alpha(x) \approx \sqrt{\frac{2}{\pi x}} \sin\left(x - \frac{\pi}{4} - \frac{\alpha\pi}{2}\right). \tag{5.42b}$$

To gain intuitions over Eq. (5.42), one refers to Table 5.1. As from Eq. (5.42a), the zero of $\mathrm{J}_n(x)$, $\zeta_s^{(0)}$ can be approximated by $\left(s - \frac{1}{4}\right)\pi$, with s sufficiently large. Inserting $s = 5$ gives $\zeta_0^{(5)} \approx 14.915$. This is in contrast with the corresponding value 14.9309 presented in Table 5.1. In other words, the accuracy of using Eq. (5.42a) to compute the zeros of $\mathrm{J}_n(x)$ is already rounded to decimal places for $x \geq 15$. Therefore, formulae (5.42) should be of great values for practical use.

5.2.4 Orthogonality

As in Sects. 1.3 and 2.3, the method of separation of variables has been employed to solve the wave equation and the heat equation defined in a rectangle time–space domain ($t > 0, x \in [0, L]$), respectively. The key is to solve the corresponding eigenvalue problems, so as to derive a set of mutually orthogonal trigonometric functions, which all satisfy the given homogeneous boundary conditions. Then the solutions for the original initial–boundary value problems are expressed as linear combinations of the derived trigonometric functions (multiplied the corresponding temporal functions). In Sect. 2.3.2, the procedure of determining the eigenvalues from the method of separation of variables is conceptualised with the introduction of Sturm–Liouville system.

The idea of inducing orthogonal functions via a Sturm–Liouville system should also apply here. Actually, we will show that, for the heat-conduction problem (5.1), the resulting governing equations, after variables being separated, for both Eq. (5.4) for $\Theta(\theta)$ and Eq. (5.6) for $\mathcal{P}(r)$, are Sturm–Liouville equations.

We are now focused on problem (5.6) for $\mathcal{P}(r)$, which is rewritten by

$$\begin{cases} r^2 \dfrac{\mathrm{d}^2\mathcal{P}}{\mathrm{d}r^2} + r\dfrac{\mathrm{d}\mathcal{P}}{\mathrm{d}r} + (\lambda r^2 - n^2)\mathcal{P} = 0, \quad r \in [0, R]; \\ \mathcal{P}|_{r=R} = 0; \\ |\mathcal{P}(0)| < +\infty. \end{cases}$$

Here a natural boundary condition $|\mathcal{P}(0)| < +\infty$ is included, so as to comply with the Sturm–Liouville system outlined by Eqs. (2.76)–(2.79). Dividing the governing equation by r and combining the first two terms, we have

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}r}\left(r\dfrac{\mathrm{d}\mathcal{P}}{\mathrm{d}r}\right) - \dfrac{n^2}{r}\mathcal{P} + \lambda r\mathcal{P} = 0, \quad r \in (0, R); \\ \mathcal{P}|_{r=R} = 0; \\ |\mathcal{P}(0)| < +\infty. \end{cases} \tag{5.43}$$

A comparison with Eq. (2.76) indicates that the governing ODE of problem (5.43) is of Sturm–Liouville type. Note that when being checked with Eq. (2.76), the sign requirements on the coefficients should be met for the governing ODE of problem (5.43), too. To be specific, for any $r \in (0, R)$, a comparison between the equation of problem (5.43) with (2.76) suggests $k = r > 0$, $q = n^2/x > 0$, $\rho = r > 0$.

As for the boundary conditions, it depends on which end is in consideration. At $r = R$, $k = r > 0$. Thus, a (Dirichlet) boundary condition is imposed, which corresponds to the case identified by Eq. (2.79). At $r = 0$, the coefficient $k(r) = r$ vanishes. Thus, no extra boundary condition is needed, but we just let $\mathcal{P}(r)$ be bounded as $r \to 0$.

Therefore, problem (5.43) is verified to be a Sturm–Liouville system. Thus, those conclusions about Sturm–Liouville systems, as discussed in Sect. 2.3.2, can be drawn naturally as follows.

1. There exist a family of eigenvalues $\lambda_1^{(n)} < \lambda_2^{(n)} < \cdots < \lambda_s^{(n)} < \cdots$, such that when $\lambda = \lambda_s^{(n)}$, problem (5.43) yields nontrival solutions.
2. The corresponding non-trivial solutions, i.e. the eigenfunctions, denoted by $\mathcal{P}_1^{(n)}(r), \mathcal{P}_2^{(n)}(r), \ldots, \mathcal{P}_s^{(n)}(r), \ldots$, are mutually orthogonal.
3. Any function satisfying the boundary condition of problem (5.43) can be expressed as a series expansion in terms of the eigenfunctions.

It is worth noting again that one needs to distinguish the meaning of the superindices of $\lambda_s^{(n)}$ with its subindices.

The above-mentioned conclusions theoretically guarantee that a complete set of orthogonal functions can be formed by Bessel functions. But we still need to specify the eigenvalues and eigenfunctions for problem (5.43).

For a given integer n, as from Sect. 5.1, the solutions to the governing equation of problem (5.43) can be generally expressed by

$$\mathcal{P}^{(n)}(r) = A\mathrm{J}_n\left(\sqrt{\lambda}r\right) + B\mathrm{N}_n\left(\sqrt{\lambda}r\right), \tag{5.44}$$

where A and B are coefficients to be determined. Note that $\mathrm{N}_n\left(\sqrt{\lambda}r\right)$ is not bounded at $r = 0$. Thus to guarantee solution boundedness, we should let $B = 0$ in Eq. (5.44). Then we obtain

$$\mathcal{P}^{(n)}(r) = A\mathrm{J}_n\left(\sqrt{\lambda}r\right). \tag{5.45}$$

Incorporating Eq. (5.45) with the boundary condition $\mathcal{P}|_{r=R} = 0$ gives

$$\mathrm{J}_n\left(\sqrt{\lambda}R\right) = 0.$$

Hence, non-trivial solutions for problem (5.43) only exist when $\sqrt{\lambda}R = \zeta_s^{(n)}$, where $\zeta_s^{(n)}$ is recalled to be the sth zero of $\mathrm{J}_n(x)$. Therefore, the eigenvalues for problem (5.43) can be expressed by

$$\lambda_s^{(n)} = \left(\frac{\zeta_s^{(n)}}{R}\right)^2. \tag{5.46}$$

The eigenfunction corresponding to $\lambda_s^{(n)}$ is thus given by

$$\mathcal{P}_s^{(n)}(r) = \mathrm{J}_n\left(\frac{\zeta_s^{(n)}r}{R}\right), s = 1, 2, \cdots. \tag{5.47}$$

Here the meaning of the super-/subindices in $\mathcal{P}_s^{(n)}$ is emphasised. For any superindex n, $\{\mathcal{P}_s^{(n)}(r)\}_{s=1}^{\infty}$ form a complete set of orthogonal functions labelled in terms of s (with n fixed). For instance, when $n = 0$, $\left\{\mathcal{P}_s^{(0)}(r)\right\}_{s=1}^{\infty} = \left\{\mathrm{J}_0\left(\frac{\zeta_s^{(0)}r}{R}\right)\right\}_{s=1}^{\infty}$ form a complete set of orthogonal functions. When $n = 2$, $\left\{\mathcal{P}_s^{(2)}(r)\right\}_{s=1}^{\infty} = \left\{\mathrm{J}_2\left(\frac{\zeta_s^{(2)}r}{R}\right)\right\}_{s=1}^{\infty}$ form another orthogonal system.

In the context of Bessel functions, the conclusive items introduced by Sturm–Liouville system listed in Sect. 2.3.2 are specified as follows.

- For any given n, the eigenfunctions formulated by Eq. (5.47) are mutually orthogonal, i.e.

$$\int_0^R r\mathrm{J}_n\left(\frac{\zeta_s^{(n)}r}{R}\right)\mathrm{J}_n\left(\frac{\zeta_k^{(n)}r}{R}\right)\mathrm{d}r = 0 \tag{5.48}$$

  holds for any $s \neq k$.

- For any given n, for any continuous function $f(x)$ satisfying the boundary conditions of problem (5.43), i.e. $f(0)$ exists and $f(R) = 0$, it can be expressed as a linear combination of the eigenfunctions given by Eq. (5.47), i.e.

$$f(r) = \sum_{s=1}^{\infty} A_s^{(n)} \mathrm{J}_n\left(\frac{\zeta_s^{(n)} r}{R}\right), \tag{5.49}$$

where the coefficient $A_s^{(n)}$ is given by

$$A_s^{(n)} = \frac{1}{M_s^{(n)}} \int_0^R r f(r) \mathrm{J}_n\left(\frac{\zeta_s^{(n)} r}{R}\right) \mathrm{d}r, \tag{5.50}$$

with

$$M_s^{(n)} = \int_0^R r \mathrm{J}_n^2\left(\frac{\zeta_s^{(n)} r}{R}\right) \mathrm{d}r \tag{5.51}$$

which is known as the *modulus* of the Bessel function of the first kind $\mathrm{J}_n\left(\frac{\zeta_s^{(n)} r}{R}\right)$.

Further analysis (in the absence of its derivations) suggests that

$$M_s^{(n)} = \frac{R^2}{2}\left[\mathrm{J}_n'\left(\zeta_s^{(n)}\right)\right]^2 = \frac{R^2}{2}\left[\mathrm{J}_{n-1}\left(\zeta_s^{(n)}\right)\right]^2 = \frac{R^2}{2}\left[\mathrm{J}_{n+1}\left(\zeta_s^{(n)}\right)\right]^2, \tag{5.52}$$

where the second and the third identities are from the recurrence formulae for Bessel functions (5.34a) and (5.34b).

5.2.5 *Analogies with Sinusoidal Functions*

To this stage, Bessel functions and their properties have been introduced. Actually, a majority of the aforementioned properties are not completely new to us, as they are also shown by certain elementary functions, most notably, sinusoidal functions. In this subsection, a thorough comparison between Bessel functions and sinusoidal functions is drawn, so as to gain more insights about Bessel functions.

Governing equation

Bessel functions of both kinds are induced as the solutions to Bessel equation (5.8). Moreover, $\mathrm{J}_\alpha(\sqrt{\lambda}x)$ is shown to be the eigenfunctions of the Sturm–Liouville system governed by

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(x\frac{\mathrm{d}y}{\mathrm{d}x}\right) - \frac{\alpha^2}{x} \cdot y + \lambda x y = 0.$$

In contrast, sinusoidal functions can also be induced by a Sturm–Liouville equation, which is formulated by

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + \lambda y = 0. \tag{5.53}$$

Note that the Bessel equation contains an extra coefficient α, indicating that a "fair" comparison between sinusoidal functions and Bessel functions should be drawn in the context where α is fixed. In the upcoming discussion, we choose 0-th-order Bessel functions to compare with sinusoidal functions. As we know, $y = \cos x$ and $y = \sin x$ are two mutually independent solutions to ODE $y'' + y = 0$; i.e. they form a fundamental system of solutions to this ODE. Correspondingly, the Bessel function of the first kind $y = \mathrm{J}_0(x)$ and the Bessel function of the second kind $y = \mathrm{N}_0(x)$ form a fundamental system of solutions to the 0-th-order Bessel equation $x^2 y'' + xy' + x^2 y = 0$.

Series expansion

Equation (5.19) formulates the series expansion of the Bessel function of the first kind. It shares certain degree of similarities with that of a cosine function, e.g.

$$\cos x = \sum_{k=0} \frac{(-1)^k}{(2k)!} \cdot x^{2k}.$$

First, both series are convergent for all $x \in \mathbb{R}$. Note that the factorial coefficient $1/(2k)!$ in the series above guarantees its convergence in the whole real space. Inserting $\alpha = 0$ into Eq. (5.19) gives

$$\mathrm{J}_0(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{2^{2k}(k!)^2} \cdot x^{2k}, \tag{5.54}$$

and a similar coefficient of $1/(k!)^2$ is observed, ensuring the convergence of series (5.54) for $x \in \mathbb{R}$. According to Stirling's approximation,

$$n! \sim \sqrt{2\pi n}\left(\frac{n}{e}\right)^n,$$

as $n \to \infty$. Hence the two coefficients are further compared by using

$$\frac{1}{(2k)!} \sim \frac{1}{\sqrt{4\pi k}} \cdot \left(\frac{\mathrm{e}}{2k}\right)^{2k}, \qquad \frac{1}{(k!)^2} \sim \frac{1}{2\pi k} \cdot \left(\frac{\mathrm{e}}{2k}\right)^{2k}.$$

It can be read that the rates of convergence for $\mathrm{J}_0(x)$ and sinusoidal functions are also similar.

The second common feature shared by Bessel functions and sinusoidal functions in their series expansions is that, they both show alternating behaviour in the constituting terms of their series. Such alternating behaviour is reflected in the profile of a sinusoidal function, where the function values oscillate around 0. Similar behaviour can also be seen for Bessel functions, as shown in Fig. 5.2, where their function values oscillate around the $y = 0$ axis.

The third common feature shared by Bessel functions and sinusoidal functions in their series expansions is from the order difference between neighbouring terms in the corresponding series. In both series, a constituting term is always x^2 order lower than its subsequent term. As a result, a sinusoidal function (including the cosine function) is either odd or even. Similar behaviour is also spotted in Bessel functions of integer orders.

Zeros

The same as sinusoidal functions, Bessel functions of integer orders have their zeros symmetric about the origin. Besides, the spacings between neighbouring zeros of $y = \sin x$ are identically equal to π. As discussed in Sect. 5.2.2, the n-th-order Bessel function of the first kind yields infinitely many zeros $\{\zeta_s^{(n)}\}_{s=1}^{\infty}$. The spacing between neighbouring zeros, as $s \to \infty$, asymptotically equals π. As shown in Sect. 5.2.4, the positive zeros of $\mathrm{J}_n(x)$ are closely linked with the eigenvalues of the corresponding Sturm–Liouville system.

Orthogonal system

Both sinusoidal functions and Bessel functions (of integer order) can be modified to become the eigenfunctions of Sturm–Liouville systems, which are formed by imposing certain homogeneous boundary conditions to Eqs. (5.53) and (5.43), respectively. For the case with sinusoidal functions, two boundary conditions are needed to compliment Eq. (5.53). In contrast, for governing equation (5.43), a boundary condition is simply needed at the end of $x = R$, while the natural boundary condition should be declared at the other end of $x = 0$.

Concluding remarks

The above-listed issues suggest that, although Bessel functions are classified as "special functions", they are not fully alienated from elementary functions. Some of their key properties see their correspondence in sinusoidal functions. Systematically drawing analogies with elementary functions provides an effective means for understanding special functions.

5.3 Solving PDE Problems with Bessel Functions

In this section, two examples on solving PDE problems with Bessel functions are presented.

Example 5.1 Solve the following wave-propagation problem within a circle.

$$\begin{cases} u_{tt} - (u_{xx} + u_{yy}) = 0, \quad t > 0, \ \sqrt{x^2 + y^2} < 1; \\ u|_{\sqrt{x^2+y^2}=1} = 0; \\ u|_{t=0} = 1 - (x^2 + y^2), \quad u_t|_{t=0} = 0. \end{cases} \tag{5.55}$$

Solution First we consider rewriting problem (5.55) in polar coordinate system $[r = \sqrt{x^2 + y^2}, \theta = \tan^{-1}(\frac{y}{x})]$. Note that the initial/boundary conditions are both independent of θ. Thus, it is reasonable to assert that the solution u is actually independent of θ. Problem (5.55) is thus reformulated by

$$\begin{cases} u_{tt} - \left(u_{rr} + \dfrac{1}{r}u_r\right) = 0, \quad t > 0, \ r \in [0, 1); \\ u|_{r=1} = 0; \\ u|_{t=0} = 1 - r^2, \quad u_t|_{t=0} = 0. \end{cases} \tag{5.56}$$

Now the unknown u has two inputs: radius r and time t, and we seek for its solutions taking a variable-separated form given by

$$u(r; t) = V(r)T(t). \tag{5.57}$$

Inserting it into the governing equation of problem (5.56) gives

$$\frac{T''}{T} = \frac{1}{V}\left(V'' + \frac{V'}{r}\right) = -\lambda,$$

where $\lambda > 0$. As usual, a pair of ODEs is derived to be

$$T'' + \lambda T = 0; \tag{5.58a}$$

$$V'' + \frac{V'}{r} + \lambda V = 0. \tag{5.58b}$$

With reference to the discussion conducted towards Eqs. (5.6) and (5.7) in Sect. 5.1.1, the solution to Eq. (5.58b) can be generally represented by

$$V(r) = A\mathrm{J}_0\left(\sqrt{\lambda}r\right) + B\mathrm{N}_0\left(\sqrt{\lambda}r\right).$$

Note that $V(r)$ should be bounded at $r = 0$. Hence $B = 0$ and

$$V(r) = A\mathrm{J}_0\left(\sqrt{\lambda}r\right). \tag{5.59}$$

Inserting the boundary condition $u|_{r=1} = 0$ into Eq. (5.59) leads to $J\left(\sqrt{\lambda}r\right) = 0$, an equation for the eigenvalue λ. For non-trivial solutions to exist, $\lambda_s = (\zeta_s^{(0)})^2$,

$s = 1, 2, \cdots$, where $\zeta_s^{(0)}$ is recalled to be the sth zero of $\mathrm{J}_0(x)$. The eigenfunction corresponding to λ_s is then given by

$$y_s(r) = \mathrm{J}_0\left(\zeta_s^{(0)} r\right). \tag{5.60}$$

Now inserting the obtained eigenvalues into Eq. (5.58a) for T, we reach

$$T_s'' + \left(\zeta_s^{(0)}\right)^2 \cdot T_s = 0.$$

Hence we derive

$$T_s(t) = C_s \cos\left(\zeta_s^{(0)} t\right) + D_s \sin\left(\zeta_s^{(0)} t\right)$$

as its general solution.

Therefore, the solution for problem (5.56) can be expressed in a series form of

$$u(r; t) = \sum_{s=1}^{\infty} \left(C_s \cos\left(\zeta_s^{(0)} t\right) + D_s \sin\left(\zeta_s^{(0)} t\right)\right) \cdot \mathrm{J}_0(\zeta_s^{(0)} r). \tag{5.61}$$

Now letting $u_t|_{t=0}$ gives rise to $D_s = 0$. In order to determine the coefficient C_s, we let $u|_{t=0} = 1 - r^2$ and obtain

$$1 - r^2 = \sum_{s=1}^{\infty} C_s \mathrm{J}_0(\zeta_s^{(0)} r).$$

It has been demonstrated in Sect. 5.2.4 that the eigenfunctions $\{\mathrm{J}_0(\zeta_s^{(0)})\}_{s=1}^{\infty}$ naturally form a complete set of orthogonal functions. Thus, the coefficient C_s is calculated to be

$$C_s = \frac{1}{M_s} \int_0^1 r(1 - r^2) \mathrm{J}_0(\zeta_s^{(0)} r) \mathrm{d}r, \tag{5.62}$$

where according to Eq. (5.52),

$$M_s = \frac{\mathrm{J}_1^2\left(\zeta_s^{(0)}\right)}{2}. \tag{5.63}$$

Now one still needs to evaluate the integral appearing in Eq. (5.62). To this end, we refer to recurrence formula (5.31). For any real number β, a new variable $x = \beta r$ can be introduced. Then the first identity of Eq. (5.31) with $\alpha = 1$ reads

$$\frac{\mathrm{d}}{\mathrm{d}r}\left[r\mathrm{J}_1(\beta r)\right] = \frac{\mathrm{d}}{\mathrm{d}x}\left[x\mathrm{J}_1(x)\right] = x\mathrm{J}_0(x) = \beta r \mathrm{J}_0(\beta r),$$

where the differentiation chain rule is adopted. Dividing β on both sides implies that

$$rJ_0(\beta r) = \frac{1}{\beta}\frac{d}{dr}\left[rJ_1(\beta r)\right]. \tag{5.64a}$$

Two other formulae key to the evaluation of integrals involving Bessel functions can be derived analogically:

$$J_1(\beta r) = -\frac{1}{\beta}\frac{d}{dr}\left[J_0(\beta r)\right]; \tag{5.64b}$$

$$r^2 J_1(\beta r) = \frac{1}{\beta}\frac{d}{dr}\left[r^2 J_2(\beta r)\right]. \tag{5.64c}$$

Based on the results outlined by Eqs. (5.64), we are enabled to evaluate the following integrals by

$$\int_0^z rJ_0(\beta r)\,dr = \frac{r}{\beta}\cdot J_1(\beta r)\Big|_0^z = \frac{z}{\beta}\cdot J_1(\beta z); \tag{5.65a}$$

$$\begin{aligned}\int_0^z r^3 J_0(\beta r)\,dr &= \frac{1}{\beta}\int_0^z r^2\,d\left[rJ_1(\beta r)\right]\\ &= \frac{z^3}{\beta}J_1(\beta z) - \frac{2}{\beta}\int_0^z r^2 J_1(\beta r)\,dr = \frac{z^3}{\beta}J_1(\beta z) - \frac{2z^2}{\beta^2}J_2(\beta z).\end{aligned} \tag{5.65b}$$

Letting $z = 1$ and $\beta = \zeta_s^{(0)}$ in Eqs. (5.65a) and (5.65b), the integral in Eq. (5.62) can be finally calculated by

$$\int_0^1 r(1-r^2)J_0(\zeta_s^{(0)}r)dr = \frac{2J_2\left(\zeta_s^{(0)}\right)}{\left(\zeta_s^{(0)}\right)^2}.$$

Incorporating it with Eq. (5.62) and using Eq. (5.63), we manage to express the coefficient C_s by

$$C_s = \frac{4J_2\left(\zeta_s^{(0)}\right)}{\left(\zeta_s^{(0)}\right)^2\cdot J_1^2\left(\zeta_s^{(0)}\right)}. \tag{5.66}$$

And the solution for problem (5.55) (in Cartesian coordinate system) is finally expressed by

$$u(x, y; t) = \sum_{s=1}^{\infty} C_s \cos\left(\zeta_s^{(0)} t\right) \cdot \mathrm{J}_0\left(\zeta_s^{(0)} \sqrt{x^2 + y^2}\right),$$

where C_s is determined by Eq. (5.66). □

In the example above, one needs to evaluate integrals involving Bessel functions (multiplied by polynomials), and the key is to (repeatedly) employ the recurrence formulae for Bessel functions.

