Morten Willatzen,
Lok C. Lew Yan Voon

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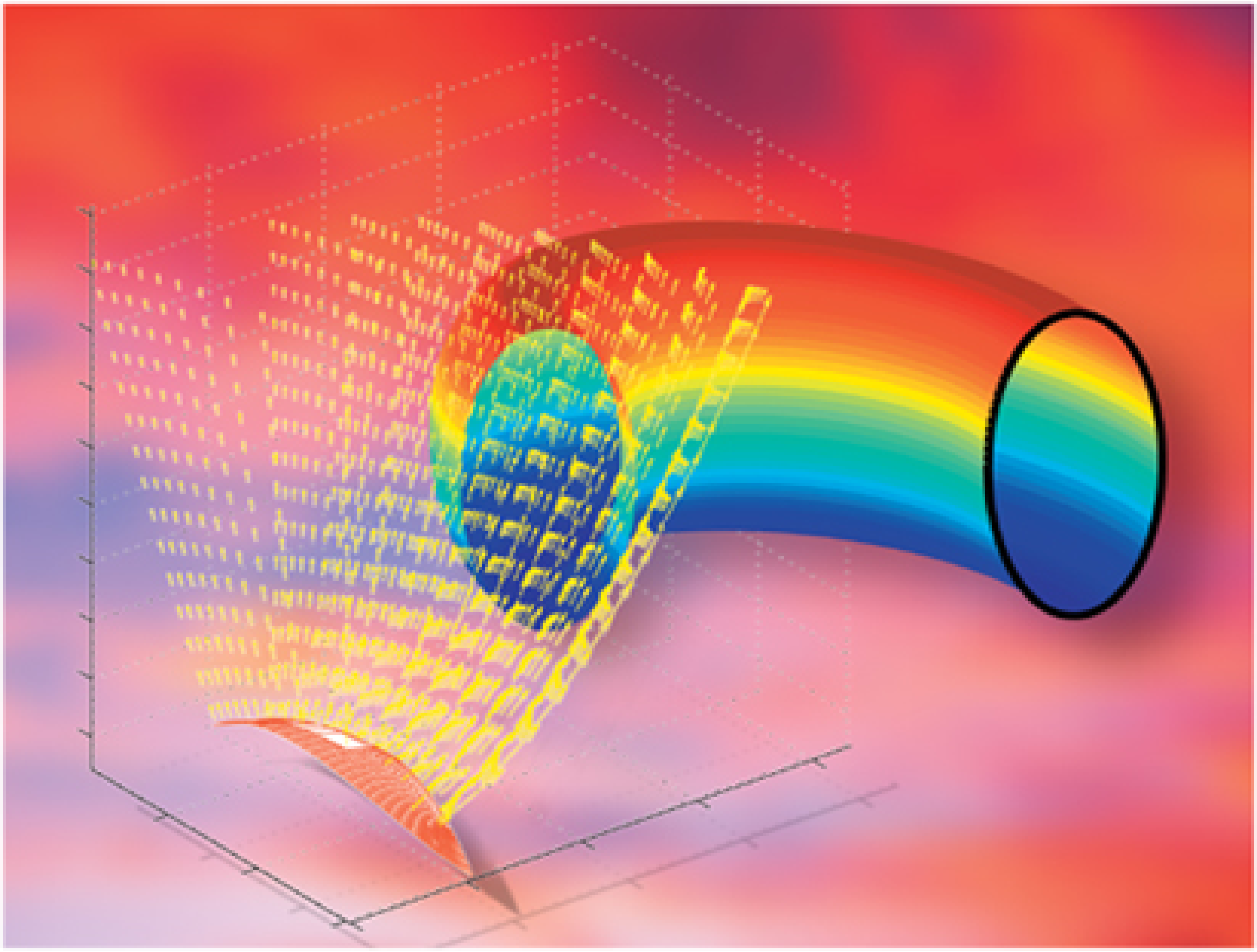
Separable Boundary-Value Problems in Physics



