METHODS OF MODERN MATHEMATICAL PHYSICS

IV
Analysis of Operators

现代数学物理方法

第4卷

Michael Reed / Barry Simon

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IV: ANALYSIS OF OPERATORS

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IV: ANALYSIS OF OPERATORS

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To David

To Rivka and Benny

Preface

. . . of making books there is no end, and much study is a weariness of the flesh
Koheleth (Ecclesiastes) 12:12

With the publication of Volumes III and IV we have completed our presentation of the material which we originally planned as "Volume II" at the time of publication of Volume I. We originally promised the publisher that the entire series would be completed nine months after we submitted Volume I. Well! We have listed the contents of future volumes below. We are not foolhardy enough to make any predictions.

We were very fortunate to have had T. Kato and R. Lavine read and criticize Chapters XII and XIII, respectively. In addition, we received valuable comments from J. Avron, P. Deift, H. Epstein, J. Ginibre, I. Herbst, and E. Trubowitz. We are grateful to these individuals and others whose comments made this book better.

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Introduction

Il libro della natura è scritto in lingua matematica. *Galileo Galilei*

The first step in the mathematical elucidation of a physical theory must be the solution of the existence problem for the basic dynamical and kinematical equations of the theory. Once that is accomplished, one would like to find general qualitative features of these solutions and also to study in detail specific special systems of physical interest.

Having discussed the general question of the existence of dynamics in Chapter X, we present methods for the study of general qualitative features of solutions in this volume and its companion (Volume III) on scattering theory. We concentrate on the Hamiltonians of nonrelativistic quantum mechanics although other systems are also treated. In Volume III, the main theme is the long-time behavior of dynamics, especially of solutions which are "asymptotically free." In this volume, the main theme involves the five kinds of spectra defined in Sections VII.2 and VII.3: the essential spectrum, σ_{ess}; the discrete spectrum, σ_{disc}; the absolutely continuous spectrum, σ_{ac}; the pure point spectrum, σ_{pp}; and the singular continuous spectrum, σ_{sing}. It turns out that the study of the absolutely continuous spectrum as well as the problem of showing that the continuous singular spectrum is empty are intimately connected with scattering theory. Thus, the separation of the material in Volumes III and IV is somewhat artificial. For this reason, we preprinted in Volume III three sections from Volume IV.

These are not the only sections in which the themes of the two volumes overlap.

In these volumes specific systems are usually presented to illustrate the application of general mathematical methods, but the detailed analysis of the specific systems is not carried very far. Mathematical physicists have to some extent neglected the detailed study of specific systems; we believe that this neglect is unfortunate, for there are many interesting unsolved problems in specific systems, even in the purely Coulombic model of atomic physics. For example, it has not been shown that H^{--} has no bound states even though the analogous classical system of one positive and three negative charges has the property that its energy is lowered by moving a suitable electron to infinity. And it is not known rigorously that the energy needed to remove the first electron from an atom is less than the energy needed to remove the second, even though this is "physically obvious." We hope that by collecting the general mathematical methods in Volumes II, III, and IV, we have made the analysis of specific systems easier and more attractive.

Nonrelativistic quantum mechanics is often viewed by physicists as an area whose qualitative structure, especially on the level treated here, is completely known. It is for this reason that a substantial fraction of the theoretical physics community would regard these volumes as exercises in pure mathematics. On the contrary, it seems to us that much of this material is an integral part of modern quantum theory. To take a specific example, consider the question of showing the absence of the singular continuous spectrum and the question of proving asymptotic completeness for the purely Coulombic model of atomic physics. The former problem was solved affirmatively by Balslev and Combes in 1970, the latter is still open. Many physicists would approach these questions with Goldberger's method: "The proof is by the method of reductio ad absurdum. Suppose asymptotic completeness is false. Why that's absurd! Q.E.D." Put more precisely: If asymptotic completeness is not valid, would we not have discovered this by observing some bizarre phenomena in atomic or molecular physics? Since physics is primarily an experimental science, this attitude should not be dismissed out of hand and, in fact, we agree that it is extremely unlikely that asymptotic completeness fails in atomic systems. But, in our opinion, theoretical physics should be a science and not an art and, furthermore, one does not fully understand a physical fact until one can derive it from first principles. Moreover, the solution of such mathematical problems can introduce new methods of calculational interest (for example, Faddeev's treatment of completeness in three-body systems and the application of his ideas in nuclear physics) and can provide important elements of clarity (for example, the physical artificiality of "adiabatic switching" in nonrigorous scattering theory and the clarifying work of Cook, Jauch, and Kato).

The general remarks about notes and problems in earlier introductions are applicable here with one addition: the bulk of the material presented in this volume is from advanced research literature, so many of the "problems" are quite substantial. Some of the starred problems summarize the contents of research papers!

