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PRINCIPLES OF QUANTUM SCATTERING THEORY

DŽEVAD BELKIĆ

ROUTLEDGE

Principles of Quantum Scattering Theory

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Dževad Belkić is a theoretical physicist. He is Professor of Mathematical Radiation Physics at Karolinska Institute in Stockholm, Sweden. His current research activities are in atomic collision physics, radiation physics, radiobiology, magnetic resonance physics and mathematical physics. In atomic collision physics, he has worked on many problems including major challenges such as the theory of charge exchange and ionization at high non-relativistic energies. *Inter alia* he used distorted wave methods, paying special attention to treatments with correct boundary conditions for scattering particles which interact through Coulomb potentials.

In radiation physics, Professor Belkić has worked on the passage of fast electrons and multiply charged ions through tissue as needed in radiation therapy in medicine. Here he has employed both deterministic methods through the Boltzmann equation and stochastic simulations via Monte Carlo computations. In radiobiology, he has worked on mathematical modelling for cell survival, and has focused on mechanistic modelling by including the main pathways for survival of cells under irradiation during radiotherapy.

In magnetic resonance physics, Professor Belkić has worked on nuclear magnetic resonance in medicine where he focused on high-resolution parametric signal processors which go beyond the conventional shape estimations of spectra. In mathematical physics, he has worked on many problems including the derivation of analytical expressions for scattering integrals or bound-free form factors, for rational response functions in signal processing, for coupling parameters in the nearest neighbour approximation which is one of the most frequently used methods in physics and chemistry, etc.

He has published more than 150 scientific publications which have received over 2000 citations. He has received a number of international awards including the triple Nobel grantee status for research grants in atomic collision theory from the Royal Swedish Academy of Sciences as approved by the Nobel Committee for Physics.

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Preface

The majority of the most important breakthroughs in physics have been made by using scattering, as one of the leading strategies for studying the structure of matter on very different fundamental levels, ranging from areas with perfectly known interactions (atomic physics) to fields with phenomenologically postulated potentials (nuclear physics). Atomic, nuclear and molecular particles, as well as their constituents, are quantum systems *per se* and, therefore, quantum scattering theory has been, and still is, overwhelmingly used in theoretical investigations on particle scatterings. The common denominators of the most influential theoretical studies in the past literature on collisions are *principles of quantum scattering theory*. Interestingly enough, scattering theory is also intensively studied in the mathematical literature, especially from the standpoint of spectral analysis. In particular, resonant scattering theory merges smoothly into spectroscopy and this provides an extraordinary opportunity for unifying these two general methodological strategies into a single quantum theory, as opposed to traditionally separate treatments. This versatile field of particle collisions is chosen for the subject of the present book, since scattering principles are a veritable cross-road for graduate physics students, future specialists on quantum scattering theory, for other non-specialist physicists, mathematical physicists, accelerator physicists, medical physicists, particle transport physicists, and researchers from neighbouring sciences, as well as from technologies or industries related to energy production (fusion reactors), to manufacturing of scanners for medical diagnostics and to radio-therapeutic devices (medical accelerators), etc.

Despite their natural and plausible introduction from both the physical and mathematical viewpoints, virtually all the theoretical principles of quantum scatterings necessitate detailed confirmation by experiments. For this reason, several principles of particle scatterings are singled out and thoroughly tested against many available experimental data in a selected branch of major atomic collisions at high non-relativistic energies. In performing such comprehensive comparisons between theory and experiment in this book, due emphasis is placed onto the main *mechanisms* that govern ion–atom energetic collisions. For example, through the remarkable phenomenon of double scattering, the reader is taken on a fascinating and illustrative journey from the time of Rutherford, Thomas, Bohr and Oppenheimer with their conjectures and intricacies all the

way to the successful resolution of a long-lasting enigma by contemporary experiments based upon single-pass translational spectroscopy and multi-pass recoil ion momentum spectroscopy. This challenging enigma was an outstanding controversy about whether one or two binary collisions eventually dominate at high-energy rearranging collisions. Unlikely as it might appear at first glance, high-energy billiard-type Thomas double collisions prevail substantially over single binary encounters, which are based upon the so-called velocity matching mechanism. Moreover, contrary to the common perception, it is emphasized in this book that the Thomas double scattering with two participating electrons and one nucleus exhibits an enhanced probability at *all* collision energies. This vigorously promotes the role of the underlying dynamic electron correlations which, in turn, can increase the chance for multi-electron transitions in ion–atom collisions, so that, e.g., several electrons could be readily ionized, as also confirmed experimentally. This remarkable dominance of double scatterings over single encounters has major ramifications for a proper formulation of quantum scattering theory, especially when charged aggregates are present in either of the channels. Furthermore, double scatterings play a very important role in collisions of charged particles with condensed matter, in plasma physics, astrophysics, particle transport physics, medical physics, radiation physics, as well as in technological disciplines such as thermonuclear fusion, etc.

An inspection of the rich literature on perturbation developments of transition matrices would reveal a totally unexpected finding that the second-order in the Born expansion for, e.g., three-body rearranging collisions yields by far inferior differential and total cross sections than those due to its first-order counterpart. This occurs even at quite high energies and throughout the angular range including the Thomas peak, despite an explicit inclusion of the free-particle Green's function which propagates the electron intermediately between two Coulomb centres before capture finally takes place. The source for this surprising occurrence, which resulted in a flagrant disagreement between the ensuing so-called second-order Brinkman–Kramers approximation and experiments, has been found to be in the neglect of the internuclear Coulomb potential for the given channel states with plane waves for the relative motion of heavy scattering aggregates. This unphysical procedure has been rectified in the literature by retaining the internuclear potential *exactly* in the usual eikonal limit. As a net result, the internuclear potential contributes rigorously nothing to the exact eikonal total cross sections, but yields an important phase factor in the related differential cross sections, in accordance with Wick's well-known conjecture from theory on charge exchange. When this modification is adequately introduced in the Born perturbation expansion, its second-order term is found to give excellent agreement with the experimentally measured differential and total cross sections. Moreover, such a boundary-corrected exact second-second Born approximation yields a substantial improvement over its first-order counterpart. This is expected, since a consistently introduced second-order in a perturbation theory contains better physics and, as such, is anticipated to display a clear superiority over the

corresponding first-order. By contrast, better physics is also taken into account in the second-order Brinkman–Kramers approximation through the Green's function propagator, but nevertheless this is fully masked, since the overall result is totally unsatisfactory due to the inconsistency between the channel states and the channel perturbations in the transition matrix. These important lessons from past experience are discussed in the present book with a special emphasis on the correct boundary conditions. These latter conditions encompass not only the proper asymptotic behaviours of the total scattering wave functions, but also the consistently introduced perturbation potentials which enable the transition to take place in a full harmony with the strict prescriptions of the so-called Dollard's asymptotic convergence problem from formal scattering theory on long-range Coulomb potentials.

The long-lasting controversy about the possible role of the inter-nuclear potential in heavy particle collisions also makes interesting reading on the level of a first-order term in a perturbation expansion. For years, the literature witnessed all sorts of results differing from each other by huge factors ranging from 2–10 to 100–1000 and this was due precisely to inadequate treatment of the internuclear potential in a wider context of violation of the correct boundary conditions. Even after the roles of the internuclear potential and the correct boundary conditions were conclusively settled in 1979 within the exact eikonal theory, a considerable degree of confusion still persisted for more than a decade. For a while the good initial trend of this exact eikonal theory seemed to be going in a reverse direction by a subsequent invention of the so-called strong potential Born approximation, which turned out to be inherently divergent. This unavoidable divergence could not be cured irrespective of whether one is resorting to a distorted wave formalism or not. The source of divergence of this model is in the ignorance of the correct boundary conditions, as dictated by the mentioned exact eikonal theory, and widely recognized later on. Had this failure been duly corrected, the strong potential Born approach would have simply been reduced to the well-known second Born approximation with the Coulomb Green's function with no intrinsic divergences. Eventually, the consensus has been reached so that the correct boundary conditions were irrevocably ingrained into atomic scattering theory. The initial results from the so-called boundary corrected first Born approximation introduced in 1979 came finally at the end of the 80's. The reported computational findings on total cross sections for electron capture by completely stripped ions from multi-electron targets showed remarkable improvements, occasionally within orders of magnitude (e.g., for proton-argon), when passing from theoretically correct to the incorrect first Born theory. Such improvements were even more dramatic than those from the mentioned second Born approximation. These essential achievements constitute 'the proof of principle' confirming the tremendous practical relevance of the asymptotic convergence problem in quantum scattering theory.

