Theory of Resonances

Principles and Applications

Reidel Texts in the Mathematical Sciences

A Ω

V. I. Kukulin,
V. M. Krasnopol'sky, and
J. Horáček

Kluwer Academic Publishers

Theory of Resonances

Reidel Texts in the Mathematical Sciences

A Graduate-Level Book Series

Theory of Resonances

Principles and Applications

by

V. I. Kukulin, V. M. Krasnopol'sky
Moscow State University, U.S.S.R.

and

J. Horáček
Charles University, Prague, Czechoslovakia

Kluwer Academic Publishers
Dordrecht / Boston / London

Library of Congress Cataloging-in-Publication Data

CIP

Kukulin, V. I.
Theory of resonances.
(Reidel texts in the mathematical sciences)
Includes index.
1. Few-body problem. 2. Resonance.
I. Krasnopol'sky, V. M. II. Horáček, J.
III. Title. IV. Series.
QC174.17.P7K85 1988 530.1'4 88–12649
ISBN 90–277–2364–8

Published by Academia, Publishing House of the Czechoslovak Academy of Sciences, Prague
in co-edition with
Kluwer Academic Publishers, P.O.Box 17, 3300 AA Dordrecht, The Netherlands.
Kluwer Academic Publishers incorporates the publishing programmes of D. Reidel, Martinus Nijhoff, Dr. W. Junk and MTP Press

Sold and distributed in the U.S.A. and Canada
by Kluwer Academic Publishers,
101 Philip Drive, Norwell, MA 02061 U.S.A.

Sold and distributed in Albania, Bulgaria, China, Czechoslovakia, Cuba, German Democratic Republic, Hungary, Mongolia, Northern Korea, Poland, Rumania, U.S.S.R., Vietnam, and Yugoslavia
by Academia, Publishing House of the Czechoslovak Academy of Sciences, Prague, Czechoslovakia.

Sold and distributed in all remaining countries
by Kluwer Academic Publishers Group,
P.O. Box 322, 3300 AH Dordrecht, The Netherlands.

Scientific Editor
Prof. Ing. Jiří Formánek, DrSc.,
Corresponding Member of the Czechoslovak Academy of Sciences

Reviewer
Prof. Ing. Milan Noga, DrSc.

Printed in Czechoslovakia.

Contents

Preface 9

Introduction 13

1. Mathematical and quantum-mechanical background 35

1.1. Some methods for regularizing divergent integrals 35
1.2. Padé approximants and their applications 40
1.2.1. Basic properties of the Padé approximants 41
1.2.2. Padé approximants of type II 47
1.2.3. Padé approximants of type III 49
1.2.4. Application of Padé approximants 50
1.3. Some methods of analytic continuation 58
1.3.1. Analytic continuation by means of power series 58
1.3.2. Analytic continuation by means of Padé approximants 61
1.3.3. Stability of analytic continuation 62
1.3.4 Analytic continuation of contour integrals 64
1.4. Scattering theory in a three-body system and the Faddeev integral equations 66
1.4.1. The features of the three-body problem as compared with the two-body problem 66
1.4.2. The Faddeev equations and their structure 68
1.5. The Hilbert-Schmidt method in the theory of integral equations 73
1.5.1. The Hilbert-Schmidt expansion for the Lippmann--Schwinger integral equation 77
1.5.2. The three-particle case 82

2. General concepts of the theory of resonance states and processes 88

2.1. Resonances in scattering theory 88
2.1.1. Parametrization of *S*-matrix in and outside the vicinity of a resonance 89
2.1.2. Resonances without *S*-matrix poles 99
2.1.3. Behaviour of scattering wave function near resonance
2.2. Quasi-stationary (Gamow or Siegert) states 102
2.2.1. Relationships between the Gamow functions and the Green function 104

2.2.2. Normalization and orthogonality of the Gamow functions 110
2.2.3. Series expansions in terms of Gamow states 113
2.3. The Kapur-Peierls formalism and the basis of eigenfunctions for the operator Green function 117
2.4. Resonances in two-level system. A model example 122
2.5. Resonance states in the *R*-matrix theory 127

3. Theory of resonance states based on the Hilbert-Schmidt expansion 134

3.1. Two-particle resonances 134
3.1.1. Perturbation theory for resonance states. Construction of normalized wave function 134
3.1.2. Determination of the Hilbert-Schmidt eigenvalues with the help of analytic continuation in energy 138
3.1.3. Calculation of the Hilbert-Schmidt eigenfunctions and eigenvalues by the method of continued fractions 142
3.2. Resonances in three-particle system 147
3.2.1. Three-particle Hilbert-Schmidt expansion and some classification of three-particle resonances 148
3.2.2. The method of analytic continuation in energy for the three-particle case 154