Our next example concerns heat conduction within a cylinder.

Example 5.2 Let Ω be a cylinder of cross-sectional radius R and height L, i.e.

$$\Omega = \left\{(x, y, z) | x^2 + y^2 \leq R,\ z \in [0, L]\right\}.$$

Suppose the domain Ω is heat-insulated from outside. We consider the thermal behaviour within Ω which can be modelled by

$$\begin{cases} u_t - a^2 \Delta u = 0, \quad t > 0,\ (x, y, z) \in \Omega; \\ \left.\dfrac{\partial u}{\partial n}\right|_{\partial\Omega} = 0; \\ u|_{t=0} = \left(1 - \dfrac{\sqrt{x^2 + y^2}}{R}\right)^2, \end{cases} \tag{5.67}$$

where $\frac{\partial u}{\partial n}|_{\partial\Omega}$ denotes the derivative of u along the outer normal directions on the cylindrical surface.

Solution As the domain of definition becomes a cylinder, the cylindrical coordinates are naturally employed, i.e.

$$r = \sqrt{x^2 + y^2},\ \theta = \tan^{-1}\left(\frac{y}{x}\right),\ z = z. \tag{5.68}$$

In the cylindrical coordinate system, $\Omega = \{(r, \theta, z) | r \leq 1,\ \theta \in [0, 2\pi),\ z \in [0, L]\}$. As suggested by Exercise 3.8, the Laplacian operator in the cylindrical coordinate system is expressed by

$$\Delta u = u_{rr} + \frac{1}{r} u_r + \frac{1}{r^2} u_{\theta\theta} + u_{zz}. \tag{5.69}$$

In this new coordinate system, the boundary conditions of problem (5.67) should be reformulated in two different situations. On the side surface, the outer normal is along the radial direction measured in r. Thus,

$$\left.\frac{\partial u}{\partial n}\right|_{r=R} = \left.\frac{\partial u}{\partial r}\right|_{r=R} = 0.$$

On the upper/bottom surfaces, the normal directions coincide with $\pm z$, i.e.

$$\left.\frac{\partial u}{\partial n}\right|_{z=0} = -\left.\frac{\partial u}{\partial z}\right|_{z=0} = 0, \quad \left.\frac{\partial u}{\partial n}\right|_{z=L} = \left.\frac{\partial u}{\partial z}\right|_{z=L} = 0.$$

It is worth noting that, the variables θ and z do not explicitly appear in both the governing equation and the initial conditions. Moreover, assuming the solution u to be independent of θ and z also meets the boundary conditions on the cylindrical surface.

Therefore, one may further let the unknown function be a binary function represented by $u = u(r; t)$. In other words, problem (5.67) can be further reformulated as

$$\begin{cases} u_t - \left(u_{rr} + \dfrac{1}{r}u_r\right) = 0, \ t > 0, \ r \in [0, 1]; \\ \left.\dfrac{\partial u}{\partial r}\right|_{r=R} = 0; \\ u|_{t=0} = \left(1 - \dfrac{r}{R}\right)^2. \end{cases} \tag{5.70}$$

For its solution, one simply lets $u(r; t) = V(r)T(t)$. Hence, one reaches an ODE in time:

$$T' + \lambda a^2 T = 0 \tag{5.71}$$

and an eigenvalue problem in radius r given by

$$\begin{cases} r^2 V'' + rV' + \lambda r^2 V = 0, \quad r \in (0, R]; \\ |V(0)| < \infty, \ \left.V'\right|_{r=R} = 0. \end{cases} \tag{5.72}$$

For bounded solutions, we write

$$V(r) = A\mathrm{J}_0(\sqrt{\lambda}r). \tag{5.73}$$

Inserting the boundary condition at $r = R$ into Eq. (5.73) results in

$$\sqrt{\lambda}\left.\frac{\mathrm{dJ}_0(\sqrt{\lambda}r)}{\mathrm{d}r}\right|_{r=R} = 0.$$

On using recurrence formula (5.64b), the identity above becomes

$$\mathrm{J}_1(\sqrt{\lambda}R) = 0.$$

The eigenvalues are then calculated by

$$\lambda_s = \left(\frac{\zeta_s^{(1)}}{R}\right)^2, \; s = 0, 1, \ldots, \tag{5.74}$$

where $\zeta_s^{(1)}$ is the sth zero of $\mathrm{J}_1(x)$. Note that constant-valued functions are also non-trivial solutions for problem (5.72), and the corresponding eigenvalue is $\lambda_0 = \zeta_0^{(1)} = 0$.

The corresponding eigenfunctions are then outlined by

$$y_0(r) = 1, \quad y_s(r) = \mathrm{J}_0\left(\frac{\zeta_s^{(1)} r}{R}\right), \; s = 1, 2, \ldots. \tag{5.75}$$

Since the eigenvalue problem (5.72) is a Sturm–Liouville system, $\{y_s(r)\}_{s=0}^{\infty}$ naturally form a complete set of orthogonal functions.

Then we insert the eigenvalues into Eq. (5.71) for T and derive

$$T_s = C_s e^{-\left(\frac{a\zeta_s^{(1)}}{R}\right)^2 t}, \; s = 0, 1, \cdots,$$

and the solution for problem (5.70) is then expressed in a series form of

$$u(r; t) = \sum_{s=0}^{\infty} T_s(t) V_s(r) = C_0 + \sum_{s=1}^{\infty} C_s e^{-\left(\frac{a\zeta_s^{(1)}}{R}\right)^2 t} \mathrm{J}_0\left(\frac{\zeta_s^{(1)} r}{R}\right).$$

For determining the coefficient C_s, the initial condition is incorporated, and one obtains

$$\left(1 - \frac{r}{R}\right)^2 = C_0 + \sum_{s=1}^{\infty} C_s \mathrm{J}_0\left(\frac{\zeta_s^{(1)} r}{R}\right).$$

On using Eq. (2.90), the coefficients can then be calculated by

$$C_0 = \frac{1}{\int_0^R r \, \mathrm{d}r} \cdot \int_0^R r\left(1 - \frac{r}{R}\right)^2 \mathrm{d}r = \frac{1}{6}; \tag{5.76}$$

$$C_s = \frac{1}{M_s} \int_0^R r\left(1 - \frac{r}{R}\right)^2 \mathrm{J}_0\left(\frac{\zeta_s^{(1)} r}{R}\right) \mathrm{d}r = \frac{R^2}{M_s} \int_0^1 x\,(1 - x)^2 \mathrm{J}_0\left(\zeta_s^{(1)} x\right) \mathrm{d}x, \tag{5.77}$$

where $x = r/R$ is introduced to facilitate the derivation and the modulus M_s is calculated by

$$M_s = \int_0^R r\mathrm{J}_0^2\left(\frac{\zeta_s^{(1)} r}{R}\right)\,\mathrm{d}r = R^2\int_0^1 x\mathrm{J}_0^2\left(\zeta_s^{(1)} x\right)\,\mathrm{d}x. \tag{5.78}$$

Now we need to evaluate the integrals appearing in Eqs. (5.77) and (5.78).

We start with the integral in Eq. (5.78):

$$\begin{aligned}\int_0^1 x\mathrm{J}_0^2\left(\zeta_s^{(1)} x\right)\,\mathrm{d}x &= \frac{1}{\zeta_s^{(1)}}\int_0^1 \mathrm{J}_0\left(\zeta_s^{(1)} x\right)\,\mathrm{d}\left[x\mathrm{J}_1\left(\zeta_s^{(1)} x\right)\right]\\ &= \frac{\mathrm{J}_0\left(\zeta_s^{(1)}\right)\mathrm{J}_1\left(\zeta_s^{(1)}\right)}{\zeta_s^{(1)}} - \frac{1}{\zeta_s^{(1)}}\int_0^1 x\mathrm{J}_1\left(\zeta_s^{(1)} x\right)\frac{\mathrm{d}}{\mathrm{d}x}\left[\mathrm{J}_0\left(\zeta_s^{(1)} x\right)\right]\,\mathrm{d}x\\ &= \int_0^1 x\mathrm{J}_1^2\left(\zeta_s^{(1)} x\right)\,\mathrm{d}x,\end{aligned}$$

where the recurrence formulae (5.64a) and (5.64b) as well as $\mathrm{J}_1(\zeta_s^{(1)}) = 0$ are employed.

Here the difference between both sides of the identity above is addressed. On the left side, it is an integral involving $\mathrm{J}_0(\cdot)$, while the final result on the right side is related to $\mathrm{J}_1(\cdot)$. In fact, the right side of the last identity is just the modulus of $\mathrm{J}_1(\cdot)$. Then with reference to Eq. (5.52), the integral in Eq. (5.78) can be fully calculated by

$$\int_0^1 x\mathrm{J}_0^2\left(\zeta_s^{(1)} x\right)\,\mathrm{d}x = \frac{\mathrm{J}_0^2(\zeta_s^{(1)})}{2}.$$

Inserting it into Eq. (5.78) finally gives

$$M_s = \frac{R^2}{2}\mathrm{J}_0^2(\zeta_s^{(1)}). \tag{5.79}$$

Now we consider evaluating the integral in Eq. (5.77), that is,

$$\int_0^1 x\,(1-x)^2\,\mathrm{J}_0\left(\zeta_s^{(1)} x\right)\,\mathrm{d}x = \int_0^1 \left(x - 2x^2 + x^3\right)\mathrm{J}_0\left(\zeta_s^{(1)} x\right)\,\mathrm{d}x, \tag{5.80}$$

and the integral on the right side of Eq. (5.80) is then calculated term by term.

By letting $\beta = \zeta_s^{(1)}$ and $z = 1$ in Eq. (5.65a), we have

$$\int_0^1 x\mathrm{J}_0\left(\zeta_s^{(1)}x\right)\,\mathrm{d}x = \frac{1}{\zeta_s^{(1)}} \cdot \mathrm{J}_1(\zeta_s^{(1)}) = 0. \tag{5.81}$$

where the second identity is because $\zeta_s^{(1)}$ is just a zero of $\mathrm{J}_1(\cdot)$.

Similarly, one may use Eq. (5.65b) to derive

$$\int_0^1 x^3\mathrm{J}_0\left(\zeta_s^{(1)}x\right)\,\mathrm{d}x = \frac{\mathrm{J}_1(\zeta_s^{(1)})}{\zeta_s^{(1)}} - \frac{2\mathrm{J}_2\left(\zeta_s^{(1)}\right)}{\left(\zeta_s^{(1)}\right)^2} = -\frac{2\mathrm{J}_2\left(\zeta_s^{(1)}\right)}{\left(\zeta_s^{(1)}\right)^2}. \tag{5.82}$$

Up to this stage, we still do not know how to explicitly calculate $\int_0^1 x^2\mathrm{J}_0\left(\zeta_s^{(1)}x\right)\,\mathrm{d}x$, whose evaluation should actually involve other special functions. Nonetheless, we may derive a series to represent it. To this end, we use the series expansion of $\mathrm{J}_0(\cdot)$ given by Eq. (5.54) and write

$$\int_0^1 x^2\mathrm{J}_0\left(\zeta_s^{(1)}x\right)\,\mathrm{d}x = \sum_{k=0}^{\infty}\frac{(-1)^k\left(\zeta_s^{(1)}\right)^{2k}}{2^{2k}(k!)^2}\int_0^1 x^{2k+2}\,\mathrm{d}x = \sum_{k=0}^{\infty}\frac{(-1)^k\left(\zeta_s^{(1)}\right)^{2k}}{2^{2k}(2k+3)(k!)^2} \triangleq g\left(\zeta_s^{(1)}\right). \tag{5.83}$$

In such a manner, the integral of Eq. (5.83), or alternatively $g\left(\zeta_s^{(1)}\right)$, can be approximately evaluated.

Incorporating Eqs. (5.79), (5.81)–(5.83) into (5.77) gives

$$C_s = -\frac{4}{R^2\mathrm{J}_0^2\left(\zeta_s^{(1)}\right)} \cdot \left[g\left(\zeta_s^{(1)}\right) + \frac{\mathrm{J}_2\left(\zeta_s^{(1)}\right)}{\left(\zeta_s^{(1)}\right)^2}\right]. \tag{5.84}$$

Therefore, the solution for problem (5.67) is finally calculated to be

$$u(r;t) = \frac{1}{6} + \sum_{s=1}^{\infty} C_s e^{-\left(\frac{a\zeta_s^{(1)}}{R}\right)^2 t}\mathrm{J}_0\left(\frac{\zeta_s^{(1)}\sqrt{x^2+y^2}}{R}\right) \tag{5.85}$$

for any $z \in [0, L]$ with the coefficients C_s determined by Eq. (5.84). □

It is shown from the two examples above that, Bessel functions of integer order play an important role in analytically solving many PDE problems defind in cylinders. Hence, Bessel functions of integer order are sometimes called the *cylinder functions*.

5.4 Generalisation

5.4.1 Hankel Functions

Now we consider the following representations:

$$\mathrm{H}_\alpha^{(1)}(x) = \mathrm{J}_\alpha(x) + \mathrm{i}\mathrm{N}_\alpha(x), \quad \mathrm{H}_\alpha^{(2)}(x) = \mathrm{J}_\alpha(x) - \mathrm{i}\mathrm{N}_\alpha(x), \tag{5.86}$$

where J_α and N_α are αth order Bessel functions of both kinds, respectively; i is the imaginary unit. The functions defined by Eq. (5.86) are called *Hankel functions*, or sometimes *Bessel function of the third kind*, conventionally denoted by capital letter H. When the index α assumes real values (as we do in this book), the corresponding two Hankel functions are conjugate to each other. It is also possible to express J_α and N_α by Hankel functions:

$$\mathrm{J}_\alpha(x) = \frac{1}{2}\left(\mathrm{H}_\alpha^{(1)}(x) + \mathrm{H}_\alpha^{(2)}(x)\right), \quad \mathrm{N}_\alpha(x) = \frac{1}{2\mathrm{i}}\left(\mathrm{H}_\alpha^{(1)}(x) - \mathrm{H}_\alpha^{(2)}(x)\right). \tag{5.87}$$

Since both J_α and N_α are solutions to Bessel equation (5.8) of the αth order, Hankel functions should also satisfy the same equation, provided the imaginary unit i is "naively" envisaged as a constant. More systematic examinations on Hankel functions need to be conducted with knowledge on functions of complex variables, i.e. $\mathrm{H}(z)$, $z \in \mathbb{C}$. Under this setting, differential equation (5.8) should be defined not only on the real axis, but the whole complex plane:

$$z^2\frac{\mathrm{d}^2y}{\mathrm{d}z^2} + z\frac{\mathrm{d}y}{\mathrm{d}z} + (z^2 - \alpha^2)y = 0. \tag{5.88}$$

5.4.2 Modified Bessel Functions

If one changes the input argument of Bessel equation to ix, and again "naively" treats the imaginary unit i as a constant, Eq. (5.8) becomes

$$x^2\frac{\mathrm{d}^2y}{\mathrm{d}x^2} + x\frac{\mathrm{d}y}{\mathrm{d}x} - (x^2 + \alpha^2)y = 0, \tag{5.89}$$

which is known as the *modified Bessel equation*. For its solution, one may follow the treatment used in Sect. 5.1.2 to seek for solutions taking a series form like Eq. (5.9). It is calculated that one solution to Eq. (5.89) is given by

$$\mathrm{I}_\alpha(x) = \sum_{k=0}^{\infty} \frac{1}{k!\Gamma(\alpha + k + 1)} \cdot \left(\frac{x}{2}\right)^{\alpha+2k}, \tag{5.90}$$

which is termed as the *modified Bessel function of the first kind*, conventionally denoted by capital letter I. Similar as the definition for the Neumann function by Eq. (5.22), one can also define the *modified Bessel function of the second kind* as a limiting case by

$$\mathrm{K}_\alpha(x) = \lim_{\nu\to\alpha} \frac{\pi}{2} \frac{\mathrm{I}_{-\nu}(x) - \mathrm{I}_\nu(x)}{\sin \nu\pi}, \tag{5.91}$$

which is conventionally denoted by capital letter K.

The above-listed differential equations see their occasional applications when physical phenomena are modelled.