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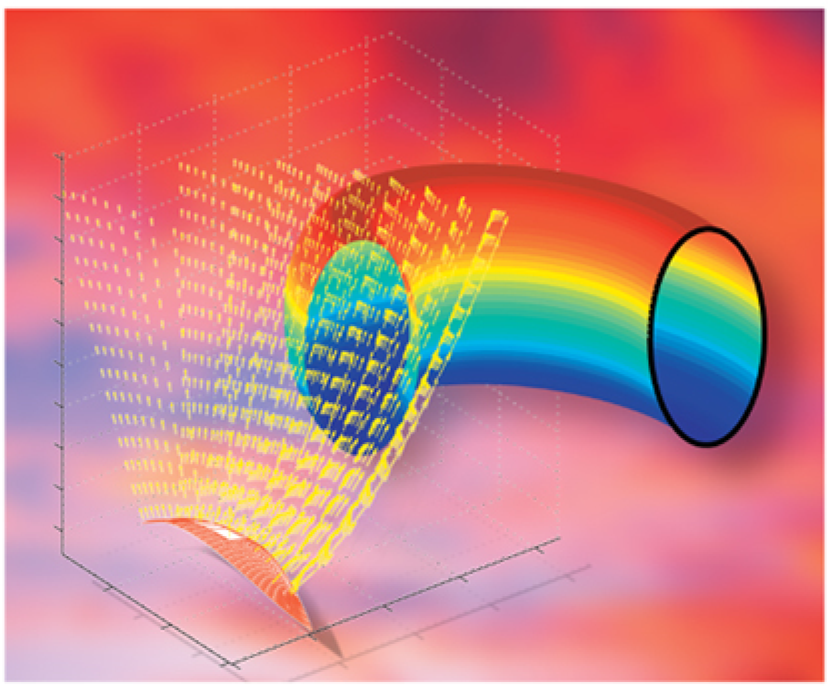

Contents

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Part Three: Three-Dimensional Coordinate Systems

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Preface

We became interested in the research that has has led to this book in 2000, when the two of us met at the ferry terminal in Tsim Tsai Tsui, Hong Kong, and discussed the problem of separability of partial differential equations. This was followed by a research visit by L.C.L.Y.V. to the Mads Clausen Institute at Syddansk Universitet in 2003, a visit funded by the Balslev Foundation. It is only fitting that L.C.L.Y.V. was invited back to the Mathematical Modeling Group of the Mads Clausen Institute on the beautiful new campus of Syddansk Universitet at Alsion to finish work on the book.

Our interaction during that time has led to numerous publications, including a few on the topic of this book and another book on the electronic properties of semiconductors. Whereas our earlier work followed the exposition of Morse and Feshbach and that of Moon and Spencer closely, we have since incorporated a more general differential-geometric approach. Both approaches are featured in this book. As mathematical physicists, it was a pleasure to put together a book that blends together knowledge in mathematics and physics going back 100 years.

The research and book writing has received generous financial support over the years. The work of M.W. has been supported by Syddansk Universitet and Sønderborg Kommune. The work of L.C.L.Y.V. has been funded by the National Science Foundation (USA), the Balslev Foundation, and Sønderborg Kommune. L.C.L.Y.V. would also like to thank the College of Science and Mathematics at Wright State University for release from duties to write this book and the hospitality of the Mads Clausen Institute at Syddansk Universitet, where most of the writing took place. Two individuals have contributed to some parts of this work. First, Prof. Jens Gravesen was an indispensable collaborator

in our work on the differential-geometric formulation and this is obvious from his coauthorship of many of our joint papers in this area. Second, we would like to thank Lars Duggen for his help in making some of the figures in the book.

Of course, none of this would have been possible without the encouragement and support of our families. Finally, we would like to thank our editors at Wiley-VCH for their wonderful job, not only with the nice product, but also with their professionalism in keeping us on track.

October 2010

Morten Willatzen
Lok C. Yan Voon

Part One

Preliminaries

Chapter 1

Introduction

This is a textbook about how to solve boundary-value problems in physics using the method of separation of variables which goes beyond the few simple coordinate systems presented in most textbook discussions. Our goal is to present an application-oriented approach to the study of the general theory of the method of separation of variables, whereby the variety of separable orthogonal coordinate systems is included to illustrate various aspects of the theory (e.g., lesser known coordinate systems, the coupling of separation constants, and solving for the boundary-value problem particularly for many-parameter surfaces) and also to discuss the variety of special functions that can result (e.g., from transcendental to Lamé functions). We will add, right upfront, that this is not a text about special functions, though sufficient results about the latter are included to make the text as self-contained as possible.