4. Projection methods 159

4.1. General projection formalism 159
4.2. Orthogonal projecting method 163
4.3. Analytic continuation of the scattering-theory equations 169
4.3.1. Continuation of the resolvent 170
4.3.2. Analytic continuation of the scattering-theory equations 172
4.3.3. Continuation of Faddeev equations 179
4.4. One-particle resonances 185
4.4.1. Equation for the resonance energy and width 185
4.4.2. Iterative inference of resonance parameters and decay amplitude 189
4.4.3. Examples 194
4.5. Resonances in three-particle system 196
4.6. Treatment of resonance states in the shell-model description of nuclear reactions 206
4.6.1. One-particle problem 208
4.6.2. Many-particle problem 211
4.7. Summary 216

5. Theory of resonance states and processes based on analytical continuation in the coupling constant 219

5.1. Two-particle resonances in real and complex potentials 220
5.1.1. Analytic properties of the energy eigenvalues as functions of the coupling constant 220
5.1.2. Analytic continuation in coupling constant and the determination of the parameters of the bound, resonance and antibound states 225
5.1.3. Determination of branch points 230
5.1.4. Wave functions of the Gamow states: orthogonality and normalization relations 232
5.1.5. Matrix elements comprising Gamow functions 235
5.1.6. Resonance in the complex potential 237
5.1.7. The resonance and near-threshold states in deformed potential 241
5.2. The structure of threshold singularities of energy eigenvalues in the presence of long-range interaction potentials 245
5.2.1. Coulombic case. Attraction 245
5.2.2. Coulombic case. Repulsion 251
5.2.3. Remarks 253
5.3. Many-particle resonance and near-threshold states in the systems with real potentials 254
5.3.1. Three-particle resonances with two-particle decay 256
5.3.2. Few-particle systems with potentials including strong repulsive core 257
5.4. Theory of quasi-stationary states with two particles in continuum 261
5.5. Scattering and the reactions involving unstable particles 264
5.5.1. Stripping to unbound state 265
5.5.2. Scattering of unstable particles by a target 268
5.6. Other examples of the application of the ACCC method in nuclear physics 270

6. *S*-matrix parametrization of scattering data. Extraction of resonance parameters from experimental data 276

6.1. Parametrization of single-channel *S*-matrix 278
6.1.1. The case of short-range interaction potential 279
6.1.2. Long-range forces 285
6.1.3. Polarization-type long-range interaction 291
6.2. Multichannel *S*-matrix parametrization 292

6.2.1. Complex phase-shift method 293
6.2.2. Multichannel *S*-matrix 295

7. Resonances in atomic physics 302
7.1. Introduction 302
7.2. Methods for calculating the resonance states 305
7.3. Variational methods in the theory of resonances 307
7.4. Stabilization method 312
7.5. Complex scaling method 316
7.5.1. Analytic model 318
7.5.2. Computational aspect of complex scaling 322
7.5.3. The Stark effect 327
7.6. Post-collision interaction model 329
7.6.1. Optical-potential approach to the post collision interaction model 334

Conclusion. Open problems 341
Appendix A 344
Index 352

Preface

It is well known that any development means specialization and differentiation. The soundness of this idea has again been substantiated by the development of quantum physics and by its applications to an ever growing number of topical problems in almost all branches of physics. This process of the differentiation of science separates the specialities, which were associated or indisciplinary as recently as thirty years ago, and makes them so far apart that people working in one of the branches are no longer interested in the problems of, and do not even understand the questions raised by the formerly associate field. We can only counter this unfortunately unavoidable specialization trend by a methodological integration, that is, by developing sufficiently universal and unified methods of studying the phenomena from different domains of physics. An excellent, but unfortunately rare, example of such a methodological unification in present-day theoretical physics is Landau and Lifshitz's ten-volume course of theoretical physics.

The development of the quantum physics of few-body systems may also be regarded as a very successful effort to counter such specialization. This quantum-physics approach, which was initiated in the early sixties by Faddeev in his mathematical works, and by Weinberg, Simonov, and many others in their pioneer studies, gradually expanded to absorb and integrate more and more fields of nuclear physics, atomic and molecular physics, and elementary particle physics in their theoretical and experimental aspects. At present, this trend has reached the status of a new and highly dynamic branch of science which unites, just on the basis of unified approaches and methods, the experts in different fields of physics. (We can get an idea of the development of this branch from the proceedings of the various international conferences on the relevant topics held regularly during the last 25-years).