Contents of Other Volumes

Volume I: Functional Analysis

Volume II: Fourier Analysis, Self-Adjointness

Volume III: Scattering Theory

Contents of Future Volumes: *Convex Sets and Functions, Commutative Banach Algebras, Introduction to Group Representations, Operator Algebras, Applications of Operator Algebras to Quantum Field Theory and Statistical Mechanics, Probabilistic Methods.*

Contents

XII: Perturbation of Point Spectra

In the thirties, under the demoralizing influence of quantum-theoretic perturbation theory, the mathematics required of a theoretical physicist was reduced to a rudimentary knowledge of the Latin and Greek alphabets. — *Res Jost*

In this chapter we shall examine the following general situation: An operator H_0 has an eigenvalue E_0, which we usually assume is in the discrete spectrum. Suppose that H_0 is perturbed a little; that is, consider $H_0 + \beta V$ where V is some other operator and $|\beta|$ is small. What eigenvalues of $H_0 + \beta V$ lie near E_0 and how are they related to V? What are their properties as functions of β? Such a situation is familiar in quantum mechanics where there are *formal* series for the perturbed eigenvalues. These **Rayleigh–Schrödinger series** are not special to quantum-mechanical operators but exist for many perturbations of the form $H_0 + \beta V$. The heart of this chapter is the second section where we shall discuss the beautiful Kato–Rellich theory of regular perturbations; this theory gives simple criteria under which one can prove that these formal series have a nonzero radius of convergence. We then discuss what the perturbation series means in cases where it is divergent or not directly related to eigenvalues.

XII.1 Finite-dimensional perturbation theory

We first discuss finite-dimensional matrices. Not only will this allow us to present explicit formulas in the simplest case, but we shall eventually treat degenerate perturbation theory by reducing it to an essentially finite-dimensional problem. Furthermore, an important difficulty already occurs in the finite-dimensional case, namely proving analyticity in β when there is a degenerate eigenvalue. Recall that E_0 is called a **degenerate eigenvalue** when the characteristic equation for H_0, $\det(H_0 - \lambda) = 0$, has a multiple root at $\lambda = E_0$. In an appendix to this section we review the theory of matrices with degenerate eigenvalues and, in particular, we discuss the Jordan normal form.

First consider the elementary example

$$T(\beta) = \begin{bmatrix} 1 & \beta \\ \beta & -1 \end{bmatrix}$$

By our definition of operator-valued analytic function in Section VI.3, $T(\beta)$ is a matrix-valued analytic function. To find its eigenvalues, we need only solve $\det(T(\beta) - \lambda) = 0$ (the **secular** or **characteristic equation**). Thus

$$\lambda_\pm(\beta) = \pm\sqrt{\beta^2 + 1}$$

are the eigenvalues. This problem has several characteristic features:

(i) Even though $T(\beta)$ is entire in β, the eigenvalues are not entire but have singularities as functions of β.

(ii) The singularities are not on the real β axis where $T(\beta)$ is self-adjoint but occur at nonreal β, namely at $\beta = \pm i$. Thus, while there are no singularities at "physical" values, the **perturbation series**, i.e., the Taylor series for $\lambda_\pm(\beta)$ at $\beta = 0$, have a finite radius of convergence due to complex singularities.

(iii) "Level crossing" takes place at the singular values of β; that is, at $\beta = \pm i$ there are fewer distinct eigenvalues, namely one, than at other points, where there are two.

(iv) At the singular values of β the matrix $T(\beta)$ is *not* diagonalizable. Explicitly

$$T(i)\begin{bmatrix} 2 \\ 2i \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \qquad T(i)\begin{bmatrix} 1 \\ -i \end{bmatrix} = \begin{bmatrix} 2 \\ 2i \end{bmatrix}$$

so the matrix of $T(i)$ in the basis $\langle 2, 2i\rangle$, $\langle 1, -i\rangle$, is

$$\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

While this "Jordan anomaly" is typical, we leave a discussion of it to the Notes; see also Problem 23.

(v) The analytic continuation of an eigenvalue is an eigenvalue.

For the remainder of this section, we shall suppose that $T(\beta)$ is a matrix-valued analytic function in a connected region R of the complex plane. Notice that we do not require $T(\beta)$ to be linear in β. Later, we shall be able to reduce the infinite-dimensional, linear, finitely degenerate perturbation problem to a finite-dimensional problem, but one that is no longer *linear* in β. Thus, greater generality at this point will be crucial.

To find the eigenvalues of $T(\beta)$ we must solve a secular equation

$$\det(T(\beta) - \lambda) = (-1)^n[\lambda^n + a_1(\beta)\lambda^{n-1} + \cdots + a_n(\beta)] = 0$$

The basic theorem about such functions is:

Theorem XII.1 Let $F(\beta, \lambda) = \lambda^n + a_1(\beta)\lambda^{n-1} + \cdots + a_n(\beta)$ be a polynomial of degree n in λ whose leading coefficient is one and whose coefficients are all analytic functions of β. Suppose that $\lambda = \lambda_0$ is a simple root of $F(\beta_0, \lambda)$. Then for β near β_0, there is exactly one root $\lambda(\beta)$ of $F(\beta, \lambda)$ near λ_0, and $\lambda(\beta)$ is analytic in β near $\beta = \beta_0$.