Inelastic atomic collisions are dominated by excitation, charge exchange and ionization as well as by various combinations of these elementary processes,

primarily double transitions, e.g., transfer-excitation transfer-ionization, two-electron capture, twofold excitation or double ionization, etc. Charge exchange (also known as charge transfer or electron capture) dominates at low energies where excitation and ionization are negligible. The relative roles of these processes are inverted at high energies where excitation and ionization dominate, whereas charge exchange becomes negligible. At intermediate energies, these three channels are competitive to each other and, therefore, this is the most challenging region to investigate. Due to the prevailing role of ionization at high energies, it is clear that charge transfer can be significantly altered whenever ionization continua are intermediately open to the electron which is ultimately captured. One of the most flexible ways to include these intermediate channels into the theory of scattering is provided by the so-called distorted waves. They represent scattering wave functions which basically describe correlation effects stemming from the simultaneous presence of the electron in the field of two Coulomb centres due to the projectile and target nucleus. Remarkably, inclusions of such distorted waves in only the *first-order* of Dodd–Greider's distorted wave perturbation expansion become equivalent to the *second-order* of the conventional undistorted Born perturbation development. This equivalence is complete both quantitatively and qualitatively when it comes to the Thomas double scattering, at least for the ground-to-ground state electron transfer at asymptotically high non-relativistic energies. The practical importance of this accomplishment is immensely augmented by the observation that the quantum-mechanical transition matrix in the ensuing continuum distorted wave approximation is obtainable by purely analytical methods in the explicit closed form. This is opposed to the equivalent second Born approximation whose transition matrix necessitates multiple numerical quadratures. Such favourable circumstances about the continuum distorted wave method attracted over the years an unprecedented number of researchers. Moreover, this method has also been extended to ionization and transfer-ionization with a remarkable success in comparisons with available experimental data. The continuum distorted wave theory of ionization has many advantages over its competitors, e.g., (i) it is mathematically well-defined, convergent and integrable, (ii) it permits the exact calculation of the transition amplitude in the analytical form, (iii) it treats the initial and final channel in a symmetric manner on the same footing, (iv) it yields the total scattering wave functions with the correct boundary conditions in both channels, (v) it accounts for the three major mechanisms via their characteristic signatures such as (1) the zero-energy peak describing a direct ejection of slow electrons, (2) electron capture to continuum yielding a cusp-shaped zero-angle peak where vectors of momenta of ejected electrons and scattered projectiles are parallel, and (3) binary encounters appearing as a binary peak when the ratio of the momenta of the electron and projectile is equal to two multiplied by cosine of the ejected electron angle. This book also openly discusses several limitations of distorted wave methods for energetic ion–atom collisions and indicates certain directions that could be undertaken for potential improvements.

Electron detachment is a special nomenclature for ionization of targets which are negatively charged ions. This is a very important sub-branch of ionizing phenomena for which experimental data are available for testing few-body quantum-mechanical scattering theories. A critical analysis of the theoretical development in this field is presented in this book, illuminating the paramount importance of consistency when linking the correctly behaving scattering wave functions with the corresponding perturbation potentials responsible for the investigated transitions. When this proper link is overlooked, entirely unphysical results were obtained some thirty years ago for the total cross sections which overestimate the experimental data and the required Bethe asymptotic limit at high energies by three orders of magnitude, despite the use of the scattering waves with the proper behaviours at asymptotically large inter-aggregate separations. This inconsistent link between scattering waves and perturbations in the transition matrix, has been identified only recently and when properly rectified, an adequate theory of detachment was finally obtained, exhibiting perfect agreement with modern experimental data from the threshold, through the Massey maximum to high energies including the Bethe asymptotic region. Again, this demonstrates that principles of quantum scattering are the key factors not only in the establishment of proper relationships among the major ingredients of the theory, but also in arriving to realistic and acceptable predictions about important experimentally measurable physical quantities.

Collisions among multiply charged ions with long range Coulomb interactions are very different from nuclear collisions characterized by short-range potentials. Consequently, the standard quantum scattering theory from nuclear physics cannot be used for atomic collisions without the essential modifications due to the presence of Coulomb interactions. This fact is emphasized in the present book by giving one of the most instructive illustrations within the well-known impulse approximation which is successful for nuclear scatterings, but fails for atomic collisions. Moreover, principles of quantum collision physics are used to illustrate in a number of important applications how this situation, which indeed significantly disturbed the customary scattering theory for a half a century, can be favourably remedied by extending the framework of the impulse hypothesis via the emergent 'reformulated impulse approximation' to match adequately all the essential peculiarities of Coulomb interactions. Most importantly, the latter fundamental reformulation, driven by the strict requirements from the principles of Coulomb scattering theory, is also fully endorsed by practice, since now both differential and total cross sections are brought into complete agreement with measurements. A wider interest in this general reformulation of scattering theory, relying upon the extended impulse hypothesis, is in the possibility to devise a myriad of new theoretical methods at high energies by merely choosing different distorting potentials. This is multi-purposely appealing, since these different methods would all belong to a common and general theoretical framework and, as such, be accessible to more direct comparative studies and to reliable assessments of their relative validity and

performance. The availability of a number of such consistently derived methods can be justified by the necessity of cross-validations of different approximations in view of the lack of the exact theory for complicated physical systems. This overall situation is highly advantageous relative to the usual occurrence, which is abundant in many apparently unrelated approximate methods occasionally introduced in a rather obscure way, such that their salient features could easily evade a proper evaluation in inter-study comparisons.

As always in physics, the most useful in diverse applications, and at the same time computationally the most difficult, is the region of intermediate energies. High-energy methods are perturbative and they truncate the series of the transition matrix, but retain scattering wave functions to all degrees for a given order of the investigated Feynman diagram. Low-energy methods develop the total state vectors on conveniently chosen quadratically integrable basis set functions and truncate this expansion, but keep the perturbation potentials to all orders. A severe drawback of such an artificial separation of theoretical procedures is that neither of these two groups of methods is adequate at the most needed intermediate energies. It would be optimal to have a single strategy which could combine the good features of low- and high-energy methods without truncating either total scattering wave functions or perturbation potentials. This book presents the possibilities for a judicious unification of scattering methods valid at low and high energies through the introduction of the variational Padé approximant applicable at all energies. Many practical methods can be derived from this novel and non-perturbative framework of scattering theory by appropriate selections of an additively factored high-energy distorted wave method with the remainder of the full transition matrix evaluated on a Sturmian basis, which is complete despite the use of exclusively discrete expansion functions. A distinct advantage of this variational unification over conventional low-energy close coupling methods is a total avoidance of the difficult and expensive problem of solving coupled systems of differential equations, but with an adequate inclusion of basically the same essential physics as the traditional expansion techniques. With the use of the hydrogenic Sturmian basis of dual functions centred on the projectile and target nucleus for three-body problems, it becomes quite impressive that the only significant numerical effort in this variationally unified quantum theory of scattering is reduced to a straightforward inversion of a matrix whose elements can all be calculated explicitly and analytically. Even this inversion can be done iteratively *en route* using a powerful method of continued fractions which is another more familiar name for the Padé approximant.

The emergence of the Padé approximant as a bridge between low- and high-energy methods in the mentioned unification is not unexpected at all, since this universal method is known to be equivalent to Schwinger's or Newton's fractional variational principles as well as to Fredholm's determinant, finite-rank separable expansions, Seaton's variation-iteration method for solving integro-differential equations in scattering problems, etc. It is anticipated that this variational Padé-based quantum scattering theory will have a multitude of applications in the future

on resonant and non-resonant atomic and nuclear collisions. Its counterpart, the Padé-based quantum spectroscopy has recently been established in the literature of spectral analysis of time signals that emanate from physical, chemical or other generic systems including living organisms and ultimately human beings scanned as patients for medical diagnostics. The present book points at this link between scattering and spectroscopy by elaborating the so-called multi-variate fast Padé transform. This transform is presently used for multi-dimensional quadratures encountered in scattering integrals, but it has already been employed elsewhere for signal processing and spectral analysis. For certain test functions, it is demonstrated that some unprecedented twelve decimal places of accuracy can be reached by the fast Padé transform as opposed to barely two exact decimals secured by the more familiar fast Fourier transform, i.e. a trapezoidal-type quadrature.

The fast Padé transform belongs to a category of deterministic methods, but this book deals intensively also with stochastic computational strategies. Here, after exhaustive computations of very complicated scattering integrals of dimensions as high as thirteen with movable and integrable singularities, Lepage's adaptive and iterative Monte Carlo algorithm VEGAS is strongly recommended for further use in collision physics and beyond. Remarkably, VEGAS which has originally been put forward in quantum electrodynamics for precise evaluations of certain corrections from Feynman's theory of graphs, can compute multi-dimensional integrals with a prescribed accuracy as if it were in a group of classical quadratures of the Gauss type. This is because VEGAS computes the standard deviation and performs the accompanying χ^2-test. The obtained results from such stochastic computations are exact within the *guaranteed* standard deviation and the overall performance is deemed acceptable whenever the χ^2-test is close to the number of iterations minus 1. The message conveyed from this book is that a wider usage of VEGAS in, e.g., atomic collision theory should lead in the near future to substantial computational breakthroughs. For example, VEGAS could be robustly employed to accurately evaluate for the first time the third-, fourth- and fifth-order Born approximations for, e.g., charge exchange in the most fundamental proton–hydrogen collisions. Since here the highest dimensions of integrals are of the order of twelve, the indicated computations are of complexity comparable to the one from the feasibility study presented in this book. This avenue is more than just a computational advantage, since it actually offers researchers a unique opportunity to probe the deeper physics of previously inaccessible higher-order effects in perturbative scattering theories.