In numerous areas of science and engineering, one has to solve a partial differential equation (PDE) for some fairly regular shape. Examples include Newtonian gravity for an ellipsoidal meteorite [1], the temperature distribution over a paraboloidal aircraft cone [2], the electric field in the vicinity of the brain modeled as an ellipsoid [3], and the electronic structure of spherical quantum dots [4]. A very powerful method is the method of separation of variables, whereby the PDE is separated into ordinary differential equations (ODEs). The latter then need to be solved, often in the form of power series, leading to special functions such as the Legendre functions and the Baer functions, and, finally, boundary conditions are applied. Even when the shape deviates from the ideal regular shape, a preliminary investigation using the regular shape is often useful both as a validation technique for some other, more numerical approach and as a first step in a, for example, perturbative approach to the exact solution. Indeed, according to Morse and Feshbach [5], the method of separation of variables is only one of two generally practical methods of solution, the other being the integral solution. Furthermore, practically all mathematical physics texts discuss the method heuristically applied to one or more of the following coordinate systems: rectangular, circular cylindrical, and spherical polar. Nevertheless, the restriction to a few coordinate systems hides a number of features of the method as well as, of course, its range of applicability. Discussion of more advanced features of the method has been reserved to a few texts [5–9]. Thus, the separability of the Helmholtz equation in 11 orthogonal coordinate systems is not generally known in spite of the utility of many of these coordinate systems for applications. Even the formal definition of "separation of variables" is rarely given. It has been argued that such a definition is needed before general results can be demonstrated [10, 11].

In this book, the problem of separating the Laplacian in various orthogonal coordinate systems in Euclidean 3-space is presented and the resulting ODEs for a number of PDEs of physical interest are given. Explicit solutions in terms of special functions are then described. Various physical problems are discussed in detail, including in acoustics, in heat conduction, in electrostatics, and in quantum mechanics, as the corresponding PDEs represent three general forms to which many other differential equations reduce (Laplace, Helmholtz, and Schrödinger). Furthermore, they represent two classes of differential equations (elliptic and hyperbolic) and different types of boundary conditions.

A unique feature of our book is the part devoted to the differential geometric formulation of PDEs and their solutions for various kinds of confined geometries and boundary conditions. Such a treatment, though not entirely new, has recently been extended by a few authors, including us, and has mostly only appeared in the research literature.

There are obviously many applications of the method of separation of variables, particularly for the common rectangular, circular cylindrical, and spherical polar coordinate systems. The general theory has also been worked out and discussed in the mathematical physics literature. Our treatment follows closely the books by Morse and Feshbach [5] and Moon and Spencer [6] in covering more than just the standard coordinate systems. The former gives an exposition of the method as applied to the Laplace, Helmholtz, and Schrödinger equations, whereas the latter lists the coordinate systems, resulting ODEs, and series solutions in a very compact and formal form, leading occasionally to less practical solutions (see, e.g., the “corrections” in [12]). We extend their treatments by giving many examples of boundary-value problems and include some more recent results mostly in the field of nanotechnology. Our book is not a comprehensive review of all the special-function literature, nor is the formal mathematical theory presented. The former is done in the many books on special functions, whereas the latter is presented in a nice book by Miller [8]. It is also worthwhile pointing out that the method of separation of variables has been applied to other PDEs such as the Dirac equation and the Klein–Gordon equation. One of the foci of the book is to emphasize that there are three distinct separability problems: that of the differential equations, that of the separation constants, and that of the boundary conditions. The separability of the differential equations is addressed by presenting the results in 11 coordinate systems (even though there can be separability in additional coordinate systems for special cases such as the Laplace equation).

The consequence of a varying degree of separability of the separation constants is made clear in connection with the boundary-value problem; this is an aspect that is missing in Moon and Spencer's treatment. Finally, the separability of the boundary conditions relates to the choice of the coordinate system. Last but not least, we present a variety of computational algorithms for the more difficult boundary-value problems that should be of practical help to readers for a complete solution to such problems. In this respect, we show the limited practical value of the series solutions in the book by Moon and Spencer and the usefulness but also restricted applicability of the algorithms given by Zhang and Jin [13]. This aspect is also not covered in the book by Morse and Feshbach.