Exercise

1. Show that if $y = F(x)$ satisfies Bessel equation (5.7), then $\mathcal{P}(r) = F(\sqrt{\lambda}r)$ satisfies Eq. (5.6).
2. Assume that the solution to the Bessel equation has a series expression as given by Eq. (5.9), where $c \leq 0$. Determine the corresponding coefficients and exponent c according to the Bessel equation, and express the resulting series [in comparison with Eq. (5.20)].
3. Determine the convergent radius for series (5.19) which defines the Bessel function of the first kind $\mathrm{J}_\alpha(x)$.
4. Show that $y = \mathrm{J}_n(ax)$ is a solution to

$$x^2y'' + xy' + (a^2x^2 - n^2)y = 0.$$

5. Verify that $y = \sqrt{x}\mathrm{J}_{\frac{1}{2}}(x)$ satisfies the ODE inducing sinusoidal functions, i.e.

$$\frac{\mathrm{d}^2y}{\mathrm{d}x^2} + y = 0.$$

6. Use the recurrence formulae for Bessel functions to express $\mathrm{J}_{\frac{3}{2}}(x)$ and $\mathrm{J}_{\frac{5}{2}}(x)$ as elementary functions.
7. Show that $y = x^{\frac{1}{2}}\mathrm{J}_n(x)$ is a solution to

$$x^2\frac{\mathrm{d}^2y}{\mathrm{d}x^2} + x^{\frac{1}{2}}\left(x^2 - \left(n^2 - \frac{1}{4}\right)\right)y = 0.$$

8. Show that $y = \mathrm{J}_\alpha\left(\frac{1}{x}\right)$ is a solution to

$$x^4\frac{\mathrm{d}^2y}{\mathrm{d}x^2} + x^3\frac{\mathrm{d}y}{\mathrm{d}x} + (1 - \alpha^2x^2)y = 0.$$

9. Use the recurrence formulae for Bessel functions to demonstrate the issues as follows.

(a) Justify Eqs. (5.64a)-(5.64c).
(b) Determine the quantity a, b and c in the following cases:

$$r^{n+1}\mathrm{J}_n(\beta r) = a\frac{\mathrm{d}}{\mathrm{d}r}\left(r^b\mathrm{J}_c(\beta r)\right),$$

$$r^{1-n}\mathrm{J}_n(\beta r) = a\frac{\mathrm{d}}{\mathrm{d}r}\left(r^b\mathrm{J}_c(\beta r)\right).$$

10. Show that $\mathrm{J}_{-\frac{1}{2}}(x)$ is an elementary function, that is Eq. (5.38), based on its series expansion.
11. Use the recurrence formulae for Bessel functions to calculate the following integrals:
    (a) $\int_0^x r^5\mathrm{J}_0(\beta r)\,\mathrm{d}r$;
    (b) $\int_0^x \mathrm{J}_1(r)\,\mathrm{d}r$;
    (c) $\int_0^x \frac{1}{r}\mathrm{J}_2(r)\,\mathrm{d}r$;
    (d) Determine the interrelationship between $\gamma > 0$ and $\alpha > 0$, such that $\int_0^x x^\gamma \mathrm{J}_\alpha(\beta r)\mathrm{d}r$ can be explicitly calculated.
    (e) In the questions above, if $\gamma < 0$, what is the corresponding interrelationship should γ satisfy with $\alpha > 0$?
12. Solve the following initial–boundary value problem with the method of separation of variables

$$\begin{cases} u_{tt} - a^2(u_{xx} + u_{yy}) = 0, \quad x^2 + y^2 < 1,\ t > 0; \\ u|_{x^2+y^2=1} = 0; \\ u|_{t=0} = \left(1 - \sqrt{x^2+y^2}\right), \quad u_t|_{t=0} = 0. \end{cases}$$

13. Solve the following boundary value problem for Laplacian equation in the cylindrical region defined by $\Omega = \{(x, y, z)|x^2 + y^2 < R^2,\ 0 < z < h\}$:

$$\begin{cases} u_{xx} + u_{yy} + u_{zz} = 0,\ \sqrt{x^2+y^2} < R,\ z \in (0, h); \\ u|_{\sqrt{x^2+y^2}=R} = 0; \\ u|_{z=0} = 0, \quad u|_{z=h} = R^2 - (x^2 + y^2). \end{cases}$$

Chapter 6
Legendre Polynomial

In this chapter, another useful set of orthogonal functions is introduced. On applying the method of separation of variables to solve PDE problems defined in a sphere, the Legendre equation is naturally introduced. Its bounded solutions, known as the Legendre polynomials, are then presented. This is followed by discussion on their properties. The topic is then extended to cover general orthogonal polynomials. Finally, solutions for a more general case, where the governing equation becomes the associated Legendre equation, are briefly examined. The contents in this chapter are summarised in the knowledge map charted by Fig. 6.1.

6.1 Legendre Equation

We now consider an initial–boundary value problem defined in a general three-dimensional domain Ω, which is governed by the wave equation, i.e.

$$\begin{cases} u_{tt} - a^2 \Delta u = 0, \quad \mathbf{r} \in \Omega \subset \mathbb{R}^3, \ t > 0; \\ u|_{t=0} = \phi(\mathbf{r}), \ \ u_t|_{t=0} = \psi(\mathbf{r}); \\ u|_{\partial\Omega} = 0, \end{cases} \tag{6.1}$$

where "Δ" denotes the three-dimensional Laplace's operator.

For implementing the method of separation of variables, we assume that

$$u(\mathbf{r}; t) = T(t)V(\mathbf{r}).$$

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Y. Zhu, *Equations and Analytical Tools in Mathematical Physics*,
https://doi.org/10.1007/978-981-16-5441-1_6

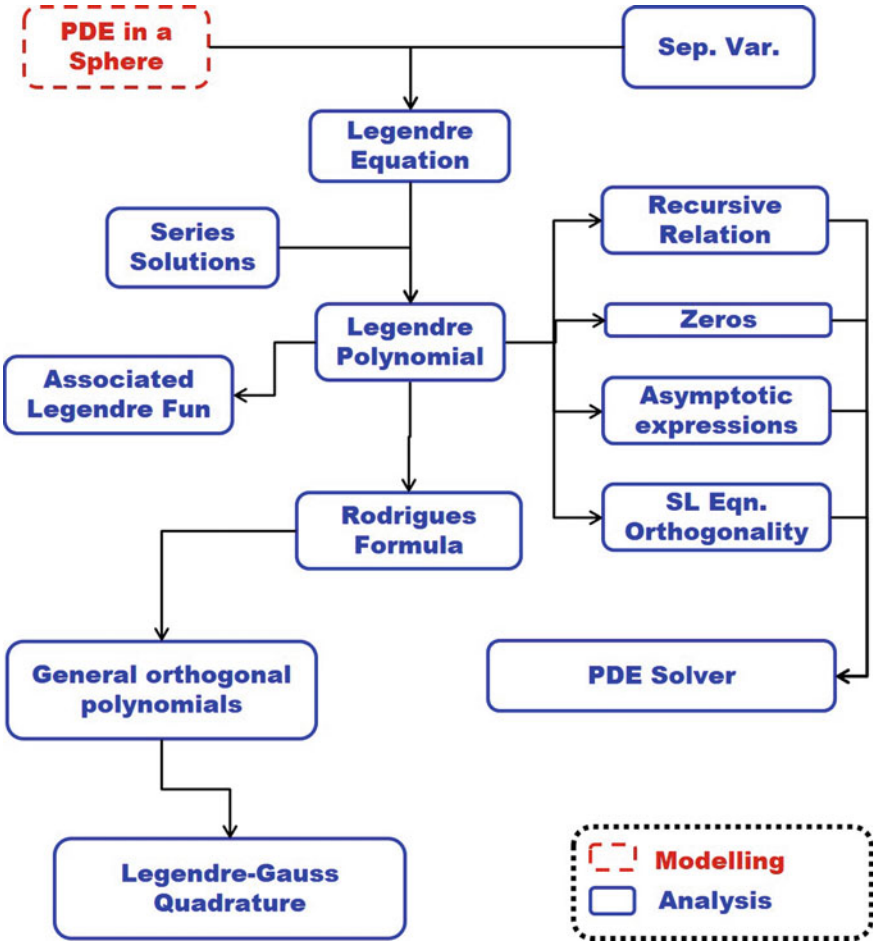

Fig. 6.1 Knowledge map—Legendre polynomial

Inserting it into the governing equation of problem (6.1) gives

$$\frac{T''}{a^2 T} = \frac{\Delta V}{V} = -\lambda. \tag{6.2}$$

Based on the previous analysis on the method of separation of variables, non-trivial solutions for the corresponding spatial problem exist only when $\lambda \geq 0$. Thus without loss of generalities, λ can be replaced by k^2, where k is termed as the *wave number* here. It has a clear physical meaning: $2\pi k$ quantifies the frequencies of the corresponding eigenfunctions.

On using $\lambda = k^2$, Eq. (6.2) leads to an ODE for the temporal function $T(t)$, given by

$$T''(t) + a^2 k^2 T = 0, \quad t > 0, \tag{6.3}$$

and a PDE for the spatial function $V(\mathbf{r})$, given by

$$\Delta V + k^2 V = 0, \quad \mathbf{r} \in \Omega. \tag{6.4}$$

Eq. (6.4) is recalled to be the Helmholtz equation. When k vanishes, the Helmholtz equation becomes Laplace's equation.

To this stage, the domain of definition Ω has yet been specified. In the previous chapter, the case where the spatial domain is a two-dimensional circle has been considered, and the Bessel equation is then derived. In this chapter, the spatial domain is set to be a sphere, say,

$$\Omega = \mathcal{O}_R = \{(x, y, z) | x^2 + y^2 + z^2 \leq R^2\}, \tag{6.5}$$

and we look for solutions to the Helmholtz equation defined in this sphere.

Naturally, spherical coordinates given by

$$\begin{cases} x = r \sin\theta \cos\varphi; \\ y = r \sin\theta \sin\varphi; \\ z = r \cos\theta, \end{cases} \tag{6.6}$$

are introduced. Laplacian operator in this spherical coordinate system, as suggested by Eq. (3.38), is expressed by

$$\Delta V = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial V}{\partial r} \right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial V}{\partial \theta} \right) + \frac{1}{r^2 \sin^2\theta} \cdot \frac{\partial^2 V}{\partial \varphi^2}. \tag{6.7}$$

With spherical coordinates, the domain of definition becomes $(r, \theta, \varphi) \in [0, R) \times [0, \pi] \times [0, 2\pi]$, which takes a cuboid shape. Thus, the method of separation of variables can be employed.

To this end, we assume that the solution V to Helmholtz equation (6.7) takes the form of

$$V(r, \theta, \varphi) = \mathcal{P}(r)\Theta(\theta)\Phi(\varphi). \tag{6.8}$$

Combining Eq. (6.8) with (6.7) and inserting the result into Eq. (6.4), we reach

$$\frac{\Theta\Phi}{r^2} \frac{\mathrm{d}}{\mathrm{d}r} \left(r^2 \frac{\mathrm{d}\mathcal{P}}{\mathrm{d}r} \right) + \frac{\mathcal{P}\Phi}{r^2 \sin\theta} \frac{\mathrm{d}}{\mathrm{d}\theta} \left(\sin\theta \frac{\mathrm{d}\Theta}{\mathrm{d}\theta} \right) + \frac{\mathcal{P}\Theta}{r^2 \sin^2\theta} \cdot \frac{\mathrm{d}^2\Phi}{\mathrm{d}\varphi^2} + k^2 \mathcal{P}\Theta\Phi = 0. \tag{6.9}$$

By multiplying $r^2/(R\Theta\Phi)$ on its both sides and sorting the terms involving $\mathcal{P}$ from the other two functions Θ and Φ, we obtain

$$\frac{1}{\mathcal{P}}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}\mathcal{P}}{\mathrm{d}r}\right)+k^2r^2=-\frac{1}{\Theta\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right)-\frac{1}{\Phi\sin^2\theta}\cdot\frac{\mathrm{d}^2\Phi}{\mathrm{d}\varphi^2}. \tag{6.10}$$

Note that the left side of Eq. (6.10) is a function solely of r, while its right side is independent of r. Hence, both sides must be equal to a constant so that Eq. (6.10) holds. In theory, we can denote this constant by λ. But the constant is conventionally chosen to be $\alpha(\alpha+1)$, where α can be a real or a complex number.

By letting the left side of Eq. (6.10) equal $\alpha(\alpha+1)$, we obtain an ODE for $\mathcal{P}(r)$, given by

$$\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}\mathcal{P}}{\mathrm{d}r}\right)+\left(k^2r^2-\alpha(\alpha+1)\right)\mathcal{P}=0. \tag{6.11a}$$

Meanwhile, a differential equation for $\Theta(\theta)$ and $\Phi(\varphi)$ is also at hand, i.e.

$$\frac{1}{\Theta\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right)+\frac{1}{\Phi\sin^2\theta}\cdot\frac{\mathrm{d}^2\Phi}{\mathrm{d}\varphi^2}+\alpha(\alpha+1)=0. \tag{6.11b}$$

The solutions to Eq. (6.11a) depend on the value of k. When $k\neq 0$, it can be checked that

$$\mathcal{P}_\alpha(r)=\frac{1}{\sqrt{r}}\left(C_1\mathrm{J}_{\alpha+\frac{1}{2}}(kr)+C_2\mathrm{N}_{\alpha+\frac{1}{2}}(kr)\right) \tag{6.12}$$

expresses the fundamental system of solutions to Eq. (6.11a), where $\mathrm{J}_{\alpha+\frac{1}{2}}(\cdot)$ and $\mathrm{N}_{\alpha+\frac{1}{2}}(\cdot)$ are recalled to be the half-integer-order Bessel functions of both kinds; C_1 and C_2 are two arbitrary constants. As from the discussion in Sect. 5.2.1, $\mathcal{P}_\alpha$ defined by Eq. (6.12) is actually an elementary function.

When $k=0$, the governing equation is effectively Laplace's equation, and Eq. (6.11a) becomes

$$r^2\frac{\mathrm{d}^2\mathcal{P}}{\mathrm{d}r^2}+2r\frac{\mathrm{d}\mathcal{P}}{\mathrm{d}r}-\alpha(\alpha+1)\mathcal{P}=0. \tag{6.13}$$

Being an ODE, Eq. (6.13) is known as the *Cauchy-Euler equation*, or *Eulerian equation* for short. It can be verified that the solution to Eq. (6.13) can be generally written by

$$\mathcal{P}_\alpha(r)=C_1r^\alpha+C_2r^{-\alpha-1}, \tag{6.14}$$

where C_1 and C_2 are arbitrary constants.

Therefore, the general solution to Eq. (6.11a) is summarised by

$$\mathcal{P}_\alpha(r)=\begin{cases}\dfrac{1}{\sqrt{r}}\left(C_1\mathrm{J}_{\alpha+\frac{1}{2}}(kr)+C_2\mathrm{N}_{\alpha+\frac{1}{2}}(kr)\right), & k>0;\\ C_1r^\alpha+C_2r^{-\alpha-1}, & k=0.\end{cases} \tag{6.15}$$

Then we proceed with solving Eq. (6.11b) by separating variables once again. Multiplying Eq. (6.11b) by $\sin^2\theta$ and separating the function of θ from that of φ, we obtain

$$\frac{\sin\theta}{\Theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right)+\alpha(\alpha+1)\sin^2\theta=-\frac{1}{\Phi}\cdot\frac{\mathrm{d}^2\Phi}{\mathrm{d}\varphi^2}. \tag{6.16}$$

In theory, both sides of Eq. (6.16) should equal a constant, say ν. However, as shown in Sect. 5.1, this constant has to be m^2, $m = 0, 1, \ldots$, such that $\Phi(\varphi)$ is periodic for $\varphi \in [0, 2\pi)$. Thus, we have

$$\frac{\mathrm{d}^2\Phi}{\mathrm{d}\varphi^2}+m^2\Phi=0 \tag{6.17a}$$

and

$$\sin\theta\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right)+(\alpha(\alpha+1)\sin^2\theta-m^2)\Theta=0. \tag{6.17b}$$

The general solution to Eq. (6.17a) is available:

$$\Phi=A_1\cos m\varphi+A_2\sin m\varphi \tag{6.18}$$

with A_1 and A_2 being two arbitrary constants.

To solve Eq. (6.17b), one may prove that if $F(x)$ satisfies

$$(1-x^2)\frac{\mathrm{d}^2F}{\mathrm{d}x^2}-2x\frac{\mathrm{d}F}{\mathrm{d}x}+\left(\alpha(\alpha+1)-\frac{m^2}{1-x^2}\right)F=0, \tag{6.19}$$

then $\Theta(\theta)=F(\cos\theta)$ is a solution to Eq. (6.17b). The ordinary differential equation given by Eq. (6.19) is called the *associated Legendre differential equation* or simply the *associated Legendre equation*.

One frequently considered case is when u is independent of φ. Then according to Eq. (6.18), $m = 0$. Therefore, Eq. (6.19) becomes

$$(1-x^2)\frac{\mathrm{d}^2F}{\mathrm{d}x^2}-2x\frac{\mathrm{d}F}{\mathrm{d}x}+\alpha(\alpha+1)F=0, \tag{6.20}$$

which is known as the *Legendre equation* of *degree* α. The term "degree" is employed because Legendre equation yields polynomial solutions when α is an integer, which just identifies the degree of the corresponding polynomial solutions.

In the upcoming section, solutions to the Legendre equation (6.20) will be investigated.

6.2 Legendre Polynomial

In this section, we consider finding solutions to the Legendre equation. Similar as in the case of the Bessel equation, we look for its solution expressed by means of series expansion. It is interesting to find that, under certain circumstances, solutions to the Legendre equation become polynomials.

6.2.1 Series Solution to the Legendre Equation

For conventional purpose, the dependent variable of the Legendre equation given by Eq. (6.20) is changed to $y = F(x)$. Then the Legendre equation is re-expressed by

$$(1 - x^2)\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} - 2x\frac{\mathrm{d}y}{\mathrm{d}x} + \alpha(\alpha + 1)y = 0. \tag{6.21}$$

Note that the coefficients of Eq. (6.21) are formed only by polynomials. Then similar as in the case for deriving the series expansion for Bessel functions by Eq. (5.9), we assume the solution to Eq. (6.21) to take a series form of

$$y = \sum_{k=0}^{\infty} a_k x^{k+c} \tag{6.22}$$

with $a_0 \neq 0$. Equation (6.22) is valid when x falls within the convergent region of the series. Therefore, operations of summation and differentiation are interchangeable. For instance, we write

$$x\frac{\mathrm{d}y}{\mathrm{d}x} = x\sum_{k=0}^{\infty}\frac{\mathrm{d}}{\mathrm{d}x}\left(a_k x^{k+c}\right) = \sum_{k=0}^{\infty} a_k(k + c)x^{k+c} \tag{6.23}$$

and

$$\begin{aligned}(1 - x^2)\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} &= a_0 c(c - 1)x^{c-2} + a_1 c(c + 1)x^{c-1} \\ &\quad + \sum_{k=0}^{\infty}\left(a_{k+2}(k + c + 2)(k + c + 1) - a_k(k + c)(k + c - 1)\right)x^{k+c},\end{aligned} \tag{6.24}$$

where the techniques of index shifting have been employed to derive Eq. (6.24).

Incorporating Eqs. (6.22)–(6.24) into (6.21) and combining the two involved series, we obtain

$$\begin{aligned} 0 &= a_0 c(c-1)x^{c-2} + a_1 c(c+1)x^{c-1} \\ &\quad + \sum_{k=0}^{\infty} \big(a_{k+2}(k+c+2)(k+c+1) - a_k((k+c)(k+c+1) - \alpha(\alpha+1))\big)\, x^{k+c}. \end{aligned} \tag{6.25}$$

Now the unknowns become the coefficient a_k and the exponent c which can be sequentially solved for from the lowest order.

Letting the coefficient in Eq. (6.25) for x^{c-2} vanish, we have $c = 0$ or $c = 1$, with $a_0 \neq 0$ still being an unspecified constant.

We consider the case with $c = 0$ first. When $c = 0$, the coefficient for x^{c-1} in Eq. (6.25) vanishes automatically. Hence, we can proceed to the next order with a_1 as another unspecified constant.

Inserting $c = 0$ into Eq. (6.25) gives

$$\sum_{k=0}^{\infty} (a_{k+2}(k+2)(k+1) - a_k(k(k+1) - \alpha(\alpha+1)))\, x^k = 0. \tag{6.26}$$

Note that $k(k+1) - \alpha(\alpha+1) = (k-\alpha)(k+\alpha+1)$. By letting the coefficients for x^{k+c} vanish, a recurrence relation is established by

$$a_{k+2} = \frac{(k-\alpha)(k+\alpha+1)}{(k+2)(k+1)} \cdot a_k. \tag{6.27}$$

Eq. (6.27) implies that the coefficients a_k, $k \geq 2$, should alternatingly thread to the two undetermined constants a_0 and a_1. This introduces two sets of coefficients. The first set consists of

$$\begin{aligned} a_2 &= -\frac{\alpha(\alpha+1)}{2!} \cdot a_0, \\ a_4 &= \frac{\alpha(\alpha-2)(\alpha+1)(\alpha+3)}{4!} \cdot a_0, \\ &\cdots, \\ a_{2m} &= (-1)^m \frac{\alpha(\alpha-2)\cdots(\alpha-2m+2)\cdot(\alpha+1)(\alpha+3)\cdots(\alpha+2m-1)}{(2m)!} \cdot a_0, \\ &\cdots. \end{aligned} \tag{6.28}$$

The second set consists of

$$
\begin{aligned}
a_3 &= -\frac{(\alpha-1)(\alpha+2)}{3!}\cdot a_1,\\
a_5 &= \frac{(\alpha-1)(\alpha-3)(\alpha+2)(\alpha+4)}{5!}\cdot a_1,\\
&\cdots,\\
a_{2m+1} &= (-1)^m\frac{(\alpha-1)(\alpha-3)\cdots(\alpha-2m+1)\cdot(\alpha+2)(\alpha+4)\cdots(\alpha+2m)}{(2m+1)!}\cdot a_1,\\
&\cdots.
\end{aligned}
\tag{6.29}
$$

Incorporating them into series (6.22), we express the solution to Legendre equation (6.21) by

$$
\begin{aligned}
y = a_0&\left(1-\frac{\alpha(\alpha+1)}{2!}\cdot x^2+\frac{\alpha(\alpha-2)(\alpha+1)(\alpha+3)}{4!}\cdot x^4+\cdots\right)\\
&+a_1\left(x-\frac{(\alpha-1)(\alpha+2)}{3!}\cdot x^3+\frac{(\alpha-1)(\alpha-3)(\alpha+2)(\alpha+4)}{5!}\cdot x^5+\cdots\right).
\end{aligned}
\tag{6.30}
$$

Note that for deriving Eq. (6.30), one needs to sort the terms related to a_0 from those related to a_1. This entails changing the sequence of summation, whose validity is only guaranteed for a uniformly convergent series.