Another good crystallization centre of various fields of microphysics is the physics of resonance states and processes. Equally, as once vibration theory became a fruitful interdisciplinary science of general laws of vibrational processes in different branches of physics, so the theory of resonance phenomena may well become, when developed appropriately, a science of general laws of formation and decay of long-lived states in molecules, atoms, nuclei, and condensed matter and under hadronic collisions. This tendency can be seen clearly nowadays and has resulted in the first interdisciplinary international conference on the methods and models in physics and theory of resonance processes (see Lecture Notes in Physics, vol. 211: *Resonances-Models and Phenomena*, edited by S. Albeverio, L. S. Ferreira, and L. Streit, Springer, Berlin, 1984).

In this book we shall attempt, as far as we are able, to contribute to the process of integration of methods in the field of resonance physics. Since this field is represented by numerous works from most branches of present-day physics, we have abandoned outright the idea of reviewing even the most fundamental works. It is difficult even to classify this vast mass of works as typifying the methods used, because a great many of the works may be regarded as synthetic, that is they use several different methods.

Fortunately, the basic elements, which are like the building blocks of every edifice, are few so that they can well be described in a moderate volume. We have chosen just this way; that is, we have tried to describe the basic elements of the theory of resonance states and processes along with typical examples of their combination into a completed "construction". Furthermore, we have limited ourselves to the sphere of our professional interests, which is still very large, namely, the resonance states in few-body systems (mainly in atomic and nuclear physics).

The feeling of great surprise which we experienced on studying numerous works from the field of atomic, molecular and nuclear physics has also given a strong impetus to writing this book, because their authors invented again and again, for their particular uses the methods elaborated properly long ago in a neighbouring branch of physics. Avoiding specific examples, we shall still show that many articles published, say, in the Physics Review, Series A are methodically almost an exact replica of earlier works published in Series C, and vice versa, often without any references.

The domain of the physics of few-body systems characterized by methodical unity of approaches seems to us to be just a good basis for the appropriate integration of various branches of resonance theory.

At present we have numerous excellent books on scattering theory (which include the theory of many-particle scattering – see the references in the basic text of the book) where the theory of resonances and resonance processes is described in more or less detail. However, all the books deal practically with only general properties of resonance states, such as the relevance of resonances to the S-matrix poles, the time-dependent decay law, etc. At the same time, any particular work has either to find theoretically the *actual* parameters of the resonance states (or the amplitudes of the processes involving the resonances) in terms of one or another dynamic model, or to infer such parameters from experimental data. However, material of this kind, which is of major importance for practical purposes, is absent in the general-purpose books and is disseminated over a great number of original works in *different* branches of physics. Therefore, our aim is to summarize at least a fraction of this vast material, including also our investigations, in a single moderate volume and to explain it in as uniform a language as possible. We leave it to the reader to judge how far we have succeeded in doing that.

The essence of the book is reflected in the table of contents and, in more detail, in the Introduction.

The book is prefaced by a referential chapter aimed at those readers who are eager to start tackling particular problems by sparing them the difficult and tiresome search for the facts and mathematical theorems scattered over the original mathematical and physical literature where various notations and different degrees of generality and rigour are used.

Some of our colleagues and friends who assisted us in writing this book read all or individual chapters and made a number of valuable remarks. We are especially grateful to Vladimir Pomerantsev, a member of our research group at the Moscow State University whose contribution to the elaboration of many results presented in the book can hardly be overestimated. He also rendered great assistance in writing Chapter 4 of the book and looked critically through the material of other chapters. The authors are particularly indebted to Professors J. Formánek and J. Kvasnica of the Charles University, Prague, for their attentive reading of the manuscript and for numerous informative remarks allowing us to improve the text. The authors should also like to thank Professor W. Domcke, Technische Universität München, Professor N. M. Queen, The University of Birmingham and Dr. J. Blank, Charles University Prague for carefully reading parts of the manuscript and pointing out a number of errors.

Since the book is to some extent a first attempt to expound the methods of resonance theory on a uniform basis, it cannot be absolutely free from shortcomings the responsibility for which is borne by the authors alone.

In the techniques and subjects treated there exists a large amount of publications. We would like to apologize to those authors whose work is not directly or sufficiently well treated.

The Soviet authors are also grateful to the administration of Charles University for offering all necessary facilities for their work in Prague which permitted them to finish the book within an acceptable period.