Finally we ask the key question as in Ockham's razor: *why should yet another book on quantum scattering theory be added on top of a number of already existing ones*? This book is special in that it intertwines many fundamental and important strands ranging from mathematically rigorous general physical principles of quantum scattering theory, through thorough illustrations presenting the results of the most comprehensive computations to date from the leading distorted wave methods for selected major high-energy ion–atom

collisions, via comprehensive analysis of certain among the most powerful modern computational strategies, to finally paving the road for crucial links to neighbouring interdisciplinary fields of sciences and related technologies. In the present book, these links are especially illuminated towards medical physics, where scattering theory, via its description of interactions of charged particles with tissue, plays a unique and capital role. For example, the overall success of radiotherapy with charged particles depends critically upon the availability of reliable data bases of cross sections for inelastic phenomena, particularly for energetic ionizing collisions. However, only simple empirical recipes have overwhelmingly been used thus far for these cross sections, leaving the best atomic scattering theories virtually unexplored in these key problems. To overcome these obstacles for the important issue of delivering better health care to patients, the present book urges cross-fertilization of atomic collision physics and medical physics on a more proactive level. As emphasized in this book, similar cross-talks have recently been initiated encompassing spectroscopy and resonant scattering theory with the purpose of furthering progress in magnetic resonance physics for medical diagnostics. It is hoped that the attempts made in this book on versatile interconnected frontiers will be rewarded by the interest of an interdisciplinary readership.

The overall message of this specialized book is that the exposition of the selected principles of quantum scattering theory with the necessary mathematical rigour is readily comprehensible to the indicated readership, and is indispensable for a more fundamental understanding of particle scattering phenomena, as well as being of the utmost numerical importance in comparison with experiment.

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PART I

THE SELECTED MAIN PRINCIPLES AND THE BASIC THEORETICAL FRAMEWORKS FOR A NON-RELATIVISTIC QUANTUM-MECHANICAL THEORY OF SCATTERING

The key problem in quantum scattering theory is probability conservation, i.e. the unitarity of the S-matrix, which connects the initial with the final state of evolution of the considered physical system. This problem is not possible to solve if the scattering states neglect the so-called asymptotic convergence problem, which requires that the bound and free dynamics coincide with each other at infinite distances between the colliding particles. Usually quantum scattering theory is thought merely as a part of courses of quantum mechanics. However, this very important part is almost invariably presented through rather simplified concepts that are overwhelmed by heuristic formulae, with a stereotypical explanation that a rigorous mathematical formalism would merely obscure the physical arguments. This is not the case as is documented in part I of the present book, relying upon theorems of *strong topology* of vector spaces and spectral operator analysis, from which all the standard synonyms of collision theory follow directly, such as the Lippmann–Schwinger integral equations, behaviours of the scattering states, probability transition from the initial to the final state, differential as well as total cross sections, etc. Furthermore, rigour in the performed mathematical treatment is in absolute compatibility with physical argumentation as well as intuition and, moreover, this is presently established in a simple and plausible manner. These fundamental aspects are not only relevant to the foundation of a *complete* quantum-mechanical scattering theory, whose essential principles are outlined in this book, but they are also of primary significance for introducing the most adequate practical methods for various applications across interdisciplinary fields.

Chapter A

Introduction

The major themes of quantum mechanics are (i) *the physical interpretations of interactions in bound systems* and (ii) *particle scatterings*. The reason for the first part of this assertion rests upon the fact that the solutions of the standard Schrödinger eigenvalue problem, $H\Psi_n = E_n\Psi_n$, i.e. the eigenvalues E_n and eigenfunctions Ψ_n of the self-adjoint Hamilton operator H correspond to *stationary* states of an isolated system under study. In these stationary states, the energy of the whole system must be conserved. A stationary state describes *a stable* physical system, by which we understand a system which does not break up spontaneously, meaning that all its constituent parts, when they are in isolation, i.e. beyond an external influence, e.g. electromagnetic fields, remain together an infinitely large amount of time. By means of such states, one further acquires knowledge about the internal structure of the examined physical systems and, finally, about the structure of matter itself, as the ultimate goal of the theory. Stability of atoms and molecules is necessary in order that materials in nature could have any given *determined* physical and chemical properties, according to which these materials are distinguished, identified and studied. Of course, for us, the most important terms in the Hamiltonians are *interactions*, because they are the generators of the physical features of the examined systems. Within theme (i), one studies the so-called proper interactions among the constituent parts of *bound* compact, isolated systems. These interactions hold together all the particles of a given system.

However, for particle scattering[1], the situation is entirely different, since the total system is obtained from at least two subsystems, which *are not in mutually bound states*. One of the two subsystems has the role of a target, whereas the other represents a projectile. Here, it is understood that the binding energy for each of the subsystems, considered as isolated, is known from the analysis within

[1] In the old literature a terminological difference has sometimes been made between the notions of scattering and collision. The former and latter terms meant exclusively one- and multi-channel problems, respectively. Such a difference, however, has disappeared with time as purely formal, so that a linguistic dualism scattering-collision has been customarily in use for many years.

theme (i). In research area (ii), energy E of the whole system is taken as a *fixed* entry parameter, so that certain other crucial physical characteristics of the system, e.g. the S-matrix, cross sections, rate of the reactions, etc, are sought as a function of E. Hence, scattering theory studies the interacting physical systems projectile–target but in the framework of the time and/or space scale, which is *large* in comparison to the corresponding standards typical for proper interparticle interactions encountered in theme (i). For this simple reason, scattering theory is the most efficient and often the only method of investigating the microstructure of matter.

Scattering theory is something more than a simple dynamics with an account of various interactions. Dynamics of non-collisional physical systems usually develop in some finite time intervals, such as $t \in [-\tau, \tau]$ ($|\tau| < \infty$). In contrast to this, in scattering theory, one is examining special sorts of states of interacting systems, known as 'asymptotically free' scattering states, whose existence must be proven for the case before the collision, i.e. in the remote past ($t \to -\infty$), as well as when the scattering is over, i.e. in the distant future ($t \to +\infty$). In scattering problems, one performs a comparative analysis of behaviours of a given physical system projectile–target in two diametrically opposite situations, i.e. under the binding and free dynamics. The former and the latter dynamics correspond to the case with and without the interactions between the colliding particles. Free dynamics develop under the influence of the unperturbed Hamiltonian H_0, whereas the total Hamiltonian H governs the binding dynamics. Then it is clear that the difference $H - H_0$ will represent the interaction V which causes the collision to take place, provided that certain initial conditions are fulfilled. Hence, interaction V between the colliding particles naturally plays the role of a perturbation potential, which is the sole cause of the transition of the system under study from a given initial to a certain final state out of all the possible final configurations. However, although such a concept of the collision problem is formally enrolled into a standard framework of the perturbation theory, it should be realized that potential V in the expression $H = H_0 + V$ must not necessarily, in any sense, be small in regard to unperturbed Hamiltonian H_0. Even in the case when V is smaller than H_0, the collision problem requires the more difficult variant of the perturbation method for an *absolutely continuous spectrum*. This is in sharp contrast to bound-state problems, which necessitate only the discrete spectrum of a given Hamiltonian.

Standard scattering theory has originally been introduced in nuclear physics, where the interactions are of short range [1–4], so that in the asymptotic region, the aggregates can be considered as being fully *free*[2]. The same formalism is,

[2] Under the notion 'short-range potentials', we will henceforth understand a function $V(\boldsymbol{r})$ which is quadratically integrable: $\int d\boldsymbol{r} |V(\boldsymbol{r})|^2 < \infty$ or locally quadratically integrable: $\int_{r \le R} d\boldsymbol{r} |V(\boldsymbol{r})|^2 < \infty$, and which behaves as $\mathcal{O}(r^{-\beta})$, $\beta > 1$, when $r \to \infty$. In the opposite case, we shall speak of 'long-range potentials', whose general form is $V(\boldsymbol{r}) + \gamma/r$, where $V(\boldsymbol{r})$ is a short-range interaction, whereas γ/r represents the Coulomb potential (γ is the coupling strength and $r \equiv |\boldsymbol{r}|$). Here the notation $V(\boldsymbol{r}) = \mathcal{O}(r^{-\beta})$ explicitly means: $|V(\boldsymbol{r})| \le c/r^{\beta}$, where c is a certain positive constant.