Given the arbitrariness in the choice of a_0 and a_1,

$$
y_1 = 1-\frac{\alpha(\alpha+1)}{2!}\cdot x^2+\frac{\alpha(\alpha-2)(\alpha+1)(\alpha+3)}{4!}\cdot x^4+\cdots \tag{6.31a}
$$

and

$$
y_2 = x-\frac{(\alpha-1)(\alpha+2)}{3!}\cdot x^3+\frac{(\alpha-1)(\alpha-3)(\alpha+2)(\alpha+4)}{5!}\cdot x^5+\cdots \tag{6.31b}
$$

should be two mutually independent solutions to Legendre equation (6.21). This is the result for the case with $c=0$, which is solved from the leading-order equation of Eq. (6.25).

The case with $c=1$ should also be considered. Nonetheless, as we have obtained two independent solutions to the second-order linear ODE (6.21), the solutions corresponding to $c=1$ must be a linear combination of them. In fact, it is not difficult to show that the solution when $c=1$ is effectively y_2 given by Eq. (6.31b) (see Exercise 6.4).

Finally, we need to calculate the convergent radii for the series given by Eqs. (6.31a)–(6.31b). Based on Eq. (6.28), we have

$$\lim_{m\to\infty}\left|\frac{a_{2m+2}}{a_{2m}}\right| = \lim_{m\to\infty}\left|\frac{(\alpha-2m)(\alpha+2m+1)}{(2m+2)(2m+1)}\right| = 1. \tag{6.32}$$

Note that when $x = \pm 1$, the resulting series given by Eq. (6.31a) becomes divergent, as long as α is not an integer. Hence, series (6.31a) is generally convergent when $x \in (-1, 1)$, which is just the domain of definition for y_1, and a same convergent rule applies for y_2 defined by Eq. (6.31b).

6.2.2 Legendre Polynomial

Now we consider the situation when $\alpha = n$ with n being an integer. Then Legendre equation (6.21) becomes

$$(1-x^2)\frac{\mathrm{d}^2y}{\mathrm{d}x^2} - 2x\frac{\mathrm{d}y}{\mathrm{d}x} + n(n+1)y = 0. \tag{6.33}$$

In this scenario, one of the two series given by Eqs. (6.31a) and (6.31b) should degenerate to a polynomial.

To see this, we consider the case when $n \geq 0$. Replacing α by n in recurrence relation (6.27) gives

$$a_{k+2} = -\frac{(n-k)(n+k+1)}{(k+2)(k+1)} \cdot a_k. \tag{6.34}$$

Eq. (6.34) suggests that when $k = n$, $a_{n+2} = 0$. Repeatedly employing recurrence formula (6.34) for $k > n$, we see that the coefficients of a_{n+4}, a_{n+6}, ... all vanish. Therefore, when n is an even number, y_1 defined by Eq. (6.31a) becomes a polynomial of degree n, where only a_0, a_2, ..., a_n are non-zero; when n is an odd number, y_2 defined by Eq. (6.31b) becomes a polynomial of degree n, where only a_1, a_3, ..., a_n are nonzero.

At the present stage, we still have one degree of freedom, because y_1 or y_2 multiplied by a constant is still a polynomial solution to the Legendre equation. Thus, we can choose to evaluate this constant, such that the resulting polynomial equals 1 at $x = 1$. To this end, we let

$$a_n = \frac{(2n)!}{2^n(n!)^2} = \frac{1\cdot 3\cdot 5\cdots(2n-1)}{n!}. \tag{6.35}$$

Plugging Eq. (6.35) into the recurrence relation (6.34) sequentially gives

$$
\begin{aligned}
a_{n-2} &= -\frac{n(n-1)}{2(2n-1)} \cdot \frac{(2n)!}{2^n (n!)^2} = -\frac{n(n-1)}{2(2n-1)} \cdot \frac{2n(2n-1)\cdot(2n-2)!}{2^n n \cdot (n-1)! \cdot n(n-1)\cdot(n-2)!} \\
&= -\frac{(2n-2)!}{2^n (n-1)!(n-2)!}, \\
a_{n-4} &= -\frac{(n-2)(n-3)}{4(2n-3)} \cdot (-1) \frac{(2n-2)!}{2^n (n-1)!(n-2)!} \\
&= \frac{(n-2)(n-3)}{4(2n-3)} \cdot \frac{2(n-1)(2n-3)\cdot(2n-4)!}{2^n (n-1)\cdot(n-2)!\cdot(n-2)(n-3)\cdot(n-2)!} \\
&= \frac{(2n-4)!}{2^n \cdot 2(n-2)!(n-4)!}, \\
a_{n-6} &= -\frac{(n-4)(n-5)}{6(2n-5)} \cdot \frac{(2n-4)!}{2\cdot 2^n (n-2)!(n-4)!} \\
&= \frac{(n-4)(n-5)}{6(2n-5)} \cdot \frac{2(n-2)(2n-5)\cdot(2n-6)!}{2\cdot 2^n (n-2)\cdot(n-3)!\cdot(n-4)(n-5)\cdot(n-6)!} \\
&= \frac{(2n-6)!}{2^n 3!(n-3)!(n-6)!}, \\
&\cdots
\end{aligned}
\tag{6.36}
$$

A general expression for the corresponding polynomial solution to the Legendre equation is thus summarised by

$$
a_{n-2m} = (-1)^m \frac{(2n-2m)!}{2^n m!(n-m)!(n-2m)!} \tag{6.37}
$$

for all positive integers m such that $n - 2m \geq 0$.

When n is a positive even number, incorporating Eq. (6.37) with (6.31a) gives

$$
y_1 = \sum_{m=0}^{n/2} (-1)^m \frac{(2n-2m)!}{2^n m!(n-m)!(n-2m)!} \cdot x^{n-2m}; \tag{6.38}
$$

when n is an odd number, inserting Eq. (6.37) into (6.31b) gives

$$
y_2 = \sum_{m=0}^{(n-1)/2} (-1)^m \frac{(2n-2m)!}{2^n m!(n-m)!(n-2m)!} \cdot x^{n-2m}. \tag{6.39}
$$

The two cases above can be unified in one expression given by

$$
\mathrm{P}_n(x) = \sum_{m=0}^{N} (-1)^m \frac{(2n-2m)!}{2^n m!(n-m)!(n-2m)!} \cdot x^{n-2m}, \tag{6.40}
$$

with

$$N = \begin{cases} n/2, & n \text{ is an even number;} \\ (n-1)/2, & n \text{ is an odd number.} \end{cases} \tag{6.41}$$

Here $\mathrm{P}_n(x)$ defined by Eq. (6.40) is termed as the *Legendre polynomial* of degree n, which is a special case of the *Legendre function of the first kind*, whose definition is still valid for the cases when α is a non-integer. The full definition for the Legendre functions of the first kind is given in Sect. 7.2.

Three issues are mentioned here. Firstly, $\mathrm{P}_n(1) = 1$ for all $n \in \mathbb{Z}^+$ as it is defined. Secondly, the domain of definition for P_n is literally $x \in \mathbb{R}$. Nonetheless, to be consistent with the convergent radii of the series solutions given by Eqs. (6.31a) and (6.31b), we mainly consider $x \in [-1, 1]$ for P_n whenever unspecified. Thirdly, through the derivation above, it can be seen that when n assumes negative integer values, we can still derive polynomial solutions. In fact, it can be verified that

$$\mathrm{P}_n(x) = \mathrm{P}_{-n-1}(x), \; n \in \mathbb{Z}^-. \tag{6.42}$$

In the rest of this chapter, unless specified, we keep n to be a non-negative integer.

Now $\mathrm{P}_n(x)$ is identified as one solution to the Legendre equation of degree n. In order to derive its fundamental system of solutions, another solution independent of $\mathrm{P}_n(x)$ is still needed. To this end, we define

$$\mathrm{Q}_0(x) = \frac{1}{2} \ln \frac{1+x}{1-x}, \tag{6.43}$$

and a set of functions can be sequentially introduced by

$$\mathrm{Q}_n(x) = \mathrm{P}_n(x)\mathrm{Q}_0(x) - \sum_{k=0}^{n-1} \frac{(2k+1)(1-(-1)^{n+k})}{(n+k+1)(n-k)} \mathrm{P}_k(x), \tag{6.44}$$

for $n = 1, 2, \ldots$. Here we state without proof that $\mathrm{Q}_n(x)$ is a solution to Legendre equation (6.33), and $\mathrm{Q}_n(x)$ is termed as the *Legendre function of the second kind*.

Here we simply address the key features of $\mathrm{Q}_n(x)$ that are relevant to the upcoming discussion. Firstly, $\mathrm{Q}_n(x)$ is unbounded in its domain of definition $x \in (-1, 1)$. Secondly, any solutions to the Legendre equation of degree n should be expressed as a linear combination of $\mathrm{P}_n(x)$ and $\mathrm{Q}_n(x)$. For a systematic study of $\mathrm{Q}_n(x)$, one may refer to the concept of hypergeometric functions, as detailed more in Chap. 7.

6.3 Properties of Legendre Polynomial

In this subsection, several key properties about Legendre polynomials are introduced. Most of the contents considered here see their counterparts in Sect. 5.2, where the properties of the Bessel functions were studied. Actually, the issues considered in this subsection can be generalised for investigating other types of orthogonal polynomials.

6.3.1 Rodrigues Formula

Here we start by introducing the *Rodrigues formula*, an expression very useful for analysing orthogonal polynomials. The Rodrigues formula says that the Legendre polynomial of degree n can be generated by

$$\mathrm{P}_n(x) = \frac{(-1)^n}{2^n n!}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \left(1 - x^2\right)^n, \tag{6.45}$$

where $\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^n$ means "taking the nth derivative of".

To verify the Rodrigues formula, one simply uses the binomial theorem to expand $(1 - x^2)^n$. The right side of Eq. (6.45) is thus transformed into the expression of the Legendre polynomials defined by Eq. (6.40).

With the Rodrigues formula, one should quickly show that $\mathrm{P}_n(1) = 1$, $\mathrm{P}_n(-1) = (-1)^n$.

6.3.2 Key Properties at a Glance

General profiles

A quick glance at the general profiles of Legendre polynomials is made. The Legendre polynomials up to degree 5 are listed as follows:

$$\begin{aligned}
\mathrm{P}_0(x) &= 1, \\
\mathrm{P}_1(x) &= x, \\
\mathrm{P}_2(x) &= \frac{1}{2}\left(3x^2 - 1\right), \\
\mathrm{P}_3(x) &= \frac{1}{2}\left(5x^3 - 3x\right), \\
\mathrm{P}_4(x) &= \frac{1}{8}\left(35x^4 - 30x^2 + 3\right), \\
\mathrm{P}_5(x) &= \frac{1}{8}\left(63x^5 - 70x^3 + 15x\right),
\end{aligned} \tag{6.46}$$

and their profiles can be visualised in Fig. 6.2.

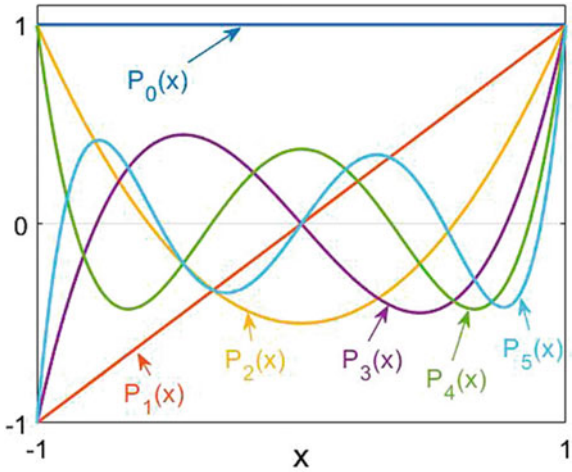

Fig. 6.2 Profiles of the Legendre polynomials up to degree 5, as formulated by Eq. (6.46)

With reference to the expression of the Legendre polynomials given by Eq. (6.40), one may quickly find that, within the domain of interest, i.e. $x \in [-1, 1]$, $\mathrm{P}_n(x)$ is an even function if n is an even number; $\mathrm{P}_n(x)$ is an odd function if n is an odd number. Such symmetry is also observed from Fig. 6.2.

Roots

Now we consider the roots of Legendre polynomials. It is well known that an n-degree polynomial should bear no more than n real roots. But for the Legendre polynomials, more attractive properties can be observed, and they are summarised as follows.

- **Completeness**—$\mathrm{P}_n(x)$ bear n mutually different real roots, say, $\zeta_1^{(n)} < \zeta_2^{(n)} < \cdots < \zeta_n^{(n)}$. They all fall within the interval of interest, i.e. $\zeta_k^{(n)} \in (-1, 1)$ for $k = 1, 2, \ldots, n$.
- **Symmetry**—If $x = a$ is one root of $\mathrm{P}_n(x)$, then $x = -a$ is also a root of $\mathrm{P}_n(x)$. This property can be naturally deduced from the symmetry of Legendre polynomials about the origin, and $x = 0$ is a root of $\mathrm{P}_n(x)$ with n being an odd number.
- **Alternating behaviour**—The roots of $\mathrm{P}_n(x)$ and $\mathrm{P}_{n+1}(x)$ alternate on the interval $(-1, 1)$. Besides, $\mathrm{P}_n(x)$ and $\mathrm{P}_{n+1}(x)$ do not have common roots. We have seen such alternating behaviour, when the zeros of Bessel functions are examined in Sect. 5.2.2.

In Fig. 6.2, the aforementioned properties can be visualised.

The roots of Legendre polynomials are of particular importance for approximately evaluating definite integrals, and the relevant concept is known as the Gauss–Legendre quadrature, which is to be detailed in Sect. 6.4.2.

Recurrence relations

The recurrence relation for polynomials enables one to express a high-degree polynomial by low-degree ones. For Legendre polynomials, one such recurrence relation is formulated by

$$\mathrm{P}_{n+1}(x) - \frac{(2n+1)x}{n+1} \cdot \mathrm{P}_n(x) + \frac{n}{n+1} \cdot \mathrm{P}_{n-1}(x) = 0, \quad n = 1, 2, \ldots. \tag{6.47}$$

Eq. (6.47) can be proved by directly inserting the general expression of the Legendre polynomials given by Eq. (6.40). But a less cumbersome proof for Eq. (6.47) can be constructed based on the concept of orthogonal polynomials, which are to be discussed in greater details in Sect. 6.3.3.

Asymptotic formula

When its degree becomes fairly high, the evaluation of $\mathrm{P}_n(x)$ involves many times of additions and multiplications, no matter which of Eq. (6.40) and the recurrence relation (6.47) is employed. Hence, deriving an approximating formula to the Legendre polynomial of high-degree n is practically meaningful for engineering use. To this end, we introduce

$$\mathrm{P}_n(\cos\theta) = \sqrt{\frac{\theta}{\sin\theta}} \cdot \mathrm{J}_0\left(\left(n + \frac{1}{2}\right)\theta\right) + \mathcal{O}(n^{-\frac{3}{2}}), \tag{6.48}$$

as $n \to \infty$, where $\mathrm{J}_0(\cdot)$ is the 0th order Bessel function of the first kind; the symbol "$\mathcal{O}$" means "a same order of magnitude to". Note that the input of P_n in Eq. (6.48) is $\cos\theta$, $\theta \in (0, \pi)$.

It is worth noting that Eq. (6.48) is more effective for θ away from 0 or π, or alternatively, x away from -1 or 1. This is because we know that $\mathrm{P}_n(\pm 1) = (\pm 1)^n$. If one wishes to evaluate $\mathrm{P}_n(1-\epsilon)$, with ϵ small, other forms of approximating formulae expanded in terms of this small ϵ should be more effective.

Equation (6.48) indicates that its approximating error is as small as $n^{-\frac{3}{2}}$. Hence, Eq. (6.48) is expected to be more effective for large n.

In Fig. 6.3, $\mathrm{P}_n(x)$, $n = 1$, 2 and 5 are drawn against their corresponding approximating formulae. It can be read that the difference between $\mathrm{P}_n(x)$ and its asymptotic formula (6.48) is barely visually distinguishable when n is as small as 5.

6.3.3 Orthogonal Systems

As seen in many previous examples, function orthogonality is a feature that is key to the use of the method of separation of variables. As recalled from Sect. 2.3.2, one way to induce a set of mutually orthogonal functions is through defining a Sturm–Liouville system. Actually, Legendre polynomials can be induced by Sturm–Liouville systems too.

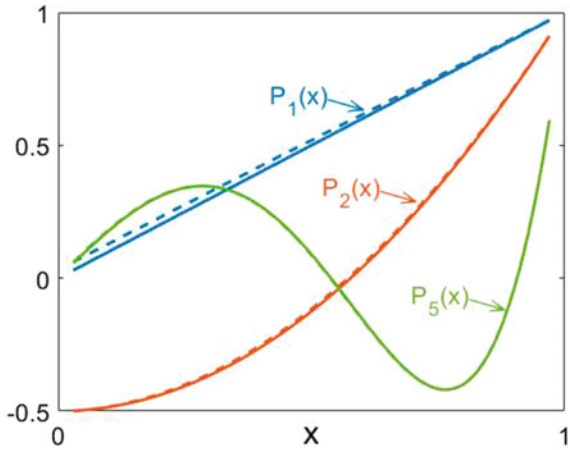

Fig. 6.3 Solid lines are produced from $P_n(x)$, and the dashed lines are produced based on the asymptotic expression by Eq. (6.48)

Sturm–Liouville system

To this end, we consider an differential equation as follows:

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\left(1-x^2\right)\frac{\mathrm{d}y}{\mathrm{d}x}\right)+\lambda y=0, \quad x\in(-1,1). \tag{6.49}$$

A comparison with Eq. (2.76) suggests that Eq. (6.49) is a Sturm–Liouville equation. Correspondingly in Eq. (2.76), $k(x)=1-x^2>0$ with $x\in(-1,1)$; $q(x)=0$; $\rho(x)=1$. Note that when $\lambda=\alpha(\alpha+1)$, Eq. (6.49) coincides with the Legendre equation of degree n, as given by Eq. (6.21).

To obtain a Sturm–Liouville system, as discussed in Sect. 2.3.2, boundary conditions are needed at $x=\pm1$ depending on the values of $k(x)=1-x^2$ there. Here $k(\pm1)=0$, indicating that only natural boundary conditions are needed, i.e. there is no need to specify the function values at $x=\pm1$, but one simply requires that the function values are bounded at the two ends.

With governing equation (6.49) and natural boundary conditions given at $x=\pm1$, a Sturm–Liouville system is developed, and the following conclusions can be drawn naturally.

- There exist a set of non-negative **eigenvalues**, say $0\le\lambda_0\le\lambda_1\le\cdots$, such that the problem defined by Eq. (6.49) has non-trivial (and bounded) solutions when $\lambda=\lambda_n$, $n=0,1,\ldots$.
- For each $\lambda=\lambda_n$, one of the corresponding (non-trivial and bounded) solution, say, $y_n(x)$, is the nth **eigenfunction** of Eq. (6.49).
- The eigenfunctions are mutually **orthogonal**. Mathematically, this is given by

$$\int_{-1}^{1} y_n(x)y_m(x)\,\mathrm{d}x=0, \quad \text{for } n\neq m. \tag{6.50}$$

Note that the orthogonality formula given by Eq. (2.88) involves a weighted function $\rho(x)$, where $\rho(x) = 1$ here.