Prague 1986

V. I. Kukulin,
V. M. Krasnopol'sky
Moscow State University

J. Horáček
Charles University

Introduction

This book is devoted to the theory of resonance states and processes expressed in terms of nonrelativistic quantum mechanics. There are already many excellent books on quantum mechanics and collision theory where, among other things, a description of general theory of resonance scattering may be found [1–6]. With rare exceptions, however, they usually discuss the parametrization of the scattering amplitude (or of the S-matrix) in the near-resonance region, for example the Breit-Wigner parametrization or the appropriate generalization to the case of many levels or many channels. At the same time, the basic problem nowadays is not to get a general parametrization of cross sections but to calculate the parameters of the resonance amplitudes (namely, widths, level shifts, S-matrix residues at resonance poles, etc.) proceeding from the fundamental interactions effective in a quantum system. It is the problem of the practical calculation of resonance parameters, however, that is explicitly given little consideration in the general-purpose manuals. They also usually omit the theory of many-body resonance states capable of decaying with emission of two or more particles, although such resonances are extensively used in atomic, molecular, nuclear and particle physics.

On the other hand, present-day pure scientific literature includes many hundreds of works devoted to methods for calculating the resonance parameters and to the general description of many-body resonances. Furthermore, many of the methods which have long been used in nuclear and particle physics are now being reinvented to describe atomic collisions, and vice versa. Therefore the aim of this book is to fill this gap between the textbooks on quantum mechanics and theory of resonance processes on the one hand and the modern-day journal publications on the other, including works from various fields of quantum physics, molecular, atomic, and nuclear physics, several sections of the book dealing with original results of the authors. In choosing the material for the book, we were guided by the desire to include the most general methods and approaches which cannot be found in the standard textbooks, but are widely used in the relevant studies. Moreover, when appropriate, we have included the results of particular numerical calculations for illustrative models bearing in mind that one simple example can well prove to be more convincing than several pages of arguments (as to the exact proofs [35], they impose highly constraining restrictions on the interactions used in most cases).

In a number of cases where lack of space prevented us from giving a detailed derivation we have tried to guide the reader by presenting basic relations and referring him to works where a completed derivation may be found. Sometimes the reader himself will probably be able to complete the derivation, which may be regarded as a good exercise. Finally, bearing in mind the main purposes of this textbook, we end each chapter with a list of references where most of the basic works on a given subject may be found.

Contents of the book. Now we shall briefly outline the contents of this book. The first Chapter of the book is auxiliary and deals with subsidiary knowledge from various areas of mathematics, such as the theory for functions of complex variables, methods of analytic continuation, estimation of divergent integrals, concise theory for the Padé approximants, and other information necessary for the subsequent sections of the book to be understood. Chapter 1 also gives necessary information about the Faddeev equations and the theory of three-particle scattering which underlie three-particle (and, generally, many-particle) resonance theory treated in the subsequent chapters of the book. (A comprehensive discussion of the basic mathematical facts, theorems, and equations concerning the modern-day scattering theory in few-body systems may be found in the latest monograph [36]).

Chapter 2 includes general information about resonance states and processes necessary both for understanding of how to detect resonances experimentally in the scattering and reaction cross sections and for learning some basic methods to describe resonance processes (the Kapur-Peierls formalism, etc.). On comparing Chapter 2 with Chapter 4 the reader can readily make sure that the Kapur-Peierls formalism and the Feschbach projection operator approach proper and its various modifications are essentially based on a single fundamental idea, namely, the decay channels of resonance states are artificially made closed, whereupon the pure stationary state is calculated. After that, the decay channels are opened again and the true quasi-stationary state is calculated (usually by the perturbation method) as a state obtainable from the initial (stationary) state when the interaction with the open channels of the continuum is included. The basic difference between the above mentioned approaches is solely that the Kapur-Peirls method is formulated in the configuration space, and the Feshbach approach in the Hilbert space (which is most probably preferable in many problems). Many other approaches (for example, the *R*-matrix method) are based on the same general idea.

Chapter 3 gives a general approach to resonance theory based on the Hilbert-Schmidt method from the theory of integral equations. This approach, developed mainly by Simonov et al., makes it possible, in a uniform way and using unified language, to formulate numerous results obtained by various methods in terms of the resonance state theory. This approach is notable for a good universality, because the given pattern permits a direct generalization in the case of three-particle resonances and allows a simple computational algorithm. The chapter describes also the readily usable methods for calculating the Hilbert-Schmidt eigenvalues and eigenfunctions proposed by the authors.

Chapter 4 describes one of the most extensively used methods to treat resonance states, namely, the projection operator formalism proposed by Feshbach, and its generalization to the many-particle resonance theory carried out by V. Pomerantsev and one of the authors of this book (V.I.K). The last section of the chapter describes the application of the Feshbach projection operator formalism to the calculation of the QBSEC-type metastable states excited in nuclei under elastic and inelastic scattering of nucleons of low and medium energies.