however, not applicable to Coulomb potentials [5,6], for which the usual S-matrix cannot be defined because the Møller wave operators $\Omega^{\pm}$, do not exist in the so-called strong limits (when $t \to \mp\infty$) of the product of the interacting $U^{\dagger}(t) = e^{iHt}$ and free $U_0(t) = e^{-iH_0t}$ evolution operator of a given conservative physical system [7]. This is a direct consequence of the fact that the Coulomb interaction never vanishes (not even for very large values of the distance between the colliding aggregates). Ignoring these special features of the Coulomb potential, which has often been done in the literature on atomic collisions [8, 9], leads to divergencies of the perturbation Born expansions of the transition amplitudes for passing from an initial to a final state of an investigated physical system. These divergencies are due to the fact that the two-particle Coulomb transition amplitude does not possess its *on-shell* limit for the case of plane waves[3]. These off-shell amplitudes are present as the kernels of the integral equations of the three-particle transition amplitudes. There have been some attempts [8, 9] to artificially remove the divergencies by subtracting an also divergent Coulomb phase factor, say Δ. This is, however, unjustified because, according to the same reasoning, one could have as well subtracted any other term of the type $\Delta + \delta$, where δ is an arbitrary *finite* quantity. This, of course, means that the final result is completely undetermined, i.e. *arbitrary*. Instead of such an unphysical approach, one should compute the two-particle *off-shell* transition amplitude with the Coulomb wave in place of the plane wave, so that the final result will always be finite and without any arbitrariness [10]. Hence, a direct taking of the definition of the S-matrix from the theory of nuclear collisions leads to singular expansions of the Coulomb amplitude for atomic scattering. This automatically implies that the first Born approximation cannot be interpreted as a mathematically meaningful first term of a perturbation series, because the latter is *divergent*. Attempts to do so have led, in a number of concrete computations for the case of charge exchange, to a flagrant disagreement between the first Born method and measurements [11, 12]. For example, for highly asymmetric charges of the nuclei of the colliding particles, the conventional first Born approximation in the form of Jackson–Schiff's [13] or Bates–Dalgarno's [14] method, predicts cross sections which overestimate the corresponding experimental data by several orders of magnitude. It then clearly follows that a substantial reformulation of the Coulomb scattering theory is necessary in accordance with the requirement of the existence of the previously mentioned strong limits of the wave operators. The first finite S-matrix time-dependent scattering theory encompassing Coulomb potentials was developed by Dollard [7] in 1964 in a rigorous mathematical form for both the one- and multi-channel case. Fundamental aspects of Dollard's [7] analysis, however, did not receive due attention for a long time, thus remaining attractive merely in the framework of the formal theory of scattering. The reason for this lies in

[3] The term *on-energy-shell* or the shorter *on-shell* signifies that the transition from an initial to a final state occurs *on the energy shell* or surface, where the energy conservation law holds true. Otherwise, when the energy is not conserved, we are talking about an event occurring *outside the energy shell*, i.e. about the so-called *off-energy shell* or the shorter *off-shell* phenomenon.

the fact that the Coulomb problem has been modified in [7], by introducing the logarithmic corrective terms for $\Omega^{\pm}$ in the form of certain integral *operators*, which are very inconvenient for practical purposes. The situation substantially changed in 1979, when Belkić *et al* [15] showed that the introduction of Dollard's logarithmic modifications of the Møller wave operators $\Omega^{\pm}$ is equivalent to the requirement of the so-called *proper boundary conditions*. These conditions impose the proper behaviours on the total scattering wavefunctions at infinitely large inter-aggregate separations, in accordance with the given physical aspects of the investigated problem. The required behaviours of the total *scattering state* are determined by the very nature of the interactions between the widely separated aggregates in the asymptotic region of scattering. In other words, for short-range potentials it is justified to employ the plane waves to describe the relative motion of the aggregates, whereas the full Coulomb wavefunctions become indispensable for long-range Coulomb potentials. These latter functions must be compatible with the eigenvalue problem in the corresponding channel of the reaction. In this manner, a complicated Dollard's [7] operator reformulation of the standard scattering theory is reduced to the relevant modifications of the wavefunctions. This is by far an easier task than the operator formalism, so that the road to applications of the proper atomic scattering theory was open, without which the formal aspects of Dollard's theory would remain empty and quantitatively unconfirmed. Moreover, in [15], an *exact* eikonal transition amplitude for three-particle rearrangement ion–atom collisions has been derived which is valid for short-range as well as long-range potentials and, as such, is applicable to problems in both atomic and nuclear physics (e.g. charge exchange, ionization, stripping, pick-up and break-up reactions, etc). An entirely analogous formalism can also be established for direct collisions, e.g. excitation of the target by the impact of heavy charged particles. Numerous applications of the scattering theory for long-range potentials, devised in the manner proposed in [15], reveal an excellent and systematic agreement with experimental data [16–19]. This will be thoroughly illustrated in part II of the present book, where the most comprehensive computations to date have been carried out for charge exchange, detachment and transfer ionization in high-energy ion–atom collisions.

Chapter B

The main physical features of collision problems

In contrast to a classical Hamiltonian, which always possesses continuous eigenvalues, a quantum-mechanical Hamiltonian can have both discrete and continuous spectra. Discrete eigenvalues correspond to stable *bound states*, whose appearance is explained by the existence of the proper interactions of sufficient strength to hold together the participating particles in a given *finite spatial domain*. This will be the case if the wavefunctions of bound states in the configuration space decrease rapidly at large values of the interparticle distance. In contrast to this, the continual spectrum is associated to *scattering states*, meaning that some of the constituent bodies will escape into the asymptotic region of *infinitely large interparticle separations*. To these *generalized free states* of particles, one customarily attaches the plane wave $\phi_{\boldsymbol{\kappa}} = \mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}\cdot\boldsymbol{r}}$ characterized by the so-called wavevector[1] or propagation vector $\boldsymbol{\kappa}$. However, plane waves are diffused throughout the space and, as such, cannot describe a particle, which must be localized in a given limited spatial region. In contrast to plane waves, the so-called wave packets $\phi(t)$, formed as a linear combination of the type $\phi(t) = \int \mathrm{d}\boldsymbol{\kappa}\overline{w}(\boldsymbol{\kappa})\phi_{\boldsymbol{\kappa}}\mathrm{e}^{-\mathrm{i}E_\kappa t}$ with a certain peaked[2] weight function $\overline{w}(\boldsymbol{\kappa})$ about the incident direction $\boldsymbol{\kappa} \approx \boldsymbol{k}_i \equiv \boldsymbol{k}$, are normalizable in the sense that they belong to a separable Hilbert state space $\mathcal{H}$. These wave packets are (indirectly) physically interpretable vector states of a finite norm, despite the fact that we are dealing with the continual spectrum of the Hamiltonian. As an illustration, we give the following example of the previously mentioned weight function: $\overline{w}(\boldsymbol{\kappa}) = N(\kappa)\mathrm{e}^{-|\boldsymbol{\kappa}-\boldsymbol{k}|^2/\kappa^2}$, where $N(\kappa)$ is the normalization factor. This Gaussian function $\overline{w}(\boldsymbol{\kappa})$ behaves like the Dirac δ-function in the region $\boldsymbol{\kappa} \approx \boldsymbol{k}$. Of course,

[1] Unless otherwise stated, throughout this work atomic units will be utilized, i.e. $\hbar = e = m_\mathrm{e} = c = 1$, where $\hbar$ is the Planck constant, whereas e and m_e represent the charge and mass of the electron, respectively.

[2] The word 'peak' is often employed in physics in the context of appearance of certain local maxima of a given function for some of the values of its argument.

it is quite obvious that the continuous spectrum of Hamiltonians exhibits its most important applications precisely in the theory of particle scattering.

B.1 Recognizable reference points of scattering theory

Every important physical theory possesses its certain 'trade mark' or emblem, i.e. some apparent and easily recognizable symbol or equation. For example in classical Newtonian mechanics that symbol is given by the expression $\boldsymbol{F} = m\boldsymbol{a}$, Einstein's theory of relativity has its symbol in the energy–mass relation $E = mc^2$, then the assignment of the quantum field theory could be some of the typical Feynman graphs, e.g. vacuum polarization or self-energy of the electron. For the very first association with quantum mechanics of bound states one would inevitably think of the Schrödinger eigenvalue problem $H\Psi_n = E_n\Psi_n$, etc. The reference point of scattering theory, however, is the Lippmann–Schwinger integral equation of the total scattering state with the well-known asymptotic behaviour in the coordinate representation:

$$\Psi_{\boldsymbol{k}}^{+}(\boldsymbol{r}) = \langle \boldsymbol{r}|\Psi_{\boldsymbol{k}}^{+}\rangle \underset{r\to\infty}{\longrightarrow} (2\pi)^{-3/2}[\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} + f(\vartheta,\varphi)\frac{\mathrm{e}^{\mathrm{i}kr}}{r}]. \qquad (\alpha)$$