- These eigenfunctions form a **complete** set of orthogonal functions, that is, for each bounded function $f(x)$ defined on the interval $(-1, 1)$, it can be expanded in terms of the eigenfunctions by

$$f(x) \sim \sum_{n=0}^{\infty} a_n y_n(x), \tag{6.51}$$

where the coefficients a_n are determined by

$$a_n = \frac{1}{M_n} \int_{-1}^{1} f(x) y_n(x)\, \mathrm{d}x, \quad \text{for } n = 0, 1, \ldots, \tag{6.52}$$

with M_n being the **modulus** of nth eigenfunction, which is given by

$$M_n = \int_{-1}^{1} y_n^2(x)\, \mathrm{d}x. \tag{6.53}$$

Orthogonal systems formed by Legendre polynomials

Now we try to build a link between the Sturm–Liouville system discussed above and Legendre polynomials. A comparison with (6.21) suggests that, when $\lambda = \alpha(\alpha + 1)$, solutions to Eq. (6.49) are expressed by the linear combination of $y_1(x)$ and $y_2(x)$, given by Eqs. (6.31a) and (6.31b), respectively. However, only bounded solutions are desired here. As a result, the cases where α is non-integer are excluded, because the series defining y_1 and y_2 have been shown divergent at $x = \pm 1$. Therefore, bounded solutions to Sturm–Liouville Eq. (6.49) only exist for $\alpha = n$ with n being integers, and the corresponding eigenvalues are

$$\lambda_n = n(n + 1), \quad n = 0, 1, \ldots. \tag{6.54}$$

Therefore, the corresponding eigenfunctions, which are just the Legendre polynomials $\{\mathrm{P}_n(x)\}_{n=0}^{\infty}$, form an complete set of orthogonal functions, and Eq. (6.50) becomes

$$\int_{-1}^{1} \mathrm{P}_n(x)\mathrm{P}_m(x)\, \mathrm{d}x = 0, \quad \text{for } n \neq m. \tag{6.55}$$

Moreover, as suggested by Eq. (6.51), any bounded function on $(-1, 1)$ can be expanded in terms of $\mathrm{P}_n(x)$. To evaluate the coefficients in the expansion, one needs to replace y_n in Eqs. (6.52) and (6.53) by $\mathrm{P}_n(x)$.

In particular, the *modulus* of the Legendre polynomial of degree n is defined by $M_n = \int_{-1}^{1} (\mathrm{P}_n(x))^2 \, \mathrm{d}x$. In order to evaluate M_n, Rodrigues formula (6.45) is employed, leading to

$$\begin{aligned}\int_{-1}^{1} (\mathrm{P}_n(x))^2 \, \mathrm{d}x &= \frac{1}{2^{2n}(n!)^2} \int_{-1}^{1} \left[\frac{\mathrm{d}^n}{\mathrm{d}x^n}(x^2-1)^n\right] \cdot \left[\frac{\mathrm{d}^n}{\mathrm{d}x^n}(x^2-1)^n\right] \mathrm{d}x \\ &= \left[\frac{\mathrm{d}^{n-1}}{\mathrm{d}x^{n-1}}(x^2-1)^n\right]\Bigg|_{-1}^{1} \cdot \left[\frac{\mathrm{d}^n}{\mathrm{d}x^n}(x^2-1)^n\right]\Bigg|_{-1}^{1} \\ &\quad - \frac{1}{2^{2n}(n!)^2} \int_{-1}^{1} \left[\frac{\mathrm{d}^{n-1}}{\mathrm{d}x^{n-1}}(x^2-1)^n\right] \cdot \left[\frac{\mathrm{d}^{n+1}}{\mathrm{d}x^{n+1}}(x^2-1)^n\right] \mathrm{d}x.\end{aligned} \tag{6.56}$$

Note that $(x^2-1)^n$ comprises n factors of (x^2-1). Thus,

$$\left[\frac{\mathrm{d}^k}{\mathrm{d}x^k}(x^2-1)^n\right]\Bigg|_{-1}^{1} = 0 \tag{6.57}$$

should hold for all integers $k < n$. Then Eq. (6.56) becomes

$$\begin{aligned}\int_{-1}^{1} (\mathrm{P}_n(x))^2 \, \mathrm{d}x &= -\frac{1}{2^{2n}(n!)^2} \int_{-1}^{1} \left[\frac{\mathrm{d}^{n-1}}{\mathrm{d}x^{n-1}}(x^2-1)^n\right] \cdot \left[\frac{\mathrm{d}^{n+1}}{\mathrm{d}x^{n+1}}(x^2-1)^n\right] \mathrm{d}x \\ &= \frac{(-1)^n}{2^{2n}(n!)^2} \int_{-1}^{1} (x^2-1)^n \left[\frac{\mathrm{d}^{2n}}{\mathrm{d}x^{2n}}(x^2-1)^n\right] \mathrm{d}x \\ &= \frac{(-1)^n (2n)!}{2^{2n}(n!)^2} \int_{-1}^{1} (x^2-1)^n \, \mathrm{d}x,\end{aligned} \tag{6.58}$$

where the second identity is obtained through repeatedly using integration by part and Eq. (6.57); the third identity stems from the fact that the $2n$th derivative of $(x^2-1)^n$ equals $(2n)!$.

To further evaluate the integral on the right side of Eq. (6.58), we set $x = \cos t$, and then $\mathrm{d}x = -\sin t \mathrm{d}t$; $(x^2-1)^n = (-1)^{2n} \sin^n t$. This results in

$$\int_{-1}^{1} (x^2-1)^n \, \mathrm{d}x = 2\int_{0}^{1} (x^2-1)^n \, \mathrm{d}x = (-1)^n \cdot 2 \int_{0}^{\frac{\pi}{2}} \sin^{2n+1} t \, \mathrm{d}t. \tag{6.59}$$

One may then calculate

$$\begin{aligned}\int_0^{\frac{\pi}{2}} \sin^{2n+1} t \,\mathrm{d}t &= -\sin^{2n} t \cos t\Big|_0^{\frac{\pi}{2}} \,\mathrm{d}t + 2n \int_0^{\frac{\pi}{2}} \sin^{2n-1} t \cos^2 t \,\mathrm{d}t \\ &= 2n \int_0^{\frac{\pi}{2}} \sin^{2n-1} t \cos^2 t \,\mathrm{d}t - 2n \int_0^{\frac{\pi}{2}} \sin^{2n+1} t \cos^2 t \,\mathrm{d}t.\end{aligned} \tag{6.60}$$

This establishes a recurrence relation of

$$\int_0^{\frac{\pi}{2}} \sin^{2n+1} t \,\mathrm{d}t = \frac{2n}{2n+1} \int_0^{\frac{\pi}{2}} \sin^{2n-1} t \,\mathrm{d}t. \tag{6.61}$$

Provided that $\int_0^{\frac{\pi}{2}} \sin t \,\mathrm{d}t = 1$, we finally reach

$$\int_0^{\frac{\pi}{2}} \sin^{2n+1} t \,\mathrm{d}t = \frac{2n \cdots 2}{(2n+1) \cdots 3} = \frac{2^{2n}(n!)^2}{(2n+1)!}. \tag{6.62}$$

Inserting Eqs. (6.59) and (6.62) into (6.58) finally gives the modulus of $\mathrm{P}_n(x)$ by

$$M_n = \int_{-1}^{1} (\mathrm{P}_n(x))^2 \,\mathrm{d}x = \frac{2}{2n+1}. \tag{6.63}$$

Therefore, for any $f(x)$ bounded on $(-1, 1)$, it can be expanded as a series summation of the Legendre polynomials by

$$f(x) = \sum_{n=0}^{\infty} a_n \mathrm{P}_n(x), \tag{6.64}$$

where the coefficients a_n are given by

$$a_n = \frac{2n+1}{2} \int_{-1}^{1} f(x) \mathrm{P}_n(x) \,\mathrm{d}x, \tag{6.65}$$

for $n = 0, 1, \ldots$.

A corollary of Eq. (6.55) is

$$\int_{-1}^{1} r(x)\mathrm{P}_n(x)\,\mathrm{d}x = 0, \tag{6.66}$$

where $r(x)$ is any polynomial whose degree is no greater than $n-1$. The proof for Eq. (6.66) is straightforward, as $r(x)$ can be expressed as a linear combination of $\{\mathrm{P}_k\}_{k=0}^{n-1}$.

Equation (6.64) implies that one may use simple polynomials to approximate any bounded functions defined on $(-1, 1)$. In fact, we have seen such polynomial approximations from Taylor's series:

$$f(x) \sim \sum_{n=0}^{\infty} \frac{f^{(n)}(x_0)}{n!} \cdot (x - x_0)^n, \tag{6.67}$$

where "$^{(n)}$" denotes "taking nth derivative of".

Generally, Taylor's series approximates a function in a "local" sense, that is, the approximating error depends on how x is close to x_0. As illustratively shown in Fig. 6.4a, Taylor series is formulated about $x_0 = 0$.

The approximating polynomials deviate from the actual function value (given by the solid curve) as x goes away from $x_0 = 0$.

In contrast, the expansion in terms of Legendre polynomials, as given by Eq. (6.64), makes the approximation in a "global" sense. As seen in Fig. 6.4b, no points from the interval $(-1, 1)$ are special, and the approximating accuracy is more uniformly

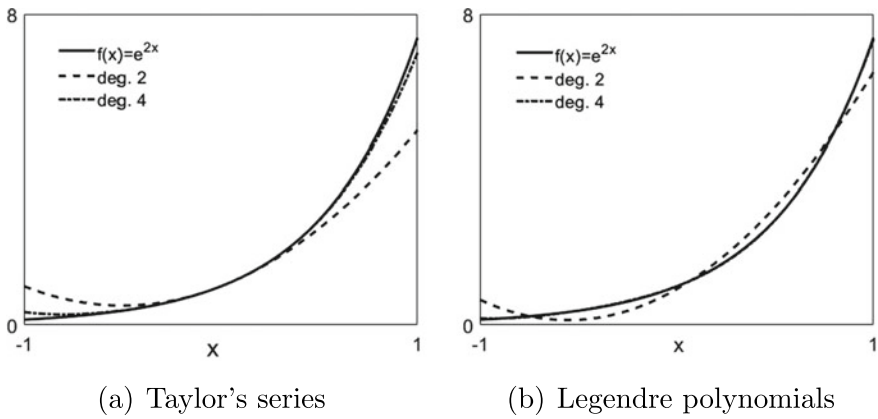

Fig. 6.4 Polynomial approximation to $f(x) = \mathrm{e}^{2x}$ using **a** Taylor series of Eq. (6.67) and **b** expansion of the Legendre polynomials of Eq. (6.64), respectively

distributed. Actually, one can barely visualise the difference between $f(x)$ and its corresponding expansion in terms of the Legendre polynomials up to degree 4.

For a further comparison between the two ways of polynomial approximations, Taylor's series enjoys a simple form. But one needs to know beforehand the values of the derivatives at x_0. Therefore, if the target $f(x)$ can not only be explicitly expressed, but is only given by data points, Taylor's series sees its limitation. In contrast, one should still approximately evaluate the integral in Eq. (6.65), even when $f(x)$ is implicitly given. Besides, as from Fig. 6.4, the convergent rates are more uniform for all points $x \in (-1, 1)$. But the computational cost for calculating the coefficient a_n by Eq. (6.65) is often higher than that for Taylor's series, especially when the target function is explicitly given. Therefore, one should decide which set of polynomials is for use, in accordance with the features of the functions of interest.

6.3.4 Discussion on General Orthogonal Polynomials

The discussion on the aforementioned issues can be generalised for studying other types of orthogonal polynomials.

Generalised Rodrigues formula

Orthogonal polynomials can find their roots in the *generalised Rodrigues formula* defined by

$$p_n(x) = \frac{1}{K_n \rho(x)} \left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \left[\rho(x)(Y(x))^n\right], \tag{6.68}$$

where $Y(x)$ is a polynomial whose coefficients do not depend on n; $\rho(x)$ is a weighted function; K_n is a number dependent of n.

Classical orthogonal polynomials can be classified, based on their domains of definition, into three groups: in an interval of finite size which can be represented by the interval $(-1, 1)$; in a semi-infinitely long interval represented by $(0, \infty)$; in a fully infinitely long interval represented by $(-\infty, \infty)$. Different choices for $\rho(x)$ and $Y(x)$ lead to the definition of various *classical orthogonal polynomials*. In Table 6.1, several types of widely used classical orthogonal polynomials are summarised.

In particular, the Legendre polynomials and the Chebyshev polynomials (of both kinds) can be viewed as special cases of the Jacobi polynomials.

Throughout the rest of this section, we use $p_n(x)$ to generally denote all classical orthogonal polynomials listed in Table 6.1, and their corresponding domains of definition are uniformly denoted by I.

Roots

Two key properties shown by the roots of these orthogonal polynomials are summarised as follows:

- p_n has n real simple roots, say, $\zeta_1^{(n)}, \ldots, \zeta_n^{(n)}$, and they all fall inside the corresponding domains of definition, i.e. $\zeta_k^{(n)} \in I$, for $k = 1, \ldots, n$.

Table 6.1 Widely used classical orthogonal polynomials generated from the generalised Rodrigues formula (6.68)

Name and notation	Domain of definition I	$Y(x)$	$\rho(x)$
Jacobi: $\mathrm{P}_n^{(\alpha,\beta)}(x)$ $(\alpha, \beta > -1)$	$(-1, 1)$	$1 - x^2$	$(1-x)^\alpha(1+x)^\beta$
Legendre: $\mathrm{P}_n(x)$	$(-1, 1)$	$1 - x^2$	1
Chebyshev: (1st kind) $\mathrm{T}_n(x)$	$(-1, 1)$	$1 - x^2$	$(1-x^2)^{-\frac{1}{2}}$
Chebyshev: (2nd kind) $\mathrm{U}_n(x)$	$(-1, 1)$	$1 - x^2$	$(1-x^2)^{\frac{1}{2}}$
Laguerre: $\mathrm{L}_n^\alpha(x)$	$(0, \infty)$	x	$x^\alpha \mathrm{e}^{-x}$
Hermite: $\mathrm{H}_n^\alpha(x)$	$(-\infty, \infty)$	1	e^{-x^2}

- The roots of p_n and p_{n+1} alternate on I and $p_n(x)$ and $p_{n+1}(x)$ do not share common roots.

Recurrence relations

Suppose that k_n represents the coefficient of x^n, the power-n term in $p_n(x)$. Then the following recurrence formula should hold:

$$p_{n+1}(x) = (a_n x + b_n)p_n + c_n p_{n-1}, \quad \text{for } n = 1, 2, \ldots, \tag{6.69}$$

where

$$a_n = \frac{k_{n+1}}{k_n}, \quad b_n = -a_n \int_I x\rho(x)(p_n(x))^2 \,\mathrm{d}x, \quad c_n = -\frac{a_n}{a_{n-1}}, \quad c_0 = 0. \tag{6.70}$$

Differential equation of induction

Similar as in the case for Legendre polynomials, classical orthogonal polynomials can be induced by second-order linear differential equations. To this end, we consider

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\rho(x)Y(x)\frac{\mathrm{d}y}{\mathrm{d}x}\right) + \lambda\rho(x)y = 0, \quad x \in I. \tag{6.71}$$

A comparison of Eq. (6.71) with the Sturm–Liouville equation (2.76) suggests that

$$k(x) = \rho(x)Y(x) > 0, \quad q(x) = 0, \quad \rho(x) = \rho(x) > 0, \text{ for } x \in I,$$

where $\rho(x)$, $Y(x)$ and the domain of definition I for each case are determined with reference to Table 6.1. Moreover, $k(x) = \rho(x)Y(x)$ tends to 0, as the boundary of the

interval I is approached for each case outlined in Table 6.1. Thus no extra boundary conditions are needed, as we are only interested in bounded solutions to Eq. (6.71).

Therefore, Eq. (6.71) actually identifies a Sturm–Liouville system for each set of $Y(x)$, $\rho(x)$ and I listed in Table 6.1.

It can be shown[1] that the classical orthogonal polynomials $p_n(x)$ listed in Table 6.1 are just the eigenfunctions for the corresponding differential equations of induction. Therefore, for any function $f(x)$ that is bounded in I, we have

$$f(x) = \sum_{n=0}^{\infty} a_n p_n(x), \tag{6.72}$$

where the coefficients a_n are given by

$$a_n = \frac{1}{M_n} \int_{-1}^{1} \rho(x) f(x) p_n(x)\, \mathrm{d}x, \tag{6.73}$$

with the modulus M_n calculated by

$$M_n = \int_{-1}^{1} \rho(x) (p_n(x))^2\, \mathrm{d}x. \tag{6.74}$$

Here only key common features shared by the classical orthogonal polynomials listed in Table 6.1 are outlined. For a systematic study over the topic, one may refer to advanced materials (e.g. [11]).

6.4 Applications with Legendre Polynomials

In this section, we consider the applications with Legendre polynomials in two aspects. First, solutions to the Helmholtz equation defined in a sphere are searched for. Second, the Gauss–Legendre quadrature, which provides an effective means for approximating definite integrals, is introduced.

6.4.1 Solving PDEs Defined in a Sphere

Here we consider a PDE problem defined in a unit sphere as follows:

$$\begin{cases} \Delta V + k^2 V = 0, \quad x^2 + y^2 + z^2 < 1; \\ V|_{\sqrt{x^2+y^2+z^2}=1} = 1 - z^2. \end{cases} \tag{6.75}$$

[1] See Sect. 6.5 of "Special functions" by N. M. Temme [11].

With the spherical coordinates given by Eq. (6.6), problem (6.75) can be rewritten by

$$\begin{cases} \dfrac{1}{r^2}\dfrac{\partial}{\partial r}\left(r^2\dfrac{\partial V}{\partial r}\right)+\dfrac{1}{r^2\sin\theta}\dfrac{\partial}{\partial\theta}\left(\sin\theta\dfrac{\partial V}{\partial\theta}\right)+\dfrac{1}{r^2\sin^2\theta}\cdot\dfrac{\partial^2 V}{\partial\varphi^2}+k^2V=0,\ r<1; \\ V|_{r=1}=1-\cos^2\theta, \end{cases} \tag{6.76}$$

where Eq. (3.38) is used to express the Laplacian operator in the spherical system.

Since the boundary condition here is independent of the angle φ, it is natural to assume that the final solution V is independent of φ. Then we search for a solution in the form of

$$V=\mathcal{P}(r)\Theta(\theta). \tag{6.77}$$

With Eq. (6.77), the governing equation of problem (6.76) becomes

$$\frac{\Theta}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}\mathcal{P}}{\mathrm{d}r}\right)+\frac{\mathcal{P}}{r^2\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right)+k^2\mathcal{P}\Theta=0, \tag{6.78}$$

which is then rearranged to a form where the variables can be separated, i.e.

$$\frac{1}{\mathcal{P}}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}\mathcal{P}}{\mathrm{d}r}\right)+k^2r^2=-\frac{1}{\Theta\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right)=n(n+1), \tag{6.79}$$

where n is an introduced constant.

Hence, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}\mathcal{P}}{\mathrm{d}r}\right)+\left(k^2r^2-n(n+1)\right)\mathcal{P}=0, \tag{6.80a}$$

and

$$\sin\theta\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right)+n(n+1)\sin^2\theta\Theta=0. \tag{6.80b}$$

As discussed in the end of Sect. 6.1, non-trivial and bounded solutions to Eq. (6.80b) only exist when the eigenvalue n is a non-negative integer, and the corresponding eigenfunction is given by

$$\Theta_n(\theta)=\mathrm{P}_n(\cos\theta). \tag{6.81}$$

Based on Eq. (6.12), solutions to Eq. (6.80a) are expressed by

$$\mathcal{P}_n(r)=\frac{1}{\sqrt{r}}\mathrm{J}_{n+\frac{1}{2}}(kr), \tag{6.82}$$

where the unbounded terms involving $\mathrm{N}_{n+\frac{1}{2}}(\cdot)$ are excluded.

Up to this stage, the solution to Eq. (6.76) is expected to be represented in a series form of

$$V = \sum_{n=0}^{\infty} \mathcal{P}_n(r)\Theta_n(\theta) = \frac{1}{\sqrt{r}} \sum_{n=0}^{\infty} C_n \mathrm{J}_{n+\frac{1}{2}}(kr)\mathrm{P}_n(\cos\theta) \tag{6.83}$$

with the coefficients C_n to be determined.