Chapter 5 deals mainly with the behaviour of the resonance poles of the S-matrix in various interaction models when the parameters of the interaction Hamiltonian vary. Most attention is paid to the ingenious approach developed by the authors and based on the analytic continuation of the S-matrix singularities in the coupling constant. In terms of this approach the resonance and virtual states are inferred from the bound states when the latter are analytically continued in the coupling constant. This approach differs from many other methods by its simplicity and wide universality because it may be applied to calculating both the resonance states proper and the amplitudes of one- and many-particle reactions involving resonances. The chapter presents numerous examples illustrating the application of the approach to various problems.

Chapter 6 discusses a method proposed by the authors and intended for actual determination of the resonance parameters (width, energies, and vertex constants) from phase shift analysis of experimental data. Particular algorithms for processing experimental phase shifts are discussed. The nuclear and atomic physics evidence exemplifies the discussion.

Finally, Chapter 7 discusses the applications of variational methods to calculating the resonance states and treats the dilatation method (i.e. the complex scale transformation method) which has enjoyed wide popularity in recent years, especially in atomic and molecular physics, and is used to study the autoionization state and other long-lived states. We are far from nursing the idea of having exhaustively expounded the above two approaches mentioned (that is the variational and dilatation methods) to which numerous publications are devoted (see the list of references to Chapter 7 which is, however, far from being complete). Our aim is more modest, namely to give some idea of the methodology in the context of this book and to cite basic references to the original works and reviews where the reader can find, if required, the necessary information. On the whole, this agrees fully with our general intention to treat the basic concepts and the calculation methods of the present-day theory of resonances in few-body systems in a comprehensible book of moderate volume. The appendix is also of mathematical character and presents some basic concepts of the theory of rigged Hilbert spaces necessary for the material of Chapter 4 to be understood more clearly. It is known (see, for example, [1]) that the theory for resonance states may also be described without using the formalism of rigged Hilbert spaces. However, the use of the language of rigged spaces makes it possible to present this theory in what is probably the most exact and logical way (see, for example, [34]). Our aim, however, is not to consistently use this ingenious formalism in all the applications, but to describe its usage in

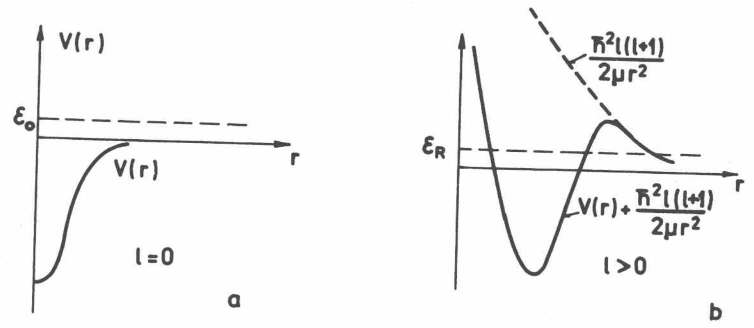

Fig. 0.1
Formation of a confining potential barrier for the superposition of a short-range attractive potential $V(r)$ (Fig. 1a) and a repulsive centrifugal potential $\hbar^2 l(l+1)/2\mu r^2$ for a non-zero particle angular momentum (Fig. 1b), $l > 0$.

constructing a resolvent operator continued to the nonphysical sheet. In the remaining chapters of the book we use a more traditional method, namely, the direct continuation of the matrix elements of operators as ordinary functions of a complex variable.

Types of long-lived states. Quantum mechanics deals with numerous types of long-lived (quasi-stationary) states. These states may be classified by the singularities of the scattering matrix, by the mechanism of their production or by the model describing them.

Let us examine briefly the most widespread types of the resonances and the long-lived states of quantum systems. The list of types given below is far from complete, but it shows the diversity of physical phenomena which we are inevitably faced with when we try to get a more or less consistent classification of long-lived states.

(i) *One-particle shape resonances*. This is the simplest and clearest type of long-lived state which arises in the case of potential scattering of a particle by an unexcited target or simply in a potential field in the presence of a confining potential barrier. The energy E of the particle has to be below or of the same order of the height of the barrier (see Fig. 0.1). The particle is captured through tunnelling to the region of strong attraction, thus forming a relatively long-lived (or quasi-stationary) state, whereupon, again through tunnelling, it leaves the inner region of interaction. The potential barrier arises, as a rule, when a strong short-range attraction is applied to a long-range repulsive potential of centrifugal (see Fig. 0.1) or Coulomb type. The lifetime τ of the quasi-statio-