Here the first term represents the incident plane wave with the initial wavevector $\boldsymbol{k}$, whereas the second contribution appears as a product of the transition amplitude $f(\vartheta,\varphi)$ and spherically scattered wave $r^{-1}\mathrm{e}^{\mathrm{i}kr}$. A detailed inspection of this first association with the scattering theory of one particle at a given local short-range potential $V(\boldsymbol{r})$ would reveal that (α) contains four pieces of basic information. *The first* relates to the superposition of the incident and scattered waves in full accord with the universal Huygens principle, which asserts that every spatial point hit by a wave becomes itself a source of new secondary spherical waves. Although simple, the Huygens principle can be, as we shall occasionally demonstrate in this book, a very useful tool in developing such basic substrates of scattering theory as, e.g., the Green function or the Lippmann–Schwinger integral equations for the total scattering wavefunctions. *The second* piece of important information is the fact that the stationary asymptotic solution $\Psi_{\boldsymbol{k}}^{+}(\boldsymbol{r})$ from (α) satisfies the time-independent Schrödinger equation but for the continuous spectrum of the Hamiltonian H. *The third* essential point from (α) is that the quantity $|f(\vartheta,\varphi)|^2$ becomes proportional to the experimentally measurable differential cross section $\mathrm{d}Q/\mathrm{d}\Omega_i$, where $\Omega_i = (\vartheta,\varphi)$ represents the solid angle around $\boldsymbol{k} = (k,\vartheta,\varphi)$, through which the incident wave is scattered:

$$\frac{\mathrm{d}Q}{\mathrm{d}\Omega_i} = \frac{\text{outgoing flux/solid angle}}{\text{incoming flux/area}} = |f(\vartheta,\varphi)|^2. \qquad (\omega)$$

Finally, *the fourth* but at the same time, for scattering theory, the most crucial insight which can be gleaned from the asymptotic form (α) is that in the remote past $(t \to -\infty)$ only the *free* wave remains from the wave packet $\Psi_{\boldsymbol{k}}^{+}(t,\boldsymbol{r}) =$

$\int d\boldsymbol{\kappa}\overline{w}(\boldsymbol{\kappa})\Psi_{\boldsymbol{\kappa}}^{+}(\boldsymbol{r})e^{-iE_{\kappa}t}$ formed by means of the stationary asymptotics (α) and a certain weight function $\overline{w}(\boldsymbol{\kappa})$ dominantly concentrated around $\boldsymbol{\kappa} \approx \boldsymbol{k}$.

The notion 'free wave' used in the previously mentioned remark is linked to the spatial asymptotics ($r \to \infty$) and this corresponds to the stationary formalism, which, from the chronological viewpoint, was the very first framework for introducing scattering theory. However, there are no valid reasons that such a road should be followed in the modern presentation of the theory of particle collisions. On the contrary, there exist two strong motivations to proceed in a different manner. First, scattering theory in its original derivation abounds with heuristic concepts, which received their justification only later, when the time-dependent formalism had been put forward. In that sense, one should critically view the asymptotics (α) for $\Psi_{\boldsymbol{k}}^{+}(\boldsymbol{r})$. Second, although the S-operator (whose matrix elements are, in fact, the probability amplitudes of finding the given colliding system in a certain state) represents the constant of motion, thus exhibiting the global stationary character of the scattering phenomenon, the collision event still effectively takes place in distinct time episodes, which naturally demand a time-dependent description as the optimal theoretical framework. The present work will thoroughly employ such a non-stationary formalism for which, instead of a search of the asymptotics of the scattering states $\Psi_{\boldsymbol{k}}^{+}(\boldsymbol{r})$ in the limit $r \to \infty$, one looks for the limiting values of the state vectors and operators (i.e. the elements of the non-commutative algebra), when the real-time variable t tends to $\mp\infty$. In any case, stationary and non-stationary scattering theory complement each other in many theoretical derivations as well as in versatile applications. The passage from non-stationary to the stationary formalism is carried out by means of Fourier transforms or through the use of Abel–Cauchy limits. This passage is especially important in the final operational part of the analysis, when one is preparing for concrete numerical computations, which are necessary for a quantitative testing of the theory in comparison with experiment. There are, however, several substantial reasons for which the very first contact with scattering theory should not be based upon the asymptotic (α) and the resulting interpretation (ω). Namely, relation (α) is interpreted by saying that the wavefunction $\Psi_{\boldsymbol{k}}^{+}(\boldsymbol{r})$ represents the sum of the incident particle beam of momentum $\boldsymbol{k}$ of a steady form described through the plane wave $e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$ and the spherically expanding scattered wave $r^{-1}e^{ikr}$ of the amplitude $f(\vartheta, \varphi)$. Interpreted only in this way, the asymptotic (α) can directly lead to the definition (ω) of the differential cross sections $dQ/d\Omega_i$. However, the wavefunction $\Psi_{\boldsymbol{k}}^{+}(\boldsymbol{r})$, which depends exclusively on one variable $\boldsymbol{r}$, can eventually represent a state of only *one given particle* and not the particle *beam*. This beam is, however, precisely necessary in the definition (ω), which rests upon *the particle flux*. Moreover, vector state $\Psi_{\boldsymbol{k}}^{+}(\boldsymbol{r})$ from (α) is not even normalizable, i.e. its norm is infinite. Therefore, the wavefunction (α) cannot in any way represent a *proper* state of a particle and, as such, it does not even belong to the appropriate separable Hilbert eigenstate space $\mathcal{H}$, whose elements must all be square integrable. This is clearly seen already on the level of the initial configuration of the projectile, which is represented by the

plane wave $e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$, playing the role of a generalized state of the operator H_0. These are also equivalently called the *improper* states, which cannot be found in the Hilbert space $\mathcal{H}$ of proper, normalizable and physically interpretable physical states. Furthermore, the wavefunction (α), which satisfies the stationary Schrödinger equation $H\Psi_{\boldsymbol{k}}^{+}(\boldsymbol{r}) = E\Psi_{\boldsymbol{k}}^{+}(\boldsymbol{r})$, corresponds to a certain model situation which is stable, i.e. unaltered with the passage of time, and this is diametrically opposite to an obvious time development of any real physical scattering problem. In addition, separate evaluation of the flux of the incoming and outgoing particle, as done in (α) and (ω), completely ignores the interference between the incident and scattered waves. This interference, however, represents an effect of primary importance for forward scattering. Namely, one of the evident characteristics of the description of a collision event within the wave formalism is that the amplitude of the incident plane wave decreases by its passage through the interaction domain. Such an effect is only possible to account for via a destructive interference of the original incident wave and the secondary spherical scattered wave. This occurs in the direction of the propagation $\boldsymbol{k}$, i.e. for forward scattering. In order to overcome all of these difficulties of the standard stationary scattering theory, it became customary to introduce *a posteriori* various artificial recipes, such as normalization of free waves in a certain box of large dimensions, then averaging the results by means of the Fourier analysis with the help of a convenient weight function, say $\overline{w}(\boldsymbol{\kappa})$, which is peaked around the incidence direction $\boldsymbol{\kappa} \approx \boldsymbol{k}$, etc. Because of these critical remarks, we shall abandon altogether the aforementioned usual, stereotypical approach to scattering theory and expose its essential principles on a modern level. Thus, for example, the correct formulation of the initial and final scattering states will be, from the onset, based upon the *wave packets*, which are the elements of $\mathcal{H}$ and, therefore, can represent proper physical states. Such a treatment is in natural harmony with the situation encountered in the collision, since the wave packets are localized in a limited spatial region, and that is the very first precondition that a given wave can describe a particle in any way. This is in contrast to the plane waves, which not only represent a physical abstraction and idealization but are also mathematically most inconvenient, since they do not belong to the Hilbert eigenstate space $\mathcal{H}$. With regard to the proposed concept on which we shall expose the major selected principles of modern scattering theory, these introductory remarks will be thoroughly worked out in the forthcoming chapters. Particular attention will be paid to the appropriate definition of the sufficient and necessary conditions for selecting (from a large class of all the quantum-mechanical particle systems) a certain subclass known as *quantum scattering systems*. The elaboration of these ideas will be accomplished by extensive use of the elements of functional analysis, strong topology and spectral analysis of the operators.

Chapter C

Universality of the scattering problem

In order to convince ourselves of the intrinsic importance of the *theory* of scattering, its universality and presence in various branches of physics and other neighbouring sciences, including technology and industry, let us give a few of the most remarkable illustrations.

First, numerous phenomena in the micro-world (nature which is unobservable to the naked eye) are the net result of collisions among mass and/or massless particles, e.g. glory, corona, etc. For a proper explanation of these and similar events, it is necessary to examine their dynamics from the viewpoint of the theory of the scattering of light on atmospheric particles. Furthermore, if dust is suspended in a liquid, it is easily *seen through a microscope* that the dust particles are moving randomly along various zig-zag paths in an entirely unpredictable manner. This is the well-known Brownian motion which, according to Einstein's explanation in this case, occurs because of a number of continuous *collisions* of the dust particles with the molecules of the neighbouring medium. Through these collisions, the dust suffers an uneven number of strikes from all sides, thus acquiring a momentum which is not compensated, so that the dust moves randomly in various directions. Hence, the phenomenon of Brownian motion is one of the most direct and *obvious* confirmations of the molecular motion of matter. Note that Brownian motion can be modelled by means of stochastic processes of the Markov type and of the Ohrnstein–Uhlenback type. The well-known Feynman theory of graphs exhibits a certain formal resemblance to the Brownian model.