Inserting the boundary condition of $V|_{r=1} = 1 - \cos^2\theta$ into Eq. (6.83) suggests

$$1 - \cos^2\theta = \sum_{n=0}^{\infty} C_n \mathrm{J}_{n+\frac{1}{2}}(k)\mathrm{P}_n(\cos\theta). \tag{6.84}$$

For simplicity, we introduce $x = \cos\theta$, and Eq. (6.84) then becomes

$$1 - x^2 = \sum_{n=0}^{\infty} C_n \mathrm{J}_{n+\frac{1}{2}}(k)\mathrm{P}_n(x). \tag{6.85}$$

For determining C_n in Eq. (6.85), we note that the left side of Eq. (6.85) is a degree 2 polynomial. Thus $C_n = 0$ for $n > 2$. Besides, since $1 - x^2$, the left side of Eq. (6.85), is an even function, $C_1 = 0$ as $\mathrm{P}_1(x)$ is an odd function. Equation (6.85) is further simplified to be

$$1 - x^2 = C_0 \mathrm{J}_{\frac{1}{2}}(k)\mathrm{P}_0(x) + C_2 \mathrm{J}_{\frac{5}{2}}(k)\mathrm{P}_2(x). \tag{6.86}$$

Incorporating it with Eq. (6.46) sets up a linear equation system for C_0 and C_2, and we obtain $C_0 = 2/(3J_{1/2}(k))$ and $C_2 = -2/(3J_{5/2}(k))$. Inserting them back into Eq. (6.83), we finally express the solution to problem (6.78) by

$$\begin{aligned} V(r,\theta) &= \frac{1}{\sqrt{r}}\left(\frac{2}{3J_{\frac{1}{2}}(k)} \cdot \mathrm{J}_{\frac{1}{2}}(kr)\mathrm{P}_0(\cos\theta) - \frac{2}{3J_{\frac{5}{2}}(k)} \cdot \mathrm{J}_{\frac{5}{2}}(kr)\mathrm{P}_2(\cos\theta)\right) \\ &= \frac{1}{\sqrt{r}}\left(\frac{2}{3J_{\frac{1}{2}}(k)} \cdot \mathrm{J}_{\frac{1}{2}}(kr) - \frac{1}{3J_{\frac{5}{2}}(k)} \cdot \mathrm{J}_{\frac{5}{2}}(kr)\left(3\cos^2\theta - 1\right)\right). \end{aligned} \tag{6.87}$$

6.4.2 Legendre–Gauss Quadrature

The concept of the Legendre–Gauss quadrature has been intensively used for evaluating definite integrals. First, we derive the rule of the Legendre–Gauss quadrature. Then the idea is extended to general orthogonal polynomials, and the rule of general Gauss quadrature is presented.

To this end, we start with evaluating $\int_{-1}^{1} f(x)\,\mathrm{d}x$, where $f(x)$ is a polynomial of degree no greater than $2n-1$. Suppose that the roots of $\mathrm{P}_n(x)$ are denoted by $-1 < \zeta_1^{(n)} < \cdots < \zeta_n^{(n)} < 1$, i.e.

$$\mathrm{P}_n(x) = (x-\zeta_1^{(n)})\cdots(x-\zeta_n^{(n)}). \tag{6.88}$$

Now we construct a function $F(x)$ through the Lagrange interpolation as

$$F(x) = \sum_{k=1}^{n} f(\zeta_k^{(n)}) \cdot \frac{\mathrm{P}_n(x)}{\mathrm{P}_n'(\zeta_k^{(n)})(x-\zeta_k^{(n)})}, \tag{6.89}$$

where P_n' denotes the first derivative of P_n. It can be checked that $F(x)$ is a polynomial of degree $n-1$ and

$$F(\zeta_k^{(n)}) = \lim_{x\to\zeta_k^{(n)}} F(x) = f(\zeta_k^{(n)}) \tag{6.90}$$

for $k = 1, \ldots, n$.

This implies that the function $F - f$ is essentially a polynomial of degree no greater than $2n-1$, and $\zeta_1^{(n)}, \ldots, \zeta_n^{(n)}$ are all its roots. In other words, the polynomial $F - f$ can be factorised by

$$F(x) - f(x) = (x-\zeta_1^{(n)})(x-\zeta_2^{(n)})\cdots(x-\zeta_n^{(n)})r(x) = \mathrm{P}_n(x)r(x), \tag{6.91}$$

where $r(x)$ is another polynomial of degree $\le n-1$, and Eq. (6.88) is employed to derive the second identity.

Replacing $F(x)$ in Eq. (6.91) by Eq. (6.89) and rearranging the result, we get

$$f(x) = \sum_{k=1}^{n} f(\zeta_k^{(n)}) \cdot \frac{\mathrm{P}_n(x)}{\mathrm{P}_n'(\zeta_k^{(n)})(x-\zeta_k^{(n)})} - r(x)\mathrm{P}_n(x). \tag{6.92}$$

Integrating both sides on $(-1, 1)$ gives

$$\int_{-1}^{1} f(x)\,\mathrm{d}x = \sum_{k=1}^{n} \omega_k^{(n)} f(\zeta_k^{(n)}) - \int_{-1}^{1} r(x)\mathrm{P}_n(x)\,\mathrm{d}x, \tag{6.93}$$

where $w_k^{(n)}$ are sometimes termed as the *Christoffel numbers* defined by

$$w_k^{(n)} = \frac{1}{\mathrm{P}_n'(\zeta_k^{(n)})} \cdot \int_{-1}^{1} \frac{\mathrm{P}_n(x)\,\mathrm{d}x}{x-\zeta_k^{(n)}}. \tag{6.94}$$

Table 6.2 Roots of the Legendre polynomials and the Christoffel numbers defined by Eq. (6.94) up to degree 5

P_n	$\zeta_k^{(n)}$	$w_k^{(n)}$
$n = 2$	$\pm\frac{1}{\sqrt{3}}$	1
$n = 3$	0	$\frac{8}{9}$
	$\pm\sqrt{\frac{3}{5}}$	$\frac{5}{9}$
$n = 4$	$\pm\sqrt{\frac{15-2\sqrt{30}}{35}}$	$\frac{1}{36}\left(18+\sqrt{30}\right)$
	$\pm\sqrt{\frac{15+2\sqrt{30}}{35}}$	$\frac{1}{36}\left(18-\sqrt{30}\right)$
$n = 5$	0	$\frac{128}{225}$
	$\pm\frac{1}{21}\sqrt{245-14\sqrt{70}}$	$\frac{1}{900}\left(322+13\sqrt{70}\right)$
	$\pm\frac{1}{21}\sqrt{245+14\sqrt{70}}$	$\frac{1}{900}\left(322-13\sqrt{70}\right)$

With reference to Eq. (6.66), the integral on the right side of Eq. (6.93) should vanish. Hence, the *rule of the Legendre–Gauss quadrature* is derived to be

$$\int_{-1}^{1} f(x)\,\mathrm{d}x = \sum_{k=1}^{n} w_k^{(n)} f(\zeta_k^{(n)}). \tag{6.95}$$

Several properties shown by the rule of the Legendre–Gauss quadrature make it particularly attractive. Firstly, the integral about a polynomial of degree $2n-1$ is simply calculated by a summation of n terms. Secondly, the Christoffel numbers $w_k^{(n)}$ do not depend on the actual form of $f(x)$, but only on the roots of P_n. Thus, they can be computed beforehand during an "offline" stage as these roots are applied for all cases of $f(x)$. During the "online" stage when the target function $f(x)$ is specified, one can directly add together the n terms on the right side of Eq. (6.95), so as to calculate the integral $\int_{-1}^{1} f(x)\,\mathrm{d}x$.

Table 6.2 lists the roots of the Legendre polynomials and the corresponding Christoffel numbers up to $n = 5$. Note that the roots that are symmetric to each other about $x = 0$ share a same Christoffel number, and $\sum_{k=1}^{n} w_k^{(n)} = 2$ which is just the length of the domain of integration. Thus, the Christoffel numbers actually correspond to a partition of the domain $(-1, 1)$, and $f(\zeta_k^n)$ can be treated as a representative function value in the kth subinterval.

Equation (6.95) is exact for $f(x)$ being a polynomial of degree $2n-1$. When $f(x)$ is an arbitrary bounded function on $(-1, 1)$, it becomes an approximation. Rigorous analysis can be made to give an upper bound for the approximating error. However, we have seen from Eq. (6.64) that $f(x)$ can be approximated by a linear combination of Legendre polynomials, as shown in demonstrative Fig. 6.4. Therefore, the approximating error is expected to diminish quickly as n is relatively large.

Table 6.3 Calculation of the integral of $\int_{-1}^{1} \mathrm{e}^{2x}\,\mathrm{d}x$ using the rule of the Legendre–Gauss quadrature by Eq. (6.95) and the corresponding relative errors

	Exact	$n = 2$	$n = 3$	$n = 4$	$n = 5$
Value	3.6269	3.4882	3.6223	3.6268	3.6269
Rel. err.	–	0.0382	0.0013	2.26×10^{-5}	1.87×10^{-7}

In Table 6.3, the computed values for $\int_{-1}^{1} \mathrm{e}^{2x}\,\mathrm{d}x$ using the rule of the Legendre–Gauss quadrature are given for various n. It is observed that the approximating accuracy on using Eq. (6.95) is up to six decimal digits as n is as small as 5. From this example, we see that the rule of the Legendre–Gauss quadrature offers an effective algorithm for evaluating definite integrals.

Finally, the derivation for Eq. (6.95) is generalisable to cope with other types of classical orthogonal polynomials. The key difference then is one needs to multiply the corresponding weighted function $\rho(x)$ when integrating Eq. (6.92). And this gives rise to the *general rule of Gauss quadrature*:

$$\int_I \rho(x) f(x)\,\mathrm{d}x = \sum_{k=1}^{n} w_k^{(n)} f(\eta_k^{(n)}), \tag{6.96}$$

where I is the domain of the orthogonal polynomial $p_n(x)$ in consideration and $\eta_k^{(n)}$ denotes the kth root of $p_n(x)$. And the Christoffel numbers then become

$$w_k^{(n)} = \frac{1}{\mathrm{P}_n'(\eta_k^{(n)})} \cdot \int_{-1}^{1} \frac{\rho(x) p_n(x)\,\mathrm{d}x}{x - \eta_k^{(n)}}. \tag{6.97}$$

6.5 The Associated Legendre Functions

In this section, we further consider the solutions to the associated Legendre equation (6.19), that is,

$$(1 - x^2)\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} - 2x\frac{\mathrm{d}y}{\mathrm{d}x} + \left(n(n+1) - \frac{m^2}{1 - x^2}\right) y = 0. \tag{6.98}$$

As discussed in Sect. 6.1, the cases when n and m are both non-negative integers are of particular importance for implementing the method of separation of variables. So the discussion in this section is confined to such situations. Since the present section is aimed to disseminate basic concepts, most of the related proofs are skipped in the main texts.

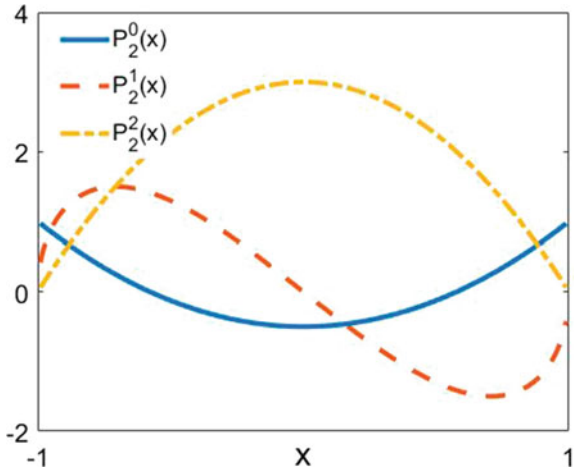

Fig. 6.5 Profiles of the associated Legendre function of the first kind $P_2^m(x)$, with $m = 0$, 1 and 2

We have demonstrated in Sect. 6.2.1 that a fundamental system of solutions to the Legendre equation (6.21) can be formed by the Legendre polynomial $P_n(x)$ given by Eq. (6.40) and the Legendre function of the second kind $Q_n(x)$ given by Eq. (6.44). Actually, the solutions to Eq. (6.98) can be induced from $P_n(x)$ and $Q_n(x)$.

For this purpose, we introduce

$$P_n^m(x) = (-1)^m \left(1 - x^2\right)^{\frac{m}{2}} \frac{d^m}{dx^m} P_n(x), \quad x \in (-1, 1) \tag{6.99}$$

and

$$Q_n^m(x) = (-1)^m \left(1 - x^2\right)^{\frac{m}{2}} \frac{d^m}{dx^m} Q_n(x), \quad x \in (-1, 1). \tag{6.100}$$

It can be checked that Eqs. (6.99) and (6.100) are both solutions to the associated Legendre equation (6.98). Here $P_n^m(x)$ is called the *associated Legendre function of the first kind*, and $Q_n^m(x)$ is called the *associated Legendre function of the second kind*. Here the integer coefficient n is termed as its *degree* and m as its *order*. Note that the term "degree" is inherited from that of Legendre polynomials, although P_n^m is not necessarily a polynomial.

From its definition (6.99), we see that $P_n^m(x)$ is uniformly zero if $n < m$. Thus, we require $n \geq m$ when defining $P_n^m(x)$. Besides, $P_n^0(x)$ is simply the Legendre polynomial of degree n. This coincides with the fact that Eq. (6.98) becomes the Legendre equation when $m = 0$.

In Fig. 6.5, the profiles of $P_2^m(x)$ up to order 2 are shown.

Some of the properties of the associated Legendre functions can be deduced straight forward from that of Legendre functions. For instance, the symmetry of $P_n^m(x)$ about $x = 0$ depends on the value of $n - m$. When $n - m$ is an odd number, $P_n^m(x)$ is an odd function. Moreover, $P_n^m(x)$ are bounded on $x \in (-1, 1)$, but $Q_n^m(x)$ are unbounded on $x \in (-1, 1)$.

Zeros

As for the zeros of $\mathrm{P}_n^m(x)$, we conclude

- $\mathrm{P}_n^m(x)$ has $(n-m)$ simple zeros within the interval $(-1, 1)$.
- The zeros of $\mathrm{P}_n^m(x)$ and $\mathrm{P}_{n+1}^m(x)$ alternate on $(-1, 1)$.
- $\mathrm{P}_n^m(x)$ and $\mathrm{P}_{n+1}^m(x)$ do not have common zeros.
- The zeros of $\mathrm{P}_n^m(x)$ are symmetric about $x = 0$.

Orthogonal systems

If replacing $n(n+1)$ in Eq. (6.98) by λ and rearranging it, we obtain an eigenvalue problem induced by a second-order linear ODE formulated by

$$\frac{\mathrm{d}}{\mathrm{d}x}\left((1-x^2)\frac{\mathrm{d}y}{\mathrm{d}x}\right) - \frac{m^2}{1-x^2}\cdot y + \lambda y = 0, \quad x \in (-1, 1). \tag{6.101}$$

A comparison of Eq. (6.101) with Eq. (2.76) [$k(x) = 1 - x^2 > 0$, $q = \frac{m^2}{1-x^2} \geq 0$ and $\rho(x) = 1$] suggests that Eq. (6.101) is a Sturm–Liouville equation. Besides, since $k(\pm 1) = 0$, only natural boundary conditions are needed.

In comparison with Eq. (6.98), the eigenvalues for Eq. (6.101) should be

$$\lambda_n = n(n+1), \quad n \geq m. \tag{6.102}$$

Since only bounded solutions are considered, the corresponding eigenfunctions are

$$y_n(x) = \mathrm{P}_n^m(x), \quad n \geq m. \tag{6.103}$$

Hence, $\{\mathrm{P}_n^m(x)\}_{n=m}^{\infty}$ should form a complete set of orthogonal functions, and the following conclusions are naturally drawn.

For a bounded function $f(x)$ defined on $x \in (-1, 1)$, it can be expressed as a series expansion of the associated Legendre polynomials of order m

$$f(x) = \sum_{n=m}^{\infty} a_n \mathrm{P}_n^m(x), \tag{6.104}$$

where the coefficient a_n is given by

$$a_n = \frac{1}{M_n^m}\int_{-1}^{1} f(x)\mathrm{P}_n^m(x)\,\mathrm{d}x \tag{6.105}$$

with the modulus M_n^m given by

$$M_n^m = \int_{-1}^{1} (\mathrm{P}_n^m(x))^2\,\mathrm{d}x = \frac{2}{2n+1}\frac{(n+m)!}{(n-m)!}. \tag{6.106}$$

It is noted that when an orthogonal system is formed, we have already fixed the order m, and the summation is made over n, with n starting from m.

The aforementioned knowledge should enable us to access the solutions to the Helmholz equation defined within a sphere for more generally imposed boundary conditions.

Exercise

1. Verify that $\mathcal{P}_\alpha(r)$ given by Eq. (6.15) solves Eq. (6.11a).
2. Take the following steps to show that $\mathcal{P}(r) = \frac{1}{\sqrt{r}} J_{\alpha+\frac{1}{2}}(kr)$ is a solution to the Cauchy–Euler equation of Eq. (6.11a), when $k \neq 0$.
   (a) Suppose $\mathcal{P}(r) = F(kr)$, and derive the governing differential equation for $y = F(x)$.
   (b) Assume a series form of $F(x) = \sum_{m=0} a_m x^{m+c}$ and show that $c = \alpha$ if the series solves Eq. (6.11a).
   (c) Carry on to determine all the coefficients a_m in the series, and finalise the proof.
3. Verify that $\Theta(\theta) = F(\cos\theta)$ solves Eq. (6.17b), where $F(\cdot)$ is a solution to the associated Legendre equation (6.19).
4. Solve the Legendre equation [Eq. (6.21)] using the following series form:

$$y = \sum_{k=1}^{\infty} a_k x^k,$$

   and show that the resulting solution is effectively y_2 given by Eq. (6.31b).
5. Verify that Q_0 and Q_n defined by Eqs. (6.43) and (6.44), respectively, solve correspondingly the Legendre equation of degree 0 and of degree n.
6. Use the Rodrigues formula (6.45) to show that $\mathrm{P}_n(1) = 1$, $\mathrm{P}_n(-1) = (-1)^n$.
7. Based on Eq. (6.46) and recurrence relation (6.47) to express the Legendre polynomials of degrees 6, 7 and 8.
8. Verify the orthogonality condition of Eq. (6.55) for Legendre polynomials with the use of Rodrigues formula (6.45).
9. Write down the orthogonality condition, in comparison with Eq. (6.55), for other types of orthogonal polynomials listed in Table 6.1.
10. Consider the Helmholtz equation $\Delta u + k^2 u = 0$ in $\mathbb{R}^3$.
    (a) Derive the general form of its radial solution, that is, $u = u(\sqrt{x^2+y^2+z^2})$;
    (b) Find one of its fundamental solution following the strategy detailed in Sect. 3.4.
11. Consider the following problem governed by Laplace's equation:

$$\begin{cases} \Delta u = 0, \text{ in } \Omega = \left\{(x, y, z) | \sqrt{x^2+y^2+z^2} < R\right\}; \\ u|_{\partial\Omega} = 1 - z^2. \end{cases}$$

(a) Solve the problem using the method of separation of variables;
(b) Solve the problem using Poisson's formula (3.74) based on the image method for electric potentials in Sect. 3.5.

12. Solve the following problem imposed with Robin boundary condition

$$\begin{cases} \Delta u = 0, \text{ in } \Omega = \left\{(x, y, z) | \sqrt{x^2 + y^2 + z^2} < 1\right\}; \\ \left(u + \dfrac{\partial u}{\partial n}\right)\Big|_{\sqrt{x^2+y^2+z^2}=1} = z. \end{cases}$$

13. Given a spherical shell of

$$\Omega = \left\{\frac{R}{2} < \sqrt{x^2 + y^2 + z^2} < R\right\},$$

use the method of separation of variables to solve

$$\begin{cases} \Delta u + k^2 u = 0, \text{ in } \Omega; \\ u|_{r=\frac{R}{2}} = 0, \ \ u|_{r=R} = z. \end{cases}$$

14. Solve the problem modelling wave propagation in a unit sphere formulated as follows:

$$\begin{cases} u_{tt} - \Delta u = 0, \text{ in } \Omega = \left\{(x, y, z) | r = \sqrt{x^2 + y^2 + z^2} < 1\right\}; \\ u|_{t=0} = r^{\frac{1}{2}}(1 - r^2), \ \ u_t|_{t=0} = 0; \\ u|_{r=1} = 0. \end{cases}$$

Chapter 7
Introduction of Hypergeometric Function

In the previous two chapters, two important classes of special functions, Bessel functions and Legendre functions with the Legendre polynomials as a special case, were discussed. In this chapter, a concise summary over general special functions is conducted from an escalated viewpoint of hypergeometric functions. We start with a review over the common features shared by both Bessel functions and Legendre functions. This is followed by a brief introduction of the general form of the Gauss hypergeometric function, and Legendre functions as one of its special cases. We then introduce the concept of confluent hypergeometric functions, which can be considered as a limiting case of the Gauss hypergeometric function. We then illustrate how the confluent hypergeometric functions induce Bessel functions, as well as many other useful functions in mathematical physics and probability theories. The contents in this chapter are summarised in the knowledge map given in Fig. 7.1.