The book is divided into four parts. The first part deals with the general theory of the method of separation of variables and also has a brief summary of the areas of physical applications discussed in the book. Part Two presents the technique in two dimensions. The solutions of the resulting ODEs are discussed in some detail, particularly when a special function appears for the first time. Part Three considers the three-dimensional coordinate systems, which include the simple three-dimensional extension of the two-dimensional systems of Part Two (rectangular and cylindrical systems) and of systems with rotational symmetry, and also the lesser known conical, ellipsoidal, and paraboloidal systems. Part Four provides an alternative formulation of the method of separation of variables in terms of differential geometry. Illustrations are provided for problems with nanowire structures and a recent perturbative theory is discussed in detail. Finally, a few key results on special functions are included in the appendices. Functions that appear directly as solutions to the separated ODEs are described in separate appendices (except for Appendix I on elliptic functions) and other useful functions which show up occasionally are collected in Appendix A on the hypergeometric function.

In summary, it is intended that this book not only contains the standard introductory topics to the study of separation of variables but will also provide a bridge to the more advanced research literature and monographs on the subject. The fundamental material presented and a few of the coordinate systems can serve as a textbook for a one-semester course on PDEs either at the senior undergraduate level or at the graduate level. It is also expected to complement the many books that have already been published on boundary-value problems and special functions (e.g., [5-9, 14-19]), particularly in the treatment of the Helmholtz problem. The chapters not covered in a course would be appropriate for self-study and even serve as sources of ideas for both undergraduate- and graduate-level research projects.

Chapter 2

General Theory

2.1 Introduction

It is widely believed that the first systematic study of the conditions required for a partial differential equation (PDE) to be separable was carried out by Stäckel [20] for the nonlinear Hamilton–Jacobi equation. This procedure was applied by Robertson to the time-independent Schrödinger equation [21], leading to the so-called Stäckel–Robertson separability conditions. Eisenhart subsequently showed that the Schrödinger equation is separable in exactly 11 curvilinear orthogonal coordinate systems, all derived from confocal quadrics [22–24].

In this chapter, we will summarize the types of PDEs to be discussed together with some possible physical applications of the said equations. We will also present key results on curvilinear differential operators and the general separability conditions in Euclidean 2- and 3-spaces, as well as the Frobenius method for series solutions.

2.2 Canonical Partial Differential Equations

We will look at the mathematical solutions to three types of canonical PDEs:

(2.1) $\nabla^2 \psi = 0$ (Laplace equation) ,

(2.2) $\nabla^2 \psi + k^2 \psi = 0$ (Helmholtz equation) ,

(2.3) $\nabla^2 \psi + k^2(r)\psi = 0$ (Schrödinger equation) ,

where ∇^2 is the Laplacian operator, ψ is a scalar field (we will only rarely mention other types of field such as vector fields), and k^2 is either a constant or a function of the spatial coordinates. The Laplace equation arises in potential-field problems such as electrostatics and Newtonian gravitation. The Helmholtz equation arises as the time-independent part of the wave equation,

$$\nabla^2 \Psi(r,t) - \frac{1}{c^2}\frac{\partial^2 \Psi(r,t)}{\partial t^2} = 0 ,$$

and the diffusion equation,

$$\nabla^2 \Psi(r,t) - \frac{1}{K}\frac{\partial \Psi(r,t)}{\partial t} = 0 .$$

The Schrödinger equation is similar to the Helmholtz equation except for the generalization of the wave number *k* to be position dependent. As given, it is the time-independent version of the time-dependent Schrödinger equation,

$$-\frac{\hbar^2}{2m}\nabla^2 \Psi(r,t) + V(r)\Psi(r,t) = i\hbar\frac{\partial \Psi(r,t)}{\partial t} .$$

This, of course, does not include all of the physical theories. For example, first-order differential equations such as the Dirac equation and higher-order equations such as for the mechanics of beam bending will not be discussed to keep this book manageable and focused.

2.3 Differential Operators in Curvilinear Coordinates

Specific forms of the differential operators will be used in the respective chapters on the various coordinate systems.

Here we provide a summary of the main expressions needed, with emphasis on orthogonal systems, as general expressions can be written down in terms of a metric. Derivations of the results below can be found in any standard mathematical physics or vector calculus textbook.

2.3.1 Metric

Given two coordinate systems, one can write the line element in both systems as

(2.4) $$\mathrm{d}s^2 = \sum_i \mathrm{d}x_i^2 = \sum_{ij} g_{ij}\,\mathrm{d}q_i\,\mathrm{d}q_j \ ,$$

where x_i(i = 1, 2, 3) represents the Cartesian set and the q_i are known as curvilinear coordinates. Then

(2.5) $$g_{ij} = h_{ij}^2 = \frac{\partial x}{\partial q_i}\frac{\partial x}{\partial q_j} + \frac{\partial y}{\partial q_i}\frac{\partial y}{\partial q_j} + \frac{\partial z}{\partial q_i}\frac{\partial z}{\partial q_j} \ .$$

g is known as the metric and, since we are only dealing with Euclidean space in this book, no distinction is made between covariant and contravariant indices (an exception will be in the differential-geometric formulation). For orthogonal systems,

(2.6) $$g_{ij} = h_{ij}^2 = 0 \text{ for } i \neq j \ ,$$

and we write h_{ii} = h_i. The latter is also known as a scale factor.

2.3.2 Gradient

The gradient of a scalar field is given by

(2.7) $$\nabla\psi\,(q_i) = e_1\frac{1}{h_1}\frac{\partial\psi}{\partial q_1} + e_2\frac{1}{h_2}\frac{\partial\psi}{\partial q_2} + e_3\frac{1}{h_3}\frac{\partial\psi}{\partial q_3} \ ,$$

where the e_i are the unit vectors of the curvilinear coordinates,

(2.8) $$e_i = \frac{1}{h_i}\frac{\partial r}{\partial q_i} \ .$$

It is often convenient to express the latter in terms of Cartesian unit vectors since the latter are constant vectors. In this case, one can write

(2.9) $$e_i = \frac{1}{h_i}\left(\frac{\partial x}{\partial q_i}e_x + \frac{\partial y}{\partial q_i}e_y + \frac{\partial z}{\partial q_i}e_z\right) .$$

2.3.3 Divergence

The divergence of a vector field $V(q_i)$ is

(2.10) $$\nabla \cdot V(q_i) = \frac{1}{h_1h_2h_3}\left[\frac{\partial}{\partial q_1}(V_1h_2h_3) + \frac{\partial}{\partial q_2}(V_2h_3h_1) + \frac{\partial}{\partial q_3}(V_3h_1h_2)\right] .$$

2.3.4 Circulation

The circulation of a vector field V is

(2.11) $$\nabla \times V = \frac{1}{h_1h_2h_3}\begin{vmatrix} e_1h_1 & e_2h_2 & e_3h_3 \\ \frac{\partial}{\partial q_1} & \frac{\partial}{\partial q_2} & \frac{\partial}{\partial q_3} \\ h_1V_1 & h_2V_2 & h_3V_3 \end{vmatrix} .$$

2.3.5 Laplacian

The Laplacian of a scalar field is obtained by combining Eqs. (2.7) and (2.10):

(2.12) $$\nabla^2\psi = \frac{1}{h_1h_2h_3}\left[\frac{\partial}{\partial q_1}\left(\frac{h_2h_3}{h_1}\frac{\partial \psi}{\partial q_1}\right) + \frac{\partial}{\partial q_2}\left(\frac{h_3h_1}{h_2}\frac{\partial \psi}{\partial q_2}\right) + \frac{\partial}{\partial q_3}\left(\frac{h_1h_2}{h_3}\frac{\partial \psi}{\partial q_3}\right)\right] .$$

2.3.5.1 Example

As an example, consider the circular cylindrical coordinate system with the following coordinates:

$$q_1 = r , \quad q_2 = \phi , \quad q_3 = z ,$$

and the relationship to the Cartesian coordinates

$$x = r\cos\phi , \quad y = r\sin\phi , \quad z = z .$$