Second, using the dynamics of certain well-studied wave and/or particle scatterings as a prototype often turns out to be of great value in examining the structure of other, more complex and otherwise directly inaccessible objects. Let us cite only a few areas: roentgen crystallography, which led to the discovery of deoxyribonucleic acid (DNA), then in positron tomography, echo cardiography, in research and the discovery of certain undersea objects by means of ultrasound, etc. In this endeavour, based on the fact that the dynamics of ultrasound are well known, one is interested in the position description as well as in the internal

structure of the matter under study using the data on scattering of ultrasound on the observed objects or on organs in a patient's body during medical examinations. Such an assumed relation could be expressed through a certain convenient functional dependence (in an ideal case this could even be reduced to some explicit formulae or equations), which, in turn, would allow one to approximately reconstruct the studied object according to the data on model scatterings. In practice, however, this process is nowadays so much simplified and standardized, that e.g. in obtaining an echo cardiogram by means of ultrasound, the commercial apparatus already contains built-in calibration for determining the depth from which the echo comes.

Third, scattering theory often represents the 'gold standard' for the very dynamics of physical systems. Thus, for example, in elementary particle physics, the dynamics are not well known due to postulated interactions and every important measurement is, in fact, the scattering experiment. Here the key question and the eliminating test of any proposed dynamics reduce to examination of the possibility of conceptually devising a scattering theory accompanied by its fundamental entities, e.g. *unitary* and convergent (meaning re-normalizable) S-matrix (scattering matrix). Such a scattering theory must be capable of explaining and interpreting the existing experimental data, thus activating its descriptive role. The latter role, however, should not be the only task of theoretical concepts which, most importantly, must promote the theory as a powerful predictor, whose results would precede the measurement and thus anticipate yet unobserved physical phenomena. In this way, scattering theory would permanently offer new challenges to experimental investigations. Hence, the previously mentioned key question is, in fact, raised to the pedestal of the type of *raison d'être* for the theory, i.e. it represents the very reason for the theory's existence. Such an assertion has certainly the most convincing justification in the example of elementary particle physics, because any real progress in this research area critically depends upon the technological feasibilities of achieving high-energy incident beams for scattering experiments, which would create new (otherwise only theoretically postulated) particles.

C.1 Fundamental aspects of collision theory

The fundamental aspects of collision theory were put forward in 1933 in the book by Mott and Massey [20], where the cornerstones were formulated in the domain of *atomic collisions*. However, numerous and very important contributions to the area of scattering followed later in other branches of physics. These contributions stemmed chiefly from (i) *quantum field theory*, which necessitates a more abstract and more general formulation of the scattering process than the one given in [20] and from (ii) *nuclear physics*, where it was indispensable to systematize the experimental data on nuclear reactions, without any knowledge of the nature of nuclear forces. Here we mainly have in mind the following achievements in the

development of scattering theory: introduction of the S-matrix concept (Wheeler [21], Heisenberg [22]), general formulation of the mathematical problem of finding the S-matrix [23–26], behaviour of cross sections in the vicinity of resonances and thresholds of reactions [27,28], obtaining the interaction potential from the S-matrix [29,30], etc. Let us emphasize that the S-matrix plays a central role in quantum mechanics and in quantum field theory, because this operator is the carrier of the actual and/or postulated *interactions* among particles as the main generators of the physical properties of matter.

Development of the mathematical concept of scattering theory proceeded quite slowly because of difficulties in the mathematical problems themselves, as well as the lack of collaboration among mathematicians and physicists. Given these circumstances, the physical literature for a long time abounded in heuristic formulae and methods, empirical equations, artificial prescriptions introduced *ad hoc*, etc. The situation, however, fundamentally improved in 1958 (Jauch [31,32]), in 1960 (Faddeev [33–35]) and in 1964 (Dollard [7]), when enormous steps were made through the formulation of the problem of one- and multi-channel collisions in a rigorous mathematical manner for short-range potentials [31–35], as well as for long-range interactions [7].

C.2 Collisions in various branches of physics

The *scattering experiment* plays one of the leading roles in the part of physics devoted to measurement, irrespective of whether one is concerned with particle collisions or with scattering of photons on various substances. To see that this statement is true, it suffices to make only a cursory inspection of the literature. For the purpose of illustration, let us quote a few of the most remarkable experimental results.

In atomic physics, Rutherford's [36] experimental discovery of the nucleus in 1911 resulted from his examination of scattering of α-particles on thin foils of gold atoms. The results of this remarkably simple measurement had far reaching consequences, which already in 1913 initiated the foundation of the Bohr [37] model of atomic hydrogen based on the concept of stationary states. The first direct confirmation of the existence of these stationary states of atoms came in 1914 through Franck–Hertz's [38] experiment on inelastic scattering of electrons on the mercury target vapour. The well-known Davisson–Germer [39] experiment on collisions of electrons with the solid surface convincingly proved the concept of electron diffraction. This latter measurement unambiguously confirmed the existence of the dualistic wave–corpuscular nature of the electron, as one of the fundamental hypotheses of quantum wave mechanics due to de Broglie.

In nuclear physics, the first clear confirmation of nuclear structure came in 1919 in Rutherford's [40] experiments on collisions of α particles with a nitrogen ($^7N^{14}$), whose nucleus decays and forms an oxygen ($^8O^{17}$) and a free proton (p), i.e. $\alpha + {}^7N^{14} \longrightarrow p + {}^8O^{17}$.

In elementary particle physics, the scattering experiment is, in fact, the principal method of creating new matter. Thus, for example a π^0 meson can be obtained in the collisional reaction of two protons: $p + p \longrightarrow p + p + \pi^0$. This experimental discovery was performed in 1947 by Lattes *et al* [41, 42], who thus confirmed Yukawa's [43] theory of mesons from 1935 for strong interactions among nucleons. More recently, in the well-known experiment on the collision between protons and anti-protons ($\bar{p}$) carried out in 1983 in CERN (Geneva), vector bosons $W^{\pm}$ and Z^0 were discovered. These latter particles together with photons, represent the mediators of the electroweak interactions. This measurement confirms Weinberg–Salam–Glashow's [44–46] theory from 1967 by which the unification of electromagnetic and weak interactions was accomplished. This is considered as one of the most significant achievements in the 65-year -old investigations in elementary particle physics [47].

C.3 Importance of collisions in atomic and molecular physics

Broadly speaking, atomic and molecular physics have the task to discover and apply the fundamental laws of nature, to acquire further knowledge and explain the structure of matter and its evolution on the *atomic and molecular level* and then, finally, to make a direct use of its own findings, as well as to pass these to other scientific disciplines and technologic branches. These goals are *predominantly* accomplished through the method of atomic collisions with or without the presence of external fields. Collision problems include at least 80% of the entire research themes and activities in the domain of atomic physics theory. The field of atomic scattering, by its original theoretical and experimental methods, as well as technical achievements and *data bases*, plays an essential role in developing other scientific disciplines in physics (plasma physics, nuclear physics, solid state physics), as well as in other branches of science (astrophysics, quantum chemistry, biophysics, medicine). From such an active role for atomic physics in the last three decades, the scientific community has witnessed the development of quantum physics of surface as a relatively autonomous field, which is a product of the synthesis of the themes and methods of atomic, molecular and solid state physics. Here also one of the most propulsive research activities is precisely the *collision* of mass and/or massless particles on the surface of solid bodies.

Phenomena on the atomic level also play an important role in preparing the experiment in the physics of elementary particles. Thus, for example, in planning investigations of hadron interactions of mesons with nucleons, essential information is necessary about the initial population of negative hadrons[1], after their capture in the atomic orbitals during the action of the field of the Coulomb potentials of the nuclei. These data are provided by the atomic

[1] The name of 'hadrons' comprises particles such as barions and mesons, which are characterized through their strong interactions.

collision field, through data based on the theoretical and experimental findings on the formation of muonic, pionic and kaonic exotic atoms of hydrogen via the mechanism of radiative recombination. Quark–antiquark interactions are successfully represented in the framework of the current confinement model (charmonium) in elementary particle physics by a linear superposition of a Coulomb field and the potentials in the form of a power function of the distance [48]. Data on muonic atoms, which are formed through rearranging collisions, are also necessary for modern studies of nuclear properties.