Note that for more comprehensive understanding over hypergeometric functions, prerequisite knowledge on the behaviour of functions with complex input arguments is needed. Here we only list, generally without proof, the key results that help gain an overview on hypergeometric functions, as well as their connections with Bessel functions and Legendre functions.

7.1 Commonalities of Bessel and Legendre Functions

Although arising with different physical backgrounds, Bessel functions and Legendre functions share a number of common features. In fact, these common features provide us hints to finding a unified formulation underlying most special functions of great use in the field of mathematical physics.

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Y. Zhu, *Equations and Analytical Tools in Mathematical Physics*,
https://doi.org/10.1007/978-981-16-5441-1_7

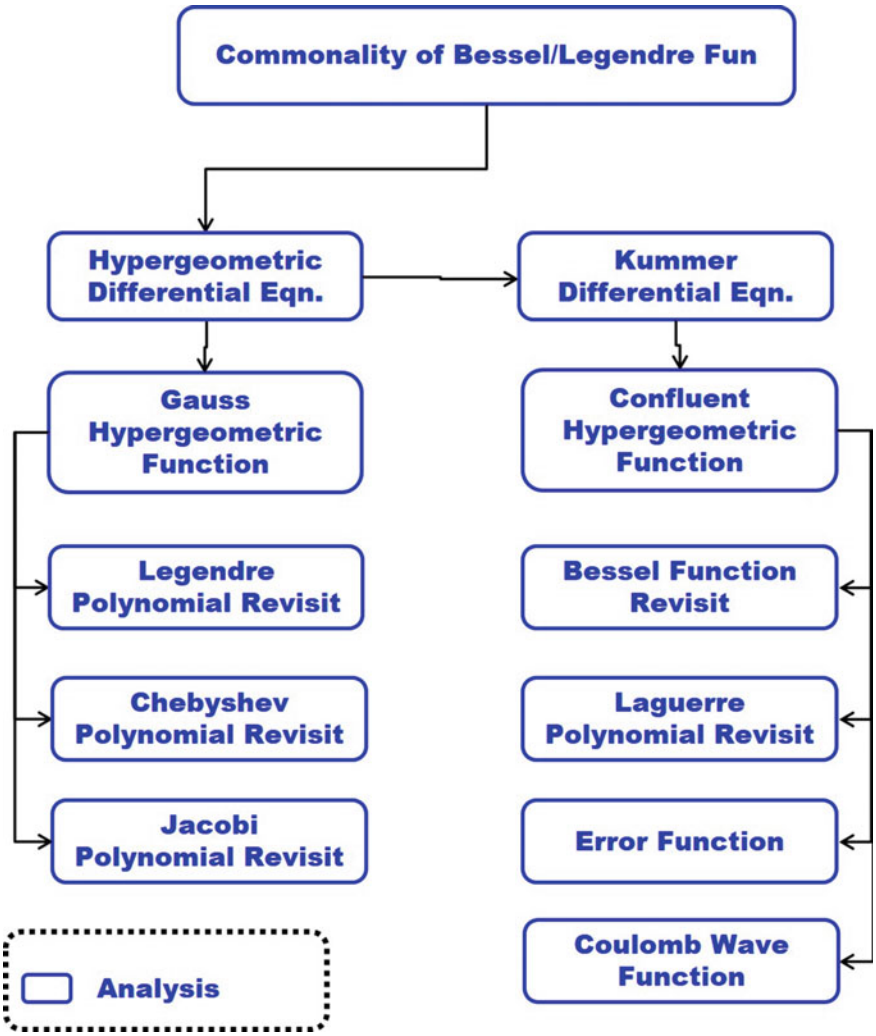

Fig. 7.1 Knowledge map—an introduction of hypergeometric function

To facilitate further discussion, the conventional *Pochhammer symbol* is introduced to denote a shifted factorial, namely

$$(a)_k = a(a+1)\cdots(a+k-1), \quad k \in \mathbb{Z}^+, \tag{7.1}$$

with $(a)_0$ set to be 1. It can be checked that

$$(a)_k = \frac{\Gamma(a+k)}{\Gamma(a)}, \tag{7.2}$$

where $\Gamma(\cdot)$ is the Gamma function defined by Eq. (5.25).

Now common features shared by Bessel functions and Legendre functions are summarised as follows.

(a) They are both induced by second-order linear ordinary differential equations whose coefficients take polynomial forms. To be specific, Bessel functions of both kinds are two mutually independent solutions to the Bessel equation given by Eq. (5.8), and (associated) Legendre functions (of both kinds) are two mutually independent solutions to the (associated) Legendre equation given by Eq. (6.19).

(b) The coefficients before the second-order derivatives vanish at the boundary points of the corresponding domains of definition for both the Bessel equation and the Legendre equation. For the Bessel equation, it happens at $x = 0$; for the Legendre equation, it happens at $x = \pm 1$. In fact, these points are just the regular singular points of the corresponding governing differential equations.

(c) They are both introduced by means of power series. Moreover, the k-th coefficients appearing in each term of the series consist of shifted factorials. For instance, the coefficient a_{2k} of Eq. (5.17) for the Bessel function of the first kind can be rewritten by

$$a_{2k} = \frac{(-1)^k a_0}{2^{2k}(\alpha+1)(\alpha+2)\cdots(\alpha+k)k!} = \frac{(-1)^k a_0}{2^{2k}(\alpha+1)_k k!}, \tag{7.3}$$

which contains two shifted factorial numbers in the denominator. Meanwhile, the coefficient a_{2k} of Eq. (6.28) appearing in the series expansion for a solution to the Legendre equation can be rewritten by

$$\begin{aligned} a_{2k} &= (-1)^k \frac{\alpha(\alpha-2)\cdots(\alpha-2k)\cdot(\alpha+1)(\alpha+3)\cdots(\alpha+2k+1)}{(2k)!}\cdot a_0 \\ &= (-1)^k 4^k a_0 \cdot \frac{\left(\frac{\alpha}{2}\right)_{k+1}\left(\frac{\alpha+1}{2}\right)_{k+1}}{(2k)!}, \end{aligned} \tag{7.4}$$

which contains three shifted factorial numbers.

The aforementioned common features imply the existence of certain underlying frameworks, at the level of which Bessel functions and Legendre functions can be formulated in a unified manner. Bearing such observations in mind, we will introduce the concept of hypergeometric functions.

7.2 Gauss Hypergeometric Function

7.2.1 Definition

Now we consider a function defined by means of a series given by

$$\mathrm{F}(a, b; c; x) = \sum_{k=0}^{\infty} \frac{(a)_k (b)_k}{(c)_k k!} x^k = 1 + \frac{ab}{c} \cdot x + \frac{a(a+1)b(b+1)}{2!c(c+1)} \cdot x^2 + \cdots, \tag{7.5}$$

where $(\cdot)_k$, as defined by Eq. (7.2), is recalled to be the Pochhammer symbol indicating a shifted factorial. A function defined by means of Eq. (7.5) is termed as a traditional *hypergeometric function* or *Gauss hypergeometric function*, conventionally denoted by the capital letter F. Here x is the free variable, which is separated from the parameters a, b and c by a semicomma in the expression of $\mathrm{F}(a, b; c; x)$. Among these three parameters, a and b appear in the numerators of the series coefficients, and they are thus separated by another semicomma from the parameter c, which appears in the denominators of the series coefficients.

Here a, b and c can assume real values, except that $c = 0, -1, \ldots$. From its definition, symmetry in the parameters a and b can be directly observed, i.e.

$$\mathrm{F}(a, b; c; x) = \mathrm{F}(b, a; c; x). \tag{7.6}$$

Moreover, when a or b assumes non-positive integer values, say, $-n$, the summation in Eq. (7.5) terminates at $k = n + 1$, and the resulting hypergeometric function becomes a polynomial. We have seen such behaviour from the derivation for Legendre polynomials in Sect. 6.2.2.

It can be readily verified that the convergent radius of the series given by Eq. (7.5) is 1. Thus, when x is permitted to assume only real values, a natural choice for the domain of definition of Gauss hypergeometric functions is $x \in (-1, 1)$.

We have seen several special cases about Gauss hypergeometric functions. For instance, the summation of a geometric sequence can be generated by

$$\mathrm{F}(1, 1; 1; x) = \sum_{k=0}^{\infty} x^k = (1 - x)^{-1}. \tag{7.7}$$

Moreover, the generalised geometric series is also a special case of the Gauss hypergeometric function given by

$$\mathrm{F}(n, b; b; x) = \sum_{k=0}^{\infty} \frac{(n + k - 1)!}{(n - 1)!k!} x^k = (1 - x)^{-n}, \; n \in \mathbb{Z}^+. \tag{7.8}$$

In fact, a high population of elementary functions can be expressed through Gauss hypergeometric functions, such as the special cases given by

$$\mathrm{F}(1, 1; 2; x) = -\frac{\log(1-x)}{x}; \tag{7.9a}$$

$$\mathrm{F}\left(\frac{1}{2}, 1; \frac{3}{2}; x^2\right) = \frac{1}{2x} \ln\left(\frac{1+x}{1-x}\right); \tag{7.9b}$$

$$F\left(\frac{1}{2}, \frac{1}{2}; \frac{3}{2}; x^2\right) = \frac{\arcsin x}{x}. \tag{7.9c}$$

For verification of the identities outlined above, one simply expresses their right sides by means of the Taylor series and then compares the resulting expansions with that of Eq. (7.5) so as to evaluate a, b and c.

It is also observed from the examples above that series (7.5) are generally divergent at $x = \pm 1$.

7.2.2 Hypergeometric Differential Equation

Definition and general solutions

Now we consider the following second-order linear ordinary differential equation for y:

$$x(1-x)\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + [c - (a+b+1)x]\frac{\mathrm{d}y}{\mathrm{d}x} - aby = 0, \tag{7.10}$$

which is termed as the *hypergeometric differential equation*, or short for the *hypergeometric equation*.

It can be checked that the Gauss hypergeometric function $\mathrm{F}(a, b; c; x)$ given by Eq. (7.5) is a solution to Eq. (7.10). For its verification, we introduce a differential operator ϑ defined by

$$\vartheta = x\frac{\mathrm{d}}{\mathrm{d}x}. \tag{7.11}$$

Thus, hypergeometric equation (7.10) is expressed by

$$\frac{1}{x}(\vartheta + c - 1)\vartheta[y] - (\vartheta + a)(\vartheta + b)[y] = 0, \tag{7.12}$$

where the square brackets imply that the input of the operator $\vartheta[\cdot]$ is a function. It can be readily checked that

$$(\vartheta + \alpha)(\vartheta + \beta)[x^k] = (k + \alpha)(k + \beta)\vartheta[x^k], \tag{7.13}$$

where α and β are two numbers. Then with reference to Eq. (7.13) and the definition of $\mathrm{F}(a, b; c; x)$ by Eq. (7.5), it is calculated that

$$\begin{aligned}\frac{1}{x}(\vartheta + c - 1)\vartheta[\mathrm{F}] &= \frac{1}{x}\sum_{k=0}^{\infty}\frac{(a)_k(b)_k}{(c)_k k!}(\vartheta + c - 1)\vartheta[x^k] \\ &= \sum_{k=1}^{\infty}\frac{(a)_k(b)_k}{(c)_k k!}k(k + c - 1)x^{k-1} = \sum_{k=1}^{\infty}\frac{(a)_k(b)_k}{(c)_{k-1}(k-1)!}x^{k-1} \\ &= \sum_{k=0}^{\infty}\frac{(k + a)(k + b)(a)_k(b)_k}{(c)_k k!}x^k = (\vartheta + \alpha)(\vartheta + \beta)\vartheta[\mathrm{F}].\end{aligned} \tag{7.14}$$

Re-arranging Eq. (7.14) just leads to Eq. (7.12), indicating that the Gauss hypergeometric function $\mathrm{F}(a, b; c; x)$ is a solution to the hypergeometric equation.

In a similar manner, it can be shown that Eq. (7.10) yields another solution given by $y_2 = x^{1-c}\mathrm{F}(a - c + 1, b - c + 1; 2 - c; x)$. But note that when $c = 1$, it coincides with the first solution $y_1 = \mathrm{F}(a, b; c; x)$. Therefore,

$$y = A\mathrm{F}(a, b; c; x) + Bx^{1-c}\mathrm{F}(a - c + 1, b - c + 1; 2 - c; x),\ c \neq 1 \tag{7.15}$$

should constitute a fundamental system to Eq. (7.10), where A and B are two constants.

When $c = 1$, Eq. (7.12) becomes

$$\frac{1}{x}\vartheta^2[y] - (\vartheta + a)(\vartheta + b)[y] = 0, \tag{7.16}$$

but extra treatments are needed for deriving its second solution [apart from $y_1 = \mathrm{F}(a, b; 1; x)$]. Following Kummer's calculations dating back to 1836, we consider a solution to Eq. (7.16) in the form of

$$y_2 = \mathrm{F}(a, b; 1; x)\ln x + \sum_{k=1}^{\infty}\frac{(a)_k(b)_k}{(k!)^2}C_k x^k,\ x \in (0, 1), \tag{7.17}$$

where C_k is the coefficients to be determined. For their determination, one may plug Eq. (7.17) into (7.16). Checking the first term on the right side of Eq. (7.17), we have

$$\begin{aligned}&\frac{1}{x}\vartheta^2[\mathrm{F}\ln x] - (\vartheta + a)(\vartheta + b)[\mathrm{F}\ln x] \\ &= \ln x\left(\frac{1}{x}\vartheta^2[\mathrm{F}] - (\vartheta + a)(\vartheta + b)[\mathrm{F}]\right) + \left(\frac{2}{x}\vartheta - (\vartheta + a) - (\vartheta + b)\right)[\mathrm{F}].\end{aligned} \tag{7.18}$$

Given Eq. (7.16), the first term of Eq. (7.18) vanishes. Then with the use of Eq. (7.5) (with $c = 1$), we have

$$
\begin{aligned}
&\frac{1}{x}\vartheta^2[\mathrm{F}\ln x] - (\vartheta + a)(\vartheta + b)[\mathrm{F}\ln x] \\
&= \sum_{k=0}^{\infty} \frac{(a)_k (b)_k}{(k!)^2} \left(\frac{2}{x}\vartheta - (\vartheta + a) - (\vartheta + b) \right) [x^k] \\
&= 2\sum_{k=0}^{\infty} \frac{(a)_{k+1}(b)_{k+1}}{(k+1)(k!)^2} x^k - \sum_{k=0}^{\infty} \frac{(a)_k (b)_k ((a+k)+(b+k))}{(k!)^2} x^k \\
&= \sum_{k=0}^{\infty} \frac{(a)_k (b)_k}{(k!)^2} \cdot \frac{(a+k)(b-1)+(a-1)(b+k)}{k+1} x^k.
\end{aligned}
\tag{7.19}
$$

Now we need to check the second part of y_2 by Eq. (7.17) with the hypergeometric equation (7.12), and we obtain

$$
\begin{aligned}
&\sum_{k=0}^{\infty} \frac{C_k (a)_k (b)_k}{(k!)^2} \left(\frac{1}{x}\vartheta^2 - (\vartheta + a)(\vartheta + b) \right) [x^k] \\
&= C_1 ab + \sum_{k=1}^{\infty} (C_{k+1} - C_k) \frac{(a)_{k+1}(b)_{k+1}}{(k!)^2} x^k.
\end{aligned}
\tag{7.20}
$$

Incorporating Eqs. (7.19) and (7.20) into (7.16) gives

$$
C_1 = \frac{1}{a} + \frac{1}{b} - 2 \tag{7.21a}
$$

and

$$
C_{k+1} = C_k - \frac{(a+k)(b-1)+(a-1)(b+k)}{(a+k)(b+k)(k+1)}. \tag{7.21b}
$$

Therefore, $\mathrm{F}(a, b; 1; x)$ and y_2 given by Eq. (7.17) form a fundamental solution system to the hypergeometric equation (7.10) with $c = 1$.

Regular singular points of a differential equation

To carry on our discussion, we need to introduce the concept of regular singular points. Note that a linear second-order differential equation can always be expressed by

$$
\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + P(x)\frac{\mathrm{d}y}{\mathrm{d}x} + Q(x)y = 0. \tag{7.22}
$$

Take the hypergeometric equation (7.10) as an example. We can divide $x(1-x)$ on both sides of it, and it is straightforward to see that $P(x) = \frac{c-(a+b+1)x}{x(1-x)}$ and $Q(x) = -\frac{ab}{x(1-x)}$.

Here we call $x = x_0$ an *regular point* of Eq. (7.22), if both $P(x)$ and $Q(x)$ assume finite values at $x = x_0$. But when either $P(x)$ or $Q(x)$ diverges as $x \to x_0$, we call $x = x_0$ a *singular point*. For a singular point $x = x_0$, if both $(x - x_0)P(x)$ and

$(x - x_0)^2 Q(x)$ become convergent as $x \to x_0$, then we call it a *regular singular point*. Examined with this definition, $x = 0$ and $x = 1$ are two regular singular points of hypergeometric equation (7.10).

Note that the point at infinity (in the complex plane) may also be a regular singular point of Eq. (7.22). To determine the function behaviour at infinity, one needs to let $\zeta = 1/x$ and transform Eq. (7.22) into an equation for $g(\zeta) = y(1/\zeta)$. If $\zeta = 0$ is a regular singular point of the resulting equation in ζ, then infinity is also said to be a regular singular point of Eq. (7.22). Examined with this definition, it can be verified that infinity is also a regular singular point of hypergeometric equation (7.10).

Potential applications

One reason that the hypergeometric equation is so attractive may be perceived from the following theorem.

Theorem 7.1 *Any homogeneous linear differential equation of the second order with at most three singular points (in the complex plane and infinity perhaps included), all of which are regular singular points, can be transformed into hypergeometric equation* (7.10).

The proof of the theorem, with $P(x)$ and $Q(x)$ in Eq. (7.22) now specified, provides an explicit guideline on how to evaluate a, b and c for the desired differential equation (7.10). By doing that, the so-called Riemann–Papperitz equation is introduced. Here detailed proof for Theorem 7.1 is not given, but key issues revealed by its proof are addressed as follows.

To meet the requirements on regular singular points of Eq. (7.22), it is shown (without proof) that $P(x)$ and $Q(x)$ can only be certain rational functions, generally expressed by

$$P(x) = \frac{p(x)}{(x-\xi)(x-\eta)(x-\zeta)}, \quad Q(x) = \frac{q(x)}{(x-\xi)^2(x-\eta)^2(x-\zeta)^2}, \tag{7.23}$$

where $p(x)$ and $q(x)$ are polynomials, and $x = \xi$, η and ζ are the three regular singular points. Note that if one of the regular singular point sits at infinity, P and Q are still rational functions given by

$$P(x) = \frac{p(x)}{(x-\xi)(x-\eta)}, \quad Q(x) = \frac{q(x)}{(x-\xi)^2(x-\eta)^2}, \tag{7.24}$$

where certain requirements on the degree of $p(x)$ and $q(x)$ should be imposed.

Interestingly, a vast majority of second-order linear differential equations, which play an important role in the theories of mathematical physics and probability, yield a form for P and Q as given by Eq. (7.23) or (7.24). Therefore, a unified framework in analysing practically useful second-order linear differential equations may be established by means of the hypergeometric differential equation (7.10). In the next subsection, we will see how Legendre functions act as a special case of hypergeometric functions.

7.2.3 Legendre Function and Legendre Polynomial—A Revisit

Legendre function

We now re-examine the Legendre equation under the framework of the hypergeometric equation. Legendre equation (6.21) can be rewritten by

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} - \frac{2x}{(1-x)(1+x)}\frac{\mathrm{d}y}{\mathrm{d}x} + \frac{\alpha(\alpha+1)}{(1-x)(1+x)}y = 0. \tag{7.25}$$

Examined with the definition for regular singular points in Sect. 7.2.2, $x = \pm 1$ are two regular singular points for Legendre equation (7.25), while its third regular singular point sits at infinity.