Proof This is a special case of the implicit function theorem. Since $F(\beta, \lambda)$ is analytic near β_0 and λ_0, we can write $F(\beta, \lambda) = \sum_{m=0}^{n} (\lambda - \lambda_0)^m f_m(\beta)$ with $f_0(\beta_0) \equiv F(\beta_0, \lambda_0) = 0$, and $f_1(\beta_0) \equiv (\partial F/\partial\lambda)(\beta_0, \lambda_0) \neq 0$ since λ_0 is a simple root. Thus to find solutions of $F(\beta, \lambda) = 0$, we need only solve the equivalent equation

$$\lambda = \lambda_0 - \frac{f_0(\beta)}{f_1(\beta)} - \sum_{m=2}^{n} (\lambda - \lambda_0)^m \frac{f_m(\beta)}{f_1(\beta)} \tag{1}$$

Because $f_1(\beta_0) \neq 0$, all the coefficients $f_k(\beta)/f_1(\beta)$ are analytic near $\beta = \beta_0$. We try to solve this last equation with a solution of the form $\lambda(\beta) = \lambda_0 + \sum_{k=1}^{\infty} \alpha_k(\beta - \beta_0)^k$. The α_k can be computed by recursive substitution into (1); for example,

$$\alpha_1 = -\left[\frac{f_0(\beta)}{f_1(\beta)}\right]'\Bigg|_{\beta=\beta_0}$$

and

$$\alpha_2 = -\frac{1}{2}\left[\frac{f_0(\beta)}{f_1(\beta)}\right]''\Bigg|_{\beta=\beta_0} - \alpha_1^2 \frac{f_2(\beta_0)}{f_1(\beta_0)}$$

It is not very hard to prove that the α's determined recursively yield a power series with a nonzero radius of convergence (Problem 1a). Uniqueness is also fairly easy (Problem 1b). ∎

Corollary Let $T(\beta)$ be a matrix-valued analytic function near β_0 and suppose λ_0 is a simple eigenvalue of $T(\beta_0)$. Then:

(a) For β near β_0, $T(\beta)$ has exactly one eigenvalue, $\lambda_0(\beta)$, near λ_0.

(b) $\lambda_0(\beta)$ is a simple eigenvalue if β is near β_0.
(c) $\lambda_0(\beta)$ is analytic near $\beta = \beta_0$.

For multiple roots, a more complicated but still straightforward analysis is necessary. We do not prove the following basic theorem for this case (proofs can be found in the references in the Notes).

Theorem XII.2 Let $F(\beta, \lambda) = \lambda^n + a_1(\beta)\lambda^{n-1} + \cdots + a_n(\beta)$ be an nth degree polynomial in λ whose leading coefficient is one and whose coefficients are all analytic functions of β. Suppose $\lambda = \lambda_0$ is a root of multiplicity m of $F(\beta_0, \lambda)$. Then for β near β_0, there are exactly m roots (counting multiplicity) of $F(\beta, \lambda)$ near λ_0 and these roots are the branches of one or more multivalued analytic functions with at worst algebraic branch points at $\beta = \beta_0$. Explicitly, there are positive integers $p_1, \ldots, p_k$ with $\sum_{i=1}^k p_i = m$ and multivalued analytic functions $\lambda_1, \ldots, \lambda_k$ (not necessarily distinct) with convergent **Puiseux series** (Taylor series in $(\beta - \beta_0)^{1/p}$)

$$\lambda_i(\beta) = \lambda_0 + \sum_{j=1}^{\infty} \alpha_j^{(i)}(\beta - \beta_0)^{j/p_i}$$

so that the m roots near λ_0 are given by the p_1 values of λ_1, the p_2 values of λ_2, etc.

Corollary If $T(\beta)$ is a matrix-valued analytic function near β_0 and if λ_0 is an eigenvalue of $T(\beta_0)$ of algebraic multiplicity m, then for β near β_0, $T(\beta)$ has exactly m eigenvalues (counting multiplicity) near λ_0. These eigenvalues are all the branches of one or more multivalued functions analytic near β_0 with at worst algebraic singularities at β_0.

If A and B are self-adjoint, the perturbed eigenvalues of $A + \beta B$ are analytic at $\beta = 0$ even if A has degenerate eigenvalues. That the branch points allowed by the last theorem do not occur in this case is a theorem of Rellich. This theorem and its sister theorem on the analyticity of the eigenvectors in this case are the really deep results of finite-dimensional perturbation theory. The example at the beginning of this section shows that branch points can occur for *nonreal* β even in the "self-adjoint case," $T(\beta)^* = T(\bar{\beta})$.

Theorem XII.3 (Rellich's theorem) Suppose that $T(\beta)$ is a matrix-valued analytic function in a region R containing a section of the real axis, and that $T(\beta)$ is self-adjoint for β on the real axis. Let λ_0 be an eigenvalue of $T(\beta_0)$ of multiplicity m. If β_0 is *real*, there are $p \le m$ distinct functions $\lambda_1(\beta), \ldots, \lambda_p(\beta)$, *single-valued* and analytic in a neighborhood of β_0, which are *all* the eigenvalues.