Research areas linked to atomic and molecular systems in external fields are of great importance from the standpoint of the advancement of the theory itself and especially in connection with numerous applications in various branches of physics and also in other sciences (astrophysics, medicine, etc), as well as in technology and industry. The interaction of radiation with matter takes a central place in these investigations. Under the notion of 'radiation', we understand the electromagnetic field in the largest sense of the word, which also comprises so-called laser radiation. If the intensity of the light source is sufficiently strong, it would be possible to observe the transitions followed by absorption, emission or scattering of one or more photons. We quote here only the experiment of Agostini *et al* [49], who succeeded in detecting the ionization of atomic hydrogen as a result of absorbing 19 photons. This type of process is called multi-photon ionization, whose detection generally requires high intensity radiation [50, 51]. Even more significant is the problem of excited states, whose distribution in atoms could substantially be modified by turning on the laser field. Namely, due to a weak binding energy, these metastable atoms are sensitive to external fields. This, in turn, offers an excellent possibility for basic testing of our actual knowledge about the atomic physics of *strong* fields. The laser technique is nowadays also used very successfully for a selective formation of atoms in highly excited Rydberg states. The problem of the Rydberg atoms in external fields represents those typical physical systems with dominantly exhibited instabilities, so that this research domain of atomic physics is, in part, tangent to problems in chaos, i.e. in nonlinear dynamics [52]. Interest in highly excited atomic states in external magnetic fields is heightened also in a larger context, such as, e.g., the possibility of incredibly strong magnetic fields in the regions near black holes, pulsars and neutron stars [53]. For these extraordinarily strong fields, the nature of atoms and molecules must be drastically modified in comparison with the normal situation without external fields. Therefore, observations of radiation lines, which are due to emission from the excited states of these highly deformed atoms, indeed represent a great challenge to experimentalists.

Due to the dominant role of scattering phenomena in research within atomic and molecular physics, it is fundamental to formulate scattering theory from *first principles*. Here we must emphasize the inapplicability of the standard concept of nuclear physics, so that the question of the investigation of the typical features of atomic interactions of *long-range* nature manifested through Coulomb interactions emerges as the most important point of departure. The peculiarity

of Coulomb interactions is transparent through the fact that their effect is felt even at infinitely large distances from the centre of scattering. This feature leads to considerable modifications of the states of those physical systems which are charged as a whole. This long-range effect has a decisive influence upon the quantitative predictions of theory, as conclusively demonstrated in [15]. In the literature, a misleading argument against the use of the correct treatment of the Coulomb potentials has, for a long time, been employed. This is the observation that, in realistic situations, all interactions are screened at large distances, so that one can introduce a sufficiently large cut-off and forget altogether about the troublesome Coulombic effects. However, such an argument is false for the following reasons. If we are about to screen a given Coulomb potential at a certain large but finite distance r_0, then all the resulting transition amplitudes derived from such a modification would only be meaningful if they do not depend upon the distance r_0. However, it is quite clear that such a cut-off of a Coulomb potential would not alter the final results, i.e. the transition amplitudes $T_{if}^{\pm}$ will be insensitive to the choice of r_0 only if r_0 represents a sufficiently large distance, so that the neighbourhood $r \sim r_0$ does not give any contribution to the values of $T_{if}^{\pm}$. However, this means, in particular, that for the spatial domain R, which includes all the points $r < r_0$ but such that r is close to r_0, one should take proper account of the long-range (because r_0 is large) Coulomb behaviour of a given potential in order to avoid spurious contributions from the region R. In other words, one is again faced with the request for the correct treatment of the Coulomb interaction but this time for the reason of eliminating the wrong contributions to the transition amplitudes coming from the *cut-off* distance r_0. This analysis illustrates how introducing a screening of the Coulomb potentials unnecessarily complicates the problem. Thus, Coulomb screening is completely undesirable. It is ironic that the cut-off procedure modifies the potential only in the region which, for consistency, must afterwards be excluded from the domains which provide physical contributions to the transition amplitudes. It then appears as the natural and easiest way to ensure that the quantities $T_{if}^{\pm}$ are identical, *with* and *without* the screening, to include the long-range behaviour of the Coulomb potential exactly from the very beginning, as in [10, 15]. In addition, the theory of [15] is general in the sense that it is applicable to various ion–atom collisions, which lead to electron transfer, excitation, ionization, Auger processes, etc. All these reactions exhibit divergent Born expansions, so that *the exact* eikonal formalism from [15] represents a universal manner of regularization of the transition amplitudes. Here, the notion *eikonal* relates to the collisions at small scattering angles. The eikonal method is otherwise a perfectly adequate framework for studying ion–atom collisions. Namely, as is well known in collisions between heavy particles, due to the large projectile mass, the incident beam deviates only slightly from its original direction. Therefore, the total cross sections obtained through integrations over given angular distributions are predominantly determined by the contributions from extremely small angles (fractions of milli-radians), in the immediate vicinity of the region of the forward scattering. The contributions from larger scattering

angles stem from the Rutherford scattering, as a result of a Coulomb repulsive interaction between the incident and target nucleus. Including this latter effect would yield a correction to the transition amplitudes $T_{if}^{\pm}$ of the order of, at the most, the values of the ratio of the masses of electron and proton ($\sim 10^{-4}$), in comparison to the major contribution from the interaction between the electron and the incident nucleus. Hence, the exact eikonal transition amplitudes account exactly for the contribution from the interaction electron–nuclei, whereas the contribution from the nucleus–nucleus potential is incorporated approximately in the eikonal sense ($\sim 1/\mu$), where μ is the reduced mass of the incident and target nucleus. Moreover, thus obtained exact eikonal transition amplitudes $T_{if}^{\pm}$ from [15] contain the entire contribution from the internuclear potential in the form of a phase factor, which modifies only the differential and not the total cross sections. In this manner, the long-standing controversy with regard to the question as to whether or not the nucleus–nucleus interaction should be taken into account [13, 14], is conclusively resolved. The definite answer given in [15], which has subsequently been accepted by others as a general fact [16–18], is that the internuclear potential yields a contribution of the order of $\mathcal{O}(1/\mu)$ to the transition amplitudes $T_{if}^{\pm}$ only if that interaction is accounted for exactly in the eikonal sense. If this basic fact is ignored, as has repeatedly been done in the literature, one obtains unphysical modifications of the observables. These modifications can sometimes be wrong by several orders of magnitudes [11, 12].

C.4 Collisions and new sources of energy

In research connected with controlled thermonuclear fusion, which represents one of the possible energy sources, the role of atomic collisions is of exceptional importance [54, 55]. The properties and behaviour of magnetically confined, high temperature thermonuclear plasmas of low density are determined by collisions among the particles in the plasma. Stability, which is one of the most essential characteristics of fusion plasmas in *tokamacs*, is substantially influenced by neutralization processes, e.g. charge exchange, as well as by collisions which can heat plasma, such as ionization. Atomic collisions to a large extent also affect: (a) the plasma radiation, as one of the dominant mechanisms of cooling of fusion plasma, (b) the transport of neutral particles in tokamacs, (c) the flux distribution of momentum and energy among the constituents of plasma, etc. Here, a particular place is reserved for collisions between multiply charged ions with hydrogen and helium. These ions are present in the peripheral edge of the plasma in tokamacs and they have a significant influence upon radiation losses and additional methods of heating by neutral beams. In fusion research, a particular emphasis is given to multi-electron correlated processes, such as simultaneous electron transfer and ionization (transfer ionization), double charge exchange, electron capture and excitation (transfer excitation), double excitation, simultaneous ionization and excitation, double ionization, etc. These processes

play a key role in modern toroidal machines for magnetic confinement of high-temperature plasmas, in the balance of energy and transport properties as well as in diagnostics [54, 55]. Of considerable importance is also obtaining original quantitative data on these processes. Such data should shed new light onto the basic *mechanisms* of the multi-electron transitions. These theoretical results should also include evaluations of the cross sections of certain typical ion–atom reactions through the use of the most successful approximations available in the literature (e.g. the *exact* second- and higher-order Born approximations, the continuum distorted wave method, the reformulated impulse approximation, etc). In the case of electron–atom collisions, encompassing both the target in its ground or metastable state, the so-called eikonal-Born series emerged, from a number of studies, as a very reliable method at intermediate and high energies [56]. However, in contrast to the exact eikonal theory of [15], which treats the electronic motion exactly, the eikonal-Born model approximates the kinetic energy of the electrons by the corresponding eikonal, linearized terms. Furthermore, we mention in regard to fusion that the diagnostic of the fusion plasma is based upon the effects produced in atomic collisions. Spectroscopic techniques, designed on *bremsstrahlung* or on the intensity of individual lines, require knowledge of the data for excitation and the whole string of other collisional processes, which lead to the population of certain energy levels in atomic systems. Active and passive diagnostic techniques with particle beams are mainly based upon the problem of scattering in which electron transfer takes place [54, 55]. There is yet another important application of the data base on atomic and molecular physics in fusion, namely study of the transport of momentum and energy in plasmas. Here atomic collisions can considerably affect the flux distributions of momentum and energy among the constituent particles of the plasma [54, 55].

Let us also point out that in 1991 in Abingdon (England), the researchers on the Joint European Torus (JET) succeeded, for the first time, to obtain a considerable quantity of electric power of the order of (1.5–2.0) MW from controlled thermonuclear fusion. This was, without any doubt, a crucial step forward in the development of fusion as a new energy source. This fusion experiment with confining magnets used a gaseous mixture of deuterium and tritium as the reactor fuel, which was heated up to the temperature of $\sim(2 \times 10^8)$ °C, i.e. about ten times higher than the temperature in the centre of the Sun. The pulse generated by fusion has reached the order of magnitude of $\sim$1 MW with a duration of 2 s and the deuterium torus exhibited stable conditions in the tokamacs in the period of 1 min. Through this milestone experiment, the several decades long effort of a large number of physicists has been successfully brought to the finishing point from the *scientific* point of view. Of course, this is not yet the end of the whole endeavour, since further fusion *technology* projects are still ongoing within the realm of the planned construction and implementation of the International Thermonuclear Experimental Reactor (ITER), which is predicted to produce more than 1000 MW of thermal energy. After this achievement, there remains yet the final goal of the engineering technology, i.e. commercial

production of electric and thermal power from the fusion processes. This will represent the culmination of one of the most profound thoughts of physicists in connecting fundamental physical phenomena with the efficient creation of new energy for the versatile needs of humankind.

C.5 Application of collisional phenomena in other sciences

Nuclear magnetic resonance (NMR) is intensively used as a non-invasive procedure in medicine, e.g. in the most reliable modern diagnostics of the disease of the brain, spinal cord and the cardiovascular system (particularly of the aorta). Here, precise magnetic-resonance pictures of the damage to various human organs are formed through radiofrequency (RF) signals, which are emitted by protons from the tissue, after its exposure to the perturbation from the incident RF pulses in the presence of strong magnetic static fields. Furthermore, computerized positron–electron tomography (PET) is considered, in the most advanced non-invasive cardiovascular diagnostics, as a revolutionary medical technique, which is a key procedure enabling inspection into the viability of damaged cardiac tissue by directly assessing metabolism of the heart. The same principle can also detect blockage of blood flow in the coronary arteries. The striking feature here is that the fundamental starting point of this fascinating application of physics in medicine, with further enormous horizons of its possible usage, is the collision of positrons e^+ with electrons e^-. The result of such a collision is the pair annihilation $e^+ - e^-$, accompanied by the emission of two photons each having the same energy of 511 keV and moving in opposite directions. Many of the most relevant modern discoveries about the influence of ionizing radiation on biological systems are based upon data stemming from the domain of investigations of atomic and molecular physics. Knowledge of the energy and angular distributions of ionizing particles during atomic collisions is of great significance in the technology of X lasers, then in biophysics and in medical physics. This is particularly true in the case of the deposition of heavy energetic ions in organic matter, then for detection of charged particles and also for the relative efficacy of the δ-rays, i.e. secondary ionized electrons [57–59]. In biophysics, collisions are important in the context of investigations linked to the surface of numerous biophysical systems. Dynamics typical of collisions are necessary for an adequate study of mobility and transport of bio-matter through the cell membranes, propagation of nerve impulses across neuronal surfaces, permeability of the cell membrane and their capability to enable the diffusion of glucose molecules and alike under conditions of even drastically reduced blood flow, etc.

In plasma physics, cross sections of a large number of collision processes are in use as the entry data, without which it would be virtually impossible to do an adequate kinetic modelling of plasmas. The most fruitful joint problematics of plasma physics and atomic–molecular physics is certainly in the domain of

controlled thermonuclear fusion research. In the physics of condensed matter, collisions of multiple charged ions with the solid surface are of considerable significance [60]. Quantum surface physics, as a new autonomous field, connects certain themes common to solid state physics, atomic and molecular physics. The interest in this research area has particularly intensified with respect to application of the results in fusion investigations which relate to the effects stemming from the interaction of plasmas with a tokamac's walls. Quantum effects on the surface of solid bodies are also important in obtaining laser radiation outside the optical domain (X lasers). Let us cite here only a few important phenomena from quantum surface physics: formation of Rydberg states of ions in the vicinity of metallic surfaces, Auger processes resulting from collisions of ions with the solid surface at small scattering angles, diagnostics of surface spin ordering and chaos in ferromagnetics, statistics of electronic emission from the metallic surface under the influence of incident ions, electronic capture into continuum states in slow collisions of ions with the metallic surface, ion neutralization at the surface, etc [60]. In collisions of heavy ions with the solid surface of tokamac walls, neutralization in the fusion plasmas frequently takes place. Of course, such an effect is undesirable and should be reduced to the smallest amount possible, since the main goal in fusion is obtaining the positive energy defect of elementary processes in tokamacs, i.e. the creation of the current flux is enabled by maintaining the constituents of the plasma in the state with non-zero charge. For technological procedures of wall construction, one needs atomic data bases for cross sections of neutralization collision processes of the fusion plasma. With these data at hand, one knows which materials exhibit the large neutralization cross sections, i.e. for which the probability of neutralization of the plasma is most significant. Such ingredients are afterwards technologically extracted from the walls of the tokamacs, so that the whole performance will be considerably improved.

In astrophysics, atomic collisions are also one of the fundamental themes of research. For example, determination of the coefficients of the reaction rate of ion capture by molecules with the permanent dipole and/or quadrupole moment at low temperatures is important for theoretical modelling of complex ion synthesis in cold interstellar clouds. The corresponding computed data on cross sections are necessary in studying the problems of radiative association [61]. In a larger class of astrophysical problems, it is possible to apply the methods originally developed in atomic and molecular physics [62–65]. When low-energy ($\leq$10 MeV amu^{-1}) cosmic rays interact with the interstellar gases (H, He, etc), particle-rearranging phenomena occur with the electron transfer, leading to formation of atoms and/or ions primarily in their excited states. These newly formed atomic systems possess one or more electrons bound to nuclei of cosmic rays [62–65]. The formed excited states are metastable, so that their subsequent radiative decays yield the emission of the x-rays. Detection of the latter radiation is of primary significance for a direct determination of the intensity of the interstellar cosmic rays. Hence, here too, knowledge of adequate theoretical predictions of cross sections for electron

capture from interstellar atoms by the impact of nuclei of cosmic radiation becomes mandatory [65]. The importance of these reliable theoretical data bases on atomic collisions is best appreciated in light of the existence of only indirect measurements connected with the influence of cosmic radiation on heating and ionization processes, as well as on formation of HD molecules [62]. For energies below 100 MeV amu^{-1}, a direct terrestrial measurement is not reliable, due to serious and undetermined modulations by the solar magnetic field. Here, theoretical results represent nowadays the only source of information about the relative intensity of cosmic radiation.

C.6 Application of collision phenomena in technology

Applications of the results from atomic and molecular physics in technology are very important and numerous, e.g. the study and refinement of materials by laser beams, laser separation of isotopes, laser-induced chemical reactions, transfer of energy and information by directed and coherent electromagnetic fields, etc. Atomic and molecular physics are also vital for a proper understanding of atmospheric and meteorological phenomena [66]. One of the net outcomes of the latter interplay is the significant contribution of atomic physics research to programmes for the preservation of the environment. We note, e.g., sensors which act from a distance using lasers and laser spectroscopy. In this way, it is feasible to monitor air pollution efficiently at a distance which is far from the source of the pollution. Data bases on atomic collisions are also important for many technological research projects, such as MHD generators, fusion machines, gaseous UV, X lasers and the technology of metal surfaces (surface features, e.g. surface 'aging', corrosion, etc).

Chapter 1

The key features of quantum systems and the Kato conditions

This chapter represents a *descriptive introduction* to the field of collision phenomena from the theoretical point of view, with the primary purpose of enumerating the fundamental themes of research as well as the relevant basic physical aspects. With this goal in mind, we shall elucidate the role of the *key features* of collision phenomena and introduce certain *basic notions* and *chief observables.*

It is methodologically justified to start first with a qualitative and intuitive description of scattering of one particle on a given potential. In this case, scattering can be imagined as a stationary or non-stationary event. In the non-stationary treatment, collision is understood as a physical phenomenon which essentially develops in three time stages. Time t will be considered as being a continuous real variable $t \in \mathbb{R}$, where $\mathbb{R}$ is the set of real numbers. In the *first* episode, we have an incident particle approaching the potential, which acts as a centre of the interacting field. In the *second* step, which is of a very short duration in comparison to the total time of the entire event, collision occurs, i.e. the incident particle is being scattered on the given potential. In the *third* stage after the collision, the particle moves away from the centre of the interaction field, in a direction which generally differs from the incident direction. This intuitive picture forms a good basis for theory of scattering. The problem is, then, in searching for the corresponding mathematical language, by which the previously outlined collision event could precisely be described.

In the stated qualitative description of scattering, we did not introduce any assumptions which would guarantee that the number and/or kind of particles should be the same before and after the collision. In addition, we did not limit the internal degrees of freedom, e.g. spin or isospin, of the particles which participate in the collision process. The mathematical apparatus, which we shall analyse in this book, will be of sufficient generality to encompass the most important cases of interest to physics. Naturally, potential scattering represents