Based on Theorem 7.1, Eq. (7.25) should be transformed into a form given by hypergeometric equation (7.10). To this end, we need to map two of its regular singular points $x = \pm 1$ onto the regular singular points of Eq. (7.10), which are 0 and 1. This can be done by letting

$$t = \frac{1-x}{2}. \tag{7.26}$$

Then we introduce $h(t) = y(x) = y(1-2t)$, and thus $\frac{\mathrm{d}y}{\mathrm{d}x} = -\frac{1}{2}\frac{\mathrm{d}h}{\mathrm{d}t}$. Hence, Legendre equation (7.25) can be re-expressed in terms of t by

$$t(1-t)\frac{\mathrm{d}^2 h}{\mathrm{d}t^2} - (1-2t)\frac{\mathrm{d}h}{\mathrm{d}t} + \alpha(\alpha+1)h = 0. \tag{7.27}$$

A comparison between Eqs. (7.27) and (7.10) suggests that $a = -\alpha$, $b = \alpha + 1$, and $c = 1$. Thus, one solution to Eq. (7.27) is given by $h(t) = \mathrm{F}(-\alpha, \alpha+1; 1; t)$ with $\mathrm{F}(\cdot, \cdot; \cdot; t)$ being the Gauss hypergeometric function given by Eq. (7.5). In other words, one solution to Legendre equation (7.25) is

$$\mathrm{P}_\alpha(x) = \mathrm{F}\left(-\alpha, \alpha+1; 1; \frac{1-x}{2}\right), \tag{7.28}$$

which actually defines the Legendre function of the first kind. As for a second solution to Eq. (7.27), one may consider using the expression by Eq. (7.17). But a more formal definition of the Legendre function of the second kind is given by

$$\mathrm{Q}_\alpha(x) = \frac{\sqrt{\pi}\,\Gamma(\alpha+1)}{\Gamma\left(\alpha+\frac{3}{2}\right)(2x)^{\alpha+1}} \cdot \mathrm{F}\left(\frac{\alpha}{2}+1, \frac{\alpha}{2}+\frac{1}{2}; \alpha+\frac{3}{2}; x^{-2}\right), \tag{7.29}$$

where $\Gamma(\cdot)$ is recalled to be the Gamma function.

When Legendre functions are available through the use of Gauss hypergeometric functions, the associated Legendre functions of both kinds of degree α, as a generalisation of Eqs. (6.99) and (6.100), are defined by

$$\mathrm{P}_\alpha^m(x) = (-1)^m \left(1 - x^2\right)^{\frac{m}{2}} \frac{\mathrm{d}^m}{\mathrm{d}x^m} \mathrm{P}_\alpha(x) \tag{7.30}$$

and

$$\mathrm{Q}_\alpha^m(x) = (-1)^m \left(1 - x^2\right)^{\frac{m}{2}} \frac{\mathrm{d}^m}{\mathrm{d}x^m} \mathrm{Q}_\alpha(x), \tag{7.31}$$

respectively, where m is restricted to assume positive integer values. It can be verified that P_α^m and Q_α^m form a fundamental solution system to associated Legendre equation (6.19).

Legendre polynomial

By letting α be an integer, say, n, we should get Legendre polynomials from Eq. (7.28), i.e.

$$\mathrm{P}_n(x) = \mathrm{F}\left(-n, n+1; 1; \frac{1-x}{2}\right). \tag{7.32}$$

This naturally agrees with our observation that the series defining the Gauss hypergeometric function (7.5) terminates at degree n provided that a or b assumes integer values. Another quick conclusion is made based on the symmetry shown by F, that is, $\mathrm{P}_n(x) = \mathrm{P}_{-n-1}(x)$, which is just Eq. (6.42).

Inserting the series form of F defined by Eq. (7.5) into (7.32), we obtain

$$\begin{aligned}
\mathrm{P}_n(x) &= \sum_{k=0}^{n} \frac{(-n)_k (n+1)_k}{(k!)^2} \left(\frac{1-x}{2}\right)^k \\
&= \sum_{k=0}^{n} (-1)^k \frac{n(n-1)\cdots(n-k+1)}{k!} \cdot \frac{(n+1)\cdots(n+k)}{k!} \cdot \left(\frac{1-x}{2}\right)^k \\
&= \sum_{k=0}^{n} \left(-\frac{1}{2}\right)^k \binom{n}{k} \binom{n+k}{k} (1-x)^k,
\end{aligned} \tag{7.33}$$

where "$\binom{\cdot}{\cdot}$" denotes the binomial coefficient. One may let $n = 0, \ldots, 5$, and check the results from Eq. (7.33) with the Legendre polynomials up to degree 5, as listed by Eqs. (6.46) (see Exercise 7.5). Interestingly, Eq. (7.33) provides a unified expression for Legendre polynomials whose degrees are either even or odd numbers.

As for the Legendre function of the second kind $\mathrm{Q}_n(x)$, one lets $\alpha = 0$ in Eq. (7.29) and obtains

$$\mathrm{Q}_0(x) = \frac{1}{2} \ln\left(\frac{1+x}{1-x}\right), \tag{7.34}$$

which reproduces Eq. (6.43). But its derivation requires advanced knowledge on operating functions of complex variables. Then it can be verified that the following representation

$$\mathrm{Q}_n(x) = \mathrm{P}_n(x)\mathrm{Q}_0(x) - W_{n-1}(x) \tag{7.35}$$

with W_{n-1} a polynomial of degree $n-1$ can be a solution to the Legendre equation (6.33) of degree n. Following a similar strategy as for deriving Eqs. (7.21), we end up with an expression for $\mathrm{Q}_n(x)$ exactly the same as Eq. (6.44).

Classical orthogonal polynomial

As an extension of the present discussion, some other orthogonal polynomials, as listed in Table 6.1, can also be expressed through the use of Gauss hypergeometric functions, and they are given by

$$\mathrm{T}_n(x) = \mathrm{F}\left(-n, n; \frac{1}{2}; \frac{1-x}{2}\right); \tag{7.36a}$$

$$\mathrm{P}_n^{\alpha,\beta}(x) = \binom{n+\alpha}{n} \cdot \mathrm{F}\left(-n, \alpha+\beta+1+n; \alpha+1; \frac{1-x}{2}\right), \tag{7.36b}$$

where T_n and $\mathrm{P}_n^{\alpha,\beta}$ are recalled to be the Chebyshev polynomial of the first kind and the Jacobi polynomial, respectively. Note that the orthogonal polynomials listed by Eqs. (7.36), along with Legendre polynomials, share a common feature that their domains of definition (with reference to Table 6.1) are all of finite size, namely $x \in (-1, 1)$. This is not a coincidence, but a feature shared by all orthogonal polynomials whose differential equations of induction bear three different regular singular points including infinity (see Exercise 7.7). As for other types of classical orthogonal polynomials outlined in Table 6.1, one may refer to the concept of confluent hypergeometric functions to be discussed in the next section.

7.3 Confluent Hypergeometric Function

7.3.1 Kummer Differential Equation and Its Solutions

A *confluent hypergeometric function* is introduced as two regular singular points of the Gauss hypergeometric equation merge at infinity. For its derivation, we let the free variable of Gauss hypergeometric function (7.5) be x/b, i.e. $\mathrm{F}(a, b; c; x/b)$, which is shown to be a solution to

$$x\left(1 - \frac{x}{b}\right)\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + \left(c - \left(1 + \frac{a+1}{b}\right)x\right)\frac{\mathrm{d}y}{\mathrm{d}x} - ay = 0. \tag{7.37}$$

Naturally, $x = b$ is a regular singular point of Eq. (7.37).

Now we consider the case as $b \to \infty$. Thus, $1/b$ tends to 0 in Eq. (7.37), which becomes

$$x\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + (c - x)\frac{\mathrm{d}y}{\mathrm{d}x} - ay = 0. \tag{7.38}$$

Eq. (7.38) is known as the *Kummer differential equation*. A natural guess to a solution to Eq. (7.38) is

$$\mathrm{M}(a; c; x) = \lim_{b\to\infty} \mathrm{F}\left(a, b; c; \frac{x}{b}\right). \tag{7.39}$$

Incorporating the series form (7.5) into Eq. (7.39) gives

$$\mathrm{M}(a; c; x) = \lim_{b\to\infty} \sum_{k=0}^{\infty} \frac{(a)_k (b)_k}{(c)_k k!} \left(\frac{x}{b}\right)^k = \sum_{k=0}^{\infty} \lim_{b\to\infty} \frac{(b)_k}{b^k} \frac{(a)_k}{(c)_k k!} x^k = \sum_{k=0}^{\infty} \frac{(a)_k}{(c)_k k!} x^k, \tag{7.40}$$

provided that the value of $|x|$ does not exceed the convergent radius of series (7.40). It is not difficult to show that Eq. (7.40) is a solution to the Kummer differential equation (7.38). The function $\mathrm{M}(a; c; x)$ defined by Eq. (7.40) is called the *Kummer function*, which is also termed as the *M-function*.

Two issues are noted concerning the Kummer function. First, definition (7.40) excludes the case where c assumes non-positive integer values, the same as the situation when a Gauss hypergeometric function is defined. Second, the convergent radius of the Kummer function is found to be infinity. Thus, Eq. (7.40) is well-defined for all $x \in \mathbb{R}^+$.

A number of functions useful in the subjects of mathematical physics or probability theories find their linkage with the Kummer function. One basic example is the exponential function: $\mathrm{M}(a; a; x) = \mathrm{e}^x$, and more examples will be shown in Sect. 7.3.2.

Now we look for a solution to the Kummer differential equation taking a different form, and it appears that the expression

$$\mathrm{U}(a; c; x) = \frac{1}{\Gamma(a)} \int_0^{\infty} \mathrm{e}^{-xt} t^{a-1} (1 + t)^{c-a-1}\, \mathrm{d}t,\ x > 0 \tag{7.41}$$

serves for this purpose, where $\Gamma(\cdot)$ is recalled to be the Gamma function. The function $\mathrm{U}(a; c; x)$ defined by Eq. (7.41) is called the *U-function*.

7.3.2 Special Cases

Our main goal here is to provide a brief overlook at useful functions in the study of mathematical physics or probability theories, which are special cases of the Kummer function. For developing a comprehensive understanding of the functions listed below, more advanced materials are suggested (e.g. [11]). Note that as the features

of the Kummer function should be fully examined with complex argument inputs, we change their input argument from x to z in the rest of the discussion.

Bessel functions—a revisit

In general, Bessel functions arise when the parameters of Eq. (7.38) satisfy $c = 2a$. Specifically, Bessel function of the first kind is linked with the Kummer function by

$$\mathrm{J}_\alpha = \frac{(z/2)^\alpha \mathrm{e}^{\mathrm{i}z}}{\Gamma(\alpha+1)} \mathrm{M}\left(\alpha + \frac{1}{2}; 2\alpha + 1; 2\mathrm{i}z\right), \tag{7.42}$$

where $\Gamma(\cdot)$ is recalled to be the Gamma function, and i is the imaginary unit.

For the modified Bessel functions of the second kind given by Eq. (5.91) in Sect. 5.4.2, we have

$$\mathrm{K}_\alpha = \sqrt{\pi}\mathrm{e}^{-z}(2z)^\alpha \mathrm{U}\left(\alpha + \frac{1}{2}; 2\alpha + 1; 2z\right). \tag{7.43}$$

Orthogonal polynomials on unbounded domain

Inherited from the Gauss hypergeometric function, the Kummer function of Eq. (7.40) becomes a polynomial, provided that a assumes non-positive integer values. We have the following representation that

$$\mathrm{L}_n^\alpha = \binom{n+\alpha}{n} \mathrm{M}(-n; \alpha + 1; z), \ n \in \mathbb{Z}^+ \cup \{0\}, \tag{7.44}$$

which is the Laguerre polynomial listed in Table 6.1.

Error functions

The *error functions* are defined by

$$\operatorname{erf} z = \frac{2}{\sqrt{\pi}} \int_0^z \mathrm{e}^{-t^2}\,\mathrm{d}t, \quad \operatorname{erfc} z = 1 - \operatorname{erf} z = \frac{2}{\sqrt{\pi}} \int_z^\infty \mathrm{e}^{-t^2}\,\mathrm{d}t. \tag{7.45}$$

The error function is of great importance in probability theories. Its connection with the Kummer function is formulated by

$$\operatorname{erf} z = \frac{2z}{\sqrt{\pi}} \mathrm{M}\left(\frac{1}{2}; \frac{3}{2}; -z^2\right). \tag{7.46}$$

Coulomb wave functions

Coulomb wave functions are of great importance in physics, especially in quantum mechanics. They are solutions to a differential equation of

$$\frac{\mathrm{d}^2 y}{\mathrm{d}z^2} + \left(1 - \frac{2\eta}{z} - \frac{\lambda(\lambda+1)}{z^2}\right) y = 0, \tag{7.47}$$

where λ and η are parameters, and the input argument z is usually employed to measure the distance to an atomic nucleus.

A pair of Coulomb wave functions, which solve Eq. (7.47), is conventionally denoted by $\mathrm{F}_\lambda(\eta; z)$ and $\mathrm{G}_\lambda(\eta; z)$. They are related to the Kummer function by

$$\mathrm{F}_\lambda(\eta; z) = A\mathrm{M}(\lambda + 1 - \mathrm{i}\eta; 2\lambda + 2; 2\mathrm{i}z) \tag{7.48a}$$

$$\mathrm{G}_\lambda(\eta; z) = \mathrm{i}\mathrm{F}_\lambda(\eta; z) + \mathrm{i}B\mathrm{U}(\lambda + 1 - \mathrm{i}\eta; 2\lambda + 2; 2\mathrm{i}z), \tag{7.48b}$$

where A and B are certain complex numbers depending on λ and η.

A number of other useful special functions, such as the Whittaker functions, the parabolic cylinder functions, the exponential integrals and the Fresnel integrals, can all find their linkage with the Kummer function, and one may refer to other materials for further studies (e.g. [11]).

7.4 Final Remarks on Hypergeometric Functions

In this chapter, a rather elementary introduction to hypergeometric functions and their related functions is presented, and our aim is to provide with preliminary knowledge underpinning further studies over the topic with more advanced materials. We conclude the chapter with several remarks as follows.

1. Hypergeometric functions and their related functions provide a unified framework under which a huge number of (special) functions arising in the subjects of mathematical physics and probability theories can be effectively analysed.
2. Hypergeometric functions and their related functions are generated from differential equations taking a relatively simple form with the coefficients no more complicated than rational functions (of degree 2). But they form a vast functional pool that seems far richer than that consisting of only elementary functions.
3. The concept of hypergeometric function can be further extended to enlarge its coverage over mathematical functions. For instance, one may introduce the *generalised hypergeometric function* as

$$_p\mathrm{F}_q(a_1, \ldots, a_p; b_1, \ldots b_q; z) = \sum_{k=0}^{\infty} \frac{(a_1)_k \cdots (a_p)_k}{(b_1)_k \cdots (b_q)_k k!} z^k, \tag{7.49}$$

where the first subindex p measures the number of parameters appearing in the numerators of the series coefficients, and the second subindex q measures the number of parameters appearing in the denominators of the series coefficients. To ensure that the series is convergent for some z, we require $p \leq q + 1$; when $p = q + 1$, the convergent domain is $|z| < 1$. When $p < q + 1$, the convergent domain becomes $|z| < \infty$. As its two special cases, the Gauss hypergeometric

function (7.5) is given by $\mathrm{F}(a, b; c; z) =_2 \mathrm{F}_1$, and the Kummer function (7.40) is given by $\mathrm{M}(a; c; z) =_1 \mathrm{F}_1$.

Exercise

1. Show that the convergent radius of the series given by Eq. (7.5) equals 1.
2. Verify the identities given by Eq. (7.9).
3. Verify that $y_2 = x^{1-c}\mathrm{F}(a - c + 1, b - c + 1; 2 - c; x)$ satisfies Eq. (7.12).
4. Show that a regular singular point of Legendre equation (7.25) sits at infinity.
   (a) For ODE (7.22), introduce $\zeta = \frac{1}{x}$ and $g(\zeta) = y(x) = y(1/\zeta)$. Then show that Eq. (7.22) is transformed into
   $$\frac{\mathrm{d}^2 g}{\mathrm{d}\zeta^2} + \left(\frac{2}{\zeta} - \frac{P(1/\zeta)}{\zeta^2}\right)\frac{\mathrm{d}g}{\mathrm{d}\zeta} + \frac{Q(1/\zeta)}{\zeta^4} g = 0.$$
   (b) Rewrite Legendre equation (7.25) in terms of ζ.
   (c) Verify that $\zeta = 0$ is a regular singular point of the resulting differential equation for $g(\zeta)$.
5. Let $n = 0, \ldots, 5$, and compare the results with the Legendre polynomials up to degree 5, as listed in Eq. (6.46).
6. Derive the expression for $\mathrm{Q}_n(x)$, which is given by Eq. (7.35).
7. Explore the differential equations inducing the orthogonal polynomials given by Eqs. (7.36).
   (a) Write down the corresponding hypergeometric differential equations they satisfy.
   (b) Show that the singular points (including infinity) of resulting differential equations are all regular singular points.
8. Verify that $\mathrm{F}(a, b; c; x/b)$ solves Eq. (7.37), provided that $\mathrm{F}(a, b; c; x)$ is a Gauss hypergeometric function satisfying Eq. (7.10).

Bibliography

1. M. Abramowitz, I.A. Stegun, *Handbook of Mathematical Functions* (Dover Publications Inc., New York, 1965)
2. B.B. Baker, E.T. Copson, *The Mathematical Theory of Huygens' Principle* (American Mathematical Society, UK, 2003)
3. R.W. Balluffi, S. Allen, W.C. Carter, *Kinetics of Materials* (Wiley, Hoboken, 2005)
4. A.V. Bitsadze, *Equations of the Mixed Type* (Pergammon, New York, 1964)
5. Y.A. Cengel, J.M. Cimbala, *Fluid Mechanics—Fundamentals and Applications*, 3rd edn. (McGraw-Hill Education, New York, 2013)
6. R. Erban, S.J. Chapman, *Stochastic Modelling of Reaction-Diffusion Processes* (Cambridge University Press, Cambridge, 2020)
7. L.C. Evans, *Partial Differential Equations*, 2nd edn. (American Mathematical Society, USA, 2010)
8. T.T. Li, T.H. Qin, *Physics and Partial Differential Equations—I* (High Education Press of China, Beijing, 2013)
9. J.R. Ockendon, S.D. Howison, A.A. Lacey, A.B. Movchan, *Applied Partial Differential Equations*, 2nd edn. (Oxford University Press, New York, 2003)
10. D. Shanks, *Solved and Unsolved Problems in Number Theory*, 4th edn. (Chelsea Pub Co., 1993)
11. N.M. Temme, *Special Functions: An Introduction to the Classical Functions of Mathematical Physics* (Wiley, New York, 1996)
12. A.N. Tikhonov, A.A. Samarskii, *Equation of Mathematical Physics* (Dover Publications Inc., New York, 1990)
13. S.P. Timoshenko, J.N. Goodier, *Theory of Elasticity*, 3rd edn. (McGraw Hill, India, 2010)
14. G.S. Was, *Fundamentals of Radiation Materials Science*, 2nd edn. (Springer, New York, 2017)
15. O.C. Zienkiewicz, R.L. Taylor, *The Finite Element for Solids and Structural Mechanics*, 7th edn. (Elsevier, Butterworth-Heinemann, 2013)
16. O.C. Zienkiewicz, R.L. Taylor, P. Nithiarasu, *The Finite Element Method for Fluid Dynamics*, 7th edn. (Elsevier, Butterworth-Heinemann, 2013)
17. O.C. Zienkiewicz, R.L. Taylor, J.Z. Zhu, *The Finite Element Method: Its Basis and Fundamentals*, 6th edn. (Elsvier, Butterworth-Heinemann, 2005)

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Y. Zhu, *Equations and Analytical Tools in Mathematical Physics*,
https://doi.org/10.1007/978-981-16-5441-1

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Y. Zhu, *Equations and Analytical Tools in Mathematical Physics*,
https://doi.org/10.1007/978-981-16-5441